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Plenary lectures

To Switch or Not To Switch - Bridging Across Scales in Ferroelectric Ceramics

Dennis Kochmann *† [1,2]

[1] California Institute of Technology (Caltech) – 1200 E. California Blvd., Pasadena, CA 91125 USA, United States
[2] ETH Zurich (ETH) – Leonhardstr. 21, 8092 Zurich, Switzerland

Ferroelectric ceramics are the enabling key to most actuator and sensor technologies, owing to their piezoelectric effect and its nonlinear extension, the ferroelectric effect. These materials convert electric voltages into mechanical deformation and, conversely, mechanical strains into electric voltage - at small amplitudes the relation between those fields is relatively simple and the mechanisms are reversible. At sufficiently large applied electric fields or mechanical stresses, a complex reorganization of the atomic-scale dipole structure results in irreversible ferroelectric switching, a process that is sensitive to loading rate and temperature. Moreover, ferroelectric ceramics possess the aforementioned properties only below their Curie temperature, above which they become unpolar through a phase transformation. Modeling the electro-thermo-mechanically-coupled behavior of ferroelectric ceramics has been a challenge that extends across multiple length and time scales: from atomic-level dipoles and thermal vibrations up to mesoscale polycrystals and, ultimately, macroscale devices. We combine information from several scales with the aim of predicting the effective material response. Using first-principles input for the energetic potentials and a statistical-mechanics formulation for the impact of finite temperature and defects, we formulate a multiphysics phase field model for ferroelectrics. The latter is employed within the framework of computational homogenization to extract from polycrystalline, mesoscale representative volume elements (RVEs) the effective, macroscale behavior. An improved Fourier spectral formulation (based on finite-difference approximations) enables the simulation of RVEs at high resolution without some of the common numerical artifacts inherent in spectral solvers. Finally, we extend the model in order to capture the material behavior near the phase transformation at the Curie point. For the purpose of validation, results are compared to in-house experimental data of both the electrical and mechanical response. Overall, much remains to be done towards a complete understanding of ferroelectric ceramics, but the theoretical-computational framework presented here provides a basis and a recipe for generalization and extensions into various directions.

Keywords: ferroelectric, phase field, homogenization, multiscale modeling

*Speaker
†Corresponding author: dmk@ethz.ch

Chemo-mechanics of metallic alloys

Dierk Raabe *† [1,2]

[1] Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH (MPIE)

The talk is about structure-chemistry interactions at lattice defects and their relevance for materials mechanics.

Internal interfaces, stacking faults and dislocations determine many mechanical, functional, and kinetic properties of alloys. These defects can be chemically manipulated by solute decoration, confined elemental partitioning and even by low-dimensional transformation phenomena, altering their energy, mobility, structure, and cohesion. Some of these phenomena are long known: Examples are Cottrell atmospheres at dislocations, Suzuki partitioning to stacking faults and grain boundary segregation according to the adsorption isotherm.

The lecture presents and discusses three aspects in that context. First, recent atomic-scale experiments show that the interplay between defect structure and chemistry can lead to a much larger variety of compositional – structural states than commonly assumed. Second, some of these states can be described by established thermodynamic and kinetic models. Third, embracing the full complexity of these defect decoration states via alloying and thermomechanical treatments establishes an approach referred to as 'segregation engineering'. In this concept defect decoration and transformation are not regarded as undesired phenomena but instead utilized to manipulate specific interface and dislocation structures, compositions and properties for advanced microstructure design with the aim to improve the mechanical properties of engineering alloys, particularly their damage tolerance.

Keywords: chemo, mechanics, metals

*Speaker
†Corresponding author: d.raabe@mpie.de

Micromechanics of deformation and fracture in highly cross-linked thermosets

Thomas Pardoen * [1], Xavier Morelle [2], Jérémy Chevalier [2], Laurence Brassart [3], Pedro Camanho [4], Christian Bailly [2], Frédéric Lani [5]

[1] Université catholique de Louvain (UCL) – Belgium
[2] Université Catholique de Louvain – Belgium
[3] Monash University – Australia
[4] Universidade do Porto – Portugal
[5] Any Shape – Belgium

Advanced constitutive models for polymers have been essentially developed for thermoplastics with relatively limited applications/extensions to thermosets. Thermosets differ from thermoplastics by the cross-linking. Recent extensions of these constitutive models provide accurate predictions over a wide range of loading configurations, strain rates and temperature, encompassing below and above transition temperature regimes, although at the prize of a very large number of parameters, often larger than 30. Still, these models, mixing phenomenological and micromechanics ingredients, are often not rich enough to capture complex behaviors such as for instance severe non-linearity upon unloading, while missing also micromechanical connection to the failure process. Based on an extensive experimental test program on the highly cross-linked RTM6 epoxy, the viscoplastic response is found very similar to thermoplastics, with hardening-softening-re-hardening, large back stress upon unloading and existence of shear band patterns at very small scale. A molecular physics-based model of the deformation process occurring through the activation of nanometer scale shear transformation zones (STZ) has been developed, borrowed from the metallic glass field. The viscoplastic deformation is the result of the cooperative activation of STZ's, sensitive to rate, temperature, stress state and stress level. This model involves only 5 parameters to identify, all with physical meaning. The model quantitatively captures all the experimental trends, even some complicated responses during creep tests performed after plastic deformation at intermediate stress levels showing backward followed by forward creep. Such as model will never replace closed form constitutive models for the treatment of large scale components but can be used to understand small scale mechanics as well as for identifying macroscopic models. In this research, a new micromechanics-based fracture model based on the attainment of a local maximum principal stress within a given volume is also proposed and validated for a wide range of stress states.

Keywords: Micromechanics, viscoplasticity, fracture, polymers

*Speaker

S1: Mechanics of polymers and metallic glasses - Experiments and models

Investigation of the contact mechanisms of High Modulus Polyethylene ropes: mechanical characterization and microstructure changes

Cédric Bain * [1], Peter Davies† [2], Yann Marco‡ [3], Guilhem Bles§ [4], Julien Barnet¶ [5]

[1] Institut de Recherche Dupuy de Lôme (IRDL - CNRS FRE 3744) – ENSTA Bretagne : rueFrançois Verny, 29200 Brest, France – France
[2] IFREMER- Laboratoire Comportement des Structure en Mer (LCSM) – Institut Français de Recherche pour l'Exploitation de la Mer (IFREMER) – Ifremer, Laboratoire des Comportement des Structure en Mer, Centre de Brest, BP 70, 29280 Plouzané, France, France
[3] Institut de Recherche Dupuy de Lôme (IRDL - CNRS FRE 3744) – ENSTA Bretagne : rueFrançois Verny, 29200 Brest, France – France
[4] Institut de Recherche Dupuy de Lôme (IRDL - CNRS FRE 3744) – ENSTA Bretagne : rueFrançois Verny, 29806 Brest, France – France
[5] INO-ROPE – INO-ROPE – 1 rue des Senneurs, 29900 CONCARNEAU, France, France

The use of synthetic ropes use is widespread for yachting applications as they have many advantages: light weight, high strength, corrosion resistance. This work is dedicated to synthetic ropes made of High Modulus PolyEthylene (HMPE). One specific property of HMPE is its very low friction, which has been exploited in the recent development of pulleys using HMPE, that consist of a loop of these ropes, in contact with a low friction ring sliding on its two strands. This is a very recent invention, so there have been few studies of the comprehension of the contact mechanisms of synthetic fiber ropes. This study aims at bringing better understanding of the mechanical behaviour of these pulleys.
HMPE braided ropes are complex and their structure presents several internal layers which introduce a complex mechanical state with friction between the fibers. Furthermore in the pulley's case, the HMPE loop is constrained by a complex loading (tension, compression, and flexion).

The study investigates the mechanical response for several scales. The first is the monofilament one. The second is at the strand level (a strand is composed of several thousands of mono-filaments twisted together). At both scales, experimental campaigns have been performed, including interrupted tension tests with numerous relaxation steps in order to identify visco-elastic behaviour, and monotonic traction tests with and without pre-stretching protocols. The purpose is here to understand the role of the different scales and that of the coatings. A second part of the study focuses on the contact area between the metallic ring and the rope, because a remarkable change occurs at the surface of the HMPE rope. This transformation can be first observed from the brightness of this area, we will call it "polishing". The first observations of polishing HMPE fibers are quite impressive. The mono-filaments are highly compacted near and in the polishing area. This compaction even leads to a prismatic cross section of the initially circular filaments. Further investigations aim to understand better if this geometric effect is the only modification or if some other changes are involved (phase change, coating melting, ...). These will also be discussed.

Keywords: HMPE, dyneema, contact, fiber, synthetic, mechanisms, interfaces

*Speaker
†Corresponding author: peter.davies@ifremer.fr
‡Corresponding author: Yann.Marco@ensta-bretagne.fr
§Corresponding author: guilhem.bles@ensta-bretange.fr
¶Corresponding author: julienbarnet@inorope.com

Effects of speed and friction on the plastic deformation of a polymer material during extrusion ECAE: Numerical study

Ramdane Boulahia * [1], Hariti Samir [2]

[1] Faculté de Génie Mécanique & Génie des procédés- Laboratoire de Mécanique Avancée (LMA/FGMGP/USTHB) – BP. 32 El-Alia, 16111, Bab-Ezzouar , Alger, Algeria
[2] Faculté de Génie-Mécanique, USTHB, – BP.32, El Alia, Bab-Ezzouar, 16111, Alger, Algeria

The ECAE process is a technique of large plastic deformation which consists of a combination of several parameters. The peculiarity of this technique is that these parameters can be changed (either separately or at the same time), to give a multitude of choices of the methods to be used for carrying out the extrusion experiments. The purpose of this work is to demonstrate the effect of two parameters, namely the extrusion rate and the friction, on the equivalent total plastic deformation induced on the extruded material.
Until now, the majority of research and development on ECAE have been conducted on metallic materials. However, given the anisotropy and the complex behavior of the polymer materials, little work is being done to solve mechanical behavior problems during the ECAE process. A study shows that changes in ECAE design parameters lead to changes in simple shear deformation mode and result in a more complicated and non-uniform stress state. In addition, there is always a vacuum in the corner of the channel (gap) between the sample and the matrix, even if we optimize the geometric parameters of the matrix. In the case of polymers, in the absence of back pressure, the gap problem is more important because of their viscous behavior; the gap is larger and leads to very curved samples at the outlet of the channel.

Using the FEM simulation, it can be seen that the speed of the piston slightly influences the homogeneity of the distribution of the equivalent plastic deformation, although a better result is obtained when the piston speed is low. However, increasing the latter parameter also increases the force required to extrude the workpiece. The influence of the friction on the change in the force of the piston is illustrated, which shows that the required force increases with increasing friction coefficient. The deformation near the lower zone decreases as the coefficient of friction increases, while for the rest of the thickness the deformation increases. However, the load necessary to carry out the extrusion process is very sensitive to this parameter. The steady state load is sensitive to the friction parameter. Indeed, the higher it is, the higher the coefficient of friction. This can be explained by the fact that the friction improves and promotes the degree of filling of the elbow (gap) . In conclusion we can see that, although the friction improves and promotes the filling of the elbow (gap) is thus increase the shear rate, the load required for extrusion have very significantly increased. Therefore, it is preferable to perform the ECAE test with a suitable lubricant to reduce the effect of friction.

Keywords: Polymer, ECAE, Friction, plastic deformation

*Speaker

Effect of photo-oxidation on deformation and fracture of bulk polyamide bars

Kenneth Cundiff * [1], Amine Benzerga [1,2]

[1] Texas A&M University, Department of Aerospace Engineering – H.R. Bright Building 701 Ross St College Station, TX 77840, United States
[2] Texas A&M University, Department of Material Science – 207 Reed McDonald Building, 575 Ross Street, Texas A&M University, College Station, TX 77843, United States

Polymers are susceptible to degradation from UV radiation. This deficiency limits possible applications where the material is exposed to a harsh environment. Improving the understanding of how the mechanical behavior of polymers is impacted by UV aging will lead to more accurate assessments of lifetime and possibly an increased number of applications. UV radiation damage is essentially a surface oxidation process catalyzed by photons. For this reason, the intrinsic mechanical behavior of aged polymers is usually accessed using thin films. However, the influence of aging on bulk behavior remains elusive, which puts into question the transferability of results to structural components. In addition, thin films are not ideal for characterizing fracture. In this study, millimeter-scale round tensile bars and compression pins of polyamide 6 (PA6) were exposed to accelerated UV radiation under controlled conditions of temperature and humidity. Each cylindrical specimen was periodically rotated about its axis in the aging chamber to ensure nominally uniform aging about the circumference. Aging times were up to 192 hours. Unaged and UV aged specimens were then monotonically loaded to fracture using whole-field strain measurements and novel video-monitored extensometry. The experimental test matrix accounts for loading mode (tension versus compression), temperature and strain rate, in addition to radiation dose. The effects of UV aging on strength, strain hardening and strain to failure were then carefully quantified using advanced post-processing methods of the mechanical tests. In addition, in situ testing enabled the deformation and fracture mechanisms to be discussed in aged bars. It was found that while the structural response was weakly sensitive to UV aging, the strain to failure was a decreasing function of radiation dose even with oxidation being confined to the surface. Contrary to current understanding in the literature, no sharp ductile-to-brittle transition was found. This points to the need of developing constitutive models that account for chemo-mechanical coupling capable of describing the gradual decrease of ductility with radiation. One such formulation is proposed and its implementation highlighted through preliminary results.

Keywords: photo, oxidation, semi, crystalline, polymers, PA 6

*Speaker

On the mode I interfacial toughness of adhesive bonds accounting for strain-softening

Sylvain Dépinoy *† [1], Thierry Massart [2], Stéphane Godet [1], Thomas Pardoen [3]

[1] 4MAT, Materials Engineering, Characterization, Processing and Recycling, Université Libre de Bruxelles – 50 Avenue FD Roosevelt, CP194/03, B-1050 Brussels, Belgium
[2] BATir, Building, Architecture & Town Planning Department, Université Libre de Bruxelles – 50 Avenue FD Roosevelt, CP 194/02, B-1050 Brussels, Belgium
[3] Institute of Mechanics, Materials and Civil Engineering, IMMC, Université catholique de Louvain – B-1348, Louvain-la-Neuve, Belgium

Adhesive bonding consists in the joining of two adherents by an adhesive, typically made of glassy thermoset or thermoplastic polymer. This technology offers many advantages over traditional joining techniques, such as a more uniform stress distribution across the bond and the possibility to join different materials. A key-factor for the design of joints lies in the determination of the toughness of the interface which can be used for structural integrity assessment. While extensive research has been performed on the effect of several material and geometrical parameters on the bond line toughness, the effect of the strain-softening arising in the polymer adhesive has not been systematically addressed yet. The question of interest is to what extent a bond line model must account for the intrinsic softening of the adhesive to provide a fair representation of the crack tip plasticity and dissipation of energy. An important side effect is that if plastic softening plays a key role on setting the toughness, then ageing of the adhesive with time, which is known to modify the magnitude of the softening, could contribute to a significant evolution of the joint toughness with time.

The mode I toughness of an interface between an adhesive material subject to strain-softening and an elastic substrate was investigated by finite element calculations. An asymptotic K-field model with cohesive zone elements simulating the fracture mechanism was used. Phenomenological hardening laws reproducing the plastic response behavior of amorphous glassy polymer involving first hardening, softening and re-hardening were used. For the sake of simplicity, rate sensitivity was not addressed. The effect of the peak hardening stress and of the softening stress on the joint toughness was investigated for different elastic mismatch values and critical stresses at the interface.

It is found that the joint toughness significantly increases with decreasing peak hardening stress and increasing amplitude of the softening. This is related to larger plastic zone sizes and higher plastic strains, hence to more energy dissipation. Increasing the interface work of fracture magnifies this effect. There is an interesting coupling between the elastic mismatch and softening, related to their influence in the fracture process zone length.

Keywords: Finite element calculations, strain softening, toughness, amorphous glassy polymer

*Speaker
†Corresponding author: sdepinoy@gmail.com

Homogenization estimates for the time harmonic response of particulate viscoelastic composites

Valentin Gallican * [1], Renald Brenner [2]

[1] Institut Jean Le Rond dÁlembert (DALEMBERT) – Université Pierre et Marie Curie - Paris 6, Centre National de la Recherche Scientifique : UMR7190 – Boite 162 4 place Jussieu 75005 Paris, France
[2] Institut Jean Le Rond d'Alembert (IJLRA) – CNRS : UMR7190, Université Pierre et Marie Curie (UPMC) - Paris VI – Boite 162 4 place Jussieu 75005 Paris, France

This study addresses the description of the time harmonic macroscopic response of composite materials made of a polymer viscoelastic matrix, described by a Zener model, and elastic spherical particles. As a first step, the asymptotic behaviour of the overall complex moduli is studied by resorting to stationary principles for complex viscoelasticity [1]. Four exact relations on the storage and loss moduli are obtained. Two of them classically correspond to the uncoupled elastic responses at low and high frequencies while the two others result from the viscoelastic coupling in the transient regime [2]. These relations only involve the strain fields which are solution of the asymptotic elastic regimes. Based on these relations, approximate homogenization estimates are proposed for the whole frequency range. They classically make use of the Prony series approximation for the overall relaxation function. However, only two homogenization problems have to be considered.
An application of this approach is presented for the generalized self-consistent (GSC) scheme in the case of incompressible isotropic consituents. On one hand, the approximate model is compared with the exact GSC estimate. This allows to assess the relevance of our minimalist approach on its own. On the other hand, both GSC estimates are compared to full-field FFT computations performed on periodic polydisperse microstructures, with high volume fraction of particles, which are obtained by a random sequential adsorption process.

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Keywords: Linear viscoelasticity, Homogenization, Particulate composites

*Speaker

Micromechanical analysis of failure in thermoplastic PC/ABS blends

Jonas Hund * [1], Thomas Seelig [2]

[1] Institute of Mechanics, Karlsruhe Institute of Technology (IfM, KIT) – Germany
[2] Institute of Mechanics, Karlsruhe Institute of Technology (IfM, KIT) – Germany

The macroscopic deformation and failure behavior of rubber-toughened thermoplastic PC / ABS blends is governed by various microscale damage mechanisms. Crazing and void growth from cavitated rubber particles prevail in the ABS phase while PC typically fails by ductile rupture at large strains [1]. Furthermore, the blend composition (PC/ABS ratio) as well as the rubber content of the ABS phase have an influence on the blend morphology as well as on the deformation and failure behavior [2]. In order to gain a better understanding of the micro-macro relationship in PC/ABS blends undergoing failure, a micromechanical RVE approach is pursued. Within this apporach the two constituents are represented as distinct phases in composition dependent RVEs. To capture the deformation behavior of each phase different plasticity models are employed. Within the PC phase the standard glassy polymer model by Boyce and co-workers [3] is utilized. The inelastic deformation behavior of ABS is described by a model that accounts for the mechanism of distributed crazing in a homogenized sense [4]. A key issue is the appropriate modeling of local failure for which different stress and strain based criteria are considered. Numerical simulations analyzing the effect of the blend composition and morphology on the overall response are compared with experimental findings.

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Keywords: polymers, multiscale, pc/abs blends, micromechanical model

*Speaker

Crack growth in low-density polyethylene

Martin Kroon * [1]

[1] Linnaeus University (LNU) – Växjö, Sweden

Polyethylene is a polymer that is widely used in the industry, and the fracture mechanics properties of this material is therefore of great interest. In the present study, we have performed a series of fracture mechanics tests on polyethylene sheets. In addition, tensile tests have been performed in order to determine the constitutive behaviour of the material. A numerical finite element model is used, in which the fracture mechanics tests are simulated, and the fracture mechanics properties of the material are determined. In the numerical simulations, crack growth is enabled through the inclusion of a cohesive zone in the finite element model of the polyethylene sheet. Through the analyses, the far-field value as well as the tip value of the J-integral are determined. It turns out, that a rate-dependent cohesive law is required if the experimental results are to be accurately reproduced in the numerical simulations.

Keywords: polyethylene, fracture, cohesive zone, rate, dependent

*Speaker

Crack arrest capability of shock-resistant PMMA under impact loading

Norazrina Mat Jali *† [1], Patrice Longère [2]

[1] Institut Clément Ader – Université de Toulouse, CNRS, INSA, ISAE-SUPAERO, Mines Albi, UPS, Toulouse France, NDUM, Kuala Lumpur, Malaysia – France
[2] Institut Clément Ader (CNRS 5312) – Institut supérieur de l'aéronautique et de l'espace [ISAE] – 3 rue Caroline Aigle 31400 Toulouse CEDEX 04, France

Analysis and understanding of failure mechanisms under high strain rate loading in engineering materials is a key point for the design of structures submitted to accidental overloads. We are here interested in the crack arrest capability under impact loading of polymers used as structural and/or protection materials. In the philosophy of the crack arrest capability considered in the present work, an engineering structure is supposed to be initially weakened by a crack and the question to answer is how this pre-cracked structure behaves when dynamically reloaded. The Kalthoff and Winkler (KW) impact test, consisting in impacting the edge of a double notched plate, was accordingly retained to that purpose A comparative study of the dynamic crack arrest capability of several grades of shock-resistant PMMA under high strain rate loading is presented evidencing the brittle feature of the material failure. High speed camera was used to record the chronology of the failure mechanisms. It is notably shown that the higher the impact velocity (in the range 50-100 m/s) the larger the number of fragments. Moreover, depending on the impact velocity, changes in the crack path and thus in the mechanisms controlling the PMMA dynamic fracture can be seen.

Keywords: shock, resistant PMMA, impact test, dynamic failure

*Speaker
†Corresponding author: Norazrina.BINTI-MAT-JALI@isae.fr

Evolution of free Surface due to Surface Tension in Viscoelastic Fluid Flows

G. Durga Prasad *† [1], K. Kannan [1]

[1] Indian Institute of Technology Madras (IITM) – Chennai 600036, India

Free surface of fluids produces traction and its magnitude changes from point to point based on the direction of normal on the free surface. Martin Rehor and Vit Prusa have done numerical study on squeeze flow of viscous fluids considering the curvature forces on the free surface [1]. The evolution of free surface of viscoelastic fluids between two parallel plates was studied using thermodynamic rate type framework which was developed by K.R. Rajagopal and coworkers [2]. Two scalar valued functions, stored energy and dissipation are parameterized using natural configuration (stress free configuration). By using these functions and the second law of thermodynamics, constitutive model as a function of left Cauchy stretch tensor related to natural configuration and evolution equation by maximizing dissipation equation were obtained. By substituting the constitutive model in balance of linear momentum and along with evolution equations, the evolution of free surface of viscoelastic fluid between two parallel plates was studied using axisymmetric boundary conditions. Fluid flow was studied assuming that there is no inertia and gravity and curvature forces were applied as boundary conditions. The curvature and curvature forces are maximum at center of parallel plates on the free surface and the change in the free surface at each time step was obtained.

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Keywords: Viscoelastic fluid, curvature, Natural configuration

*Speaker
†Corresponding author: durga.iitkgp@gmail.com

Developpement of a constitutive equation for fatigue and self-heating analysis of thermoplastic copolyester

Pierre Robard * [1], Laurent Gornet [2,3], Patrick Rozycki [2,3], Gilles Marckmann† [3]

[1] Institut de Recherche en Génie Civil et Mécanique (GeM) – Université de Nantes, Ecole Centrale de Nantes, Centre National de la Recherche Scientifique : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[2] Institut de Recherche en Génie Civil et Mécanique (GeM) – Ecole Centrale de Nantes, Université de Nantes, CNRS : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[3] Institut de Recherche en Génie Civil et Mécanique (GeM) – Université de Nantes, Ecole Centrale de Nantes, Centre National de la Recherche Scientifique : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France

1 Presentation of the context

The present work is dedicated to one of the sector market of Trelleborg Boot : the constant velocity joint boots. During their life, this type of joints is subjected to severe constraints such as wide temperature range, self-contact, friction between coils, grease. In order to increase their lifespan, Trelleborg Boot is investigating a new material and particularly a thermoplastic copolyester (TPE-E). The goal of our research is to find a fatigue criterion as well for the constitutive material as for the structure under different loading paths. The research works are split into 2 main steps : the first one corresponds to the writing of a behavior law adapted for this new material, and the second one consists to mix the previous behavior law with fatigue testing. The identification of fatigue criterion will be done using both W'ohler curves and self-heating tests. Indeed, for metallic materials, some previous research works demonstrate an equivalence between the fatigue limit coming from the self-heating tests and the W'ohler curves. Same conclusions have been noticed by other authors working on thermoplastic composite materials. Whatever the case of study, the main advantage of this methodology is its low time cost. That are some reasons why we are convinced of the benefits brought by the self-heating tests for our material and problem. In this paper, we focus only on the first step : the behavior law formulation for thermoplastic copolyester. We also suggest some results including the influence of the grease on the mechanical behavior as well as some thermomechanic studies.

2 Thermomecanical behavior law

The thermoplastic copolyester exhibits some mechanical properties similar to the rubbers which includes large deformations, viscoelasticity, incompressibility... However, the experimental campaign that we carried out on the material also shows that viscoplasticity must be taken into account. Based on a multiplicative decomposition of the deformation gradient tensor F, the behavior law is inspired by the Bergstr'om-Boyce Model. In order to find an equilibrium between research and industry expectation, the thermodynamical formalism will be the same as in S. Méo and S. Lejeunes works'. We upgrade the previous model by introducing an approach for crystalline polymer. This implementation leads to the visco-hyperelastic part of the behavior law. Concerning the hyperelastic and damage parts, the model is inspired by the GDM model [6]. Finally, the viscoplastic part is based on the work done by A.V. Shutov [7]. The whole model is formulated in lagrangian formulation. All the implementation of this model has been done at the integration point in Matlab.

Keywords: polymer, behavior lawl, numeric, viscoelastic, viscoplastic, thermoplastic, fatigue, self, heating, heat build, up

*Speaker
†Corresponding author: gilles.marckmann@ec-nantes.fr

Constitutive modelling of hyperelastic rubber-like materials considering damage

Elisabeth Toups * [1], Jaan-Willem Simon [1], Stefanie Reese [1]

[1] Institute of Applied Mechanics, RWTH Aachen University (IFAM) – Mies-van-der-Rohe-Strasse 1, 52074 Aachen, Germany, Germany

Adhesives are used in numerous applications such as in the automotive industry, packaging industry, civil engineering, and many others. Multi-side bonded joints become increasingly common to use in glass-façade structures instead of bolted point fixings [1]. One reason for that is the aesthetic value due to the increasing transparency by using bonded joints and reducing external steel brackets. Another advantage is the continuous loadbearing which prevents stress concentration.
In order to optimize the building processes, improve design methods, and expand the field of applicability of adhesives, it is essential to investigate constitutive models which ensure a representation of rubber-like material behaviour. Hence, the main goal of the present work is to develop a material model which is able to represent the particular stress-strain behaviour of hyperelastic materials with respect to large deformations and multiaxial stress states. In addition, the model should be able to also account for damage.

Several hyperelastic material models are available in the literature, the most common of which are the ones of Ogden and Mooney-Rivlin. Both models show a good fitting quality to experimental test data but they are not able to represent material damage which may occur in rubber-like materials in the form of the so-called Mullins effect. Furthermore, in the current work particular attention is paid to complex stress states since multi-axial stress states may occur in glass-façade constructions. Here, especially the interaction between tensile load and shear load is considered. Existing damage models are often only validated for uniaxial tests but not for more complex load cases. Moreover, most damage models are based on the assumption of small deformations and thus have to be extended to the large deformation regime. For this reason, different models are compared and adjusted accordingly. For example, the micromorphic based formulation of a gradient-extended two-surface damage-plasticity model developed by Brepols et al. [2] is considered, in which damage and plasticity are treated independently from each other. This fact is also very useful in order to describe the damage behaviour of hyper-elastic materials without considering plasticity if needed. This model also enables the calculation of multi-axial stress states and thus offers a good starting point for further investigations. Hence, the above mentioned model is developed and tested in its suitability by comparing it with experimental test data.

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Keywords: Hyperelasticity, rubber, like material, Mullins effect, damage, large deformations, material modelling

*Speaker

Micromechanics of oriented semicrystalline polymers

Hans Van Dommelen * [1], Mohsen Mirkhalaf [1], Leon Govaert [1], Marc Geers [1]

[1] Eindhoven University of Technology (TU/e) – PO-box 513 5600 MB Eindhoven, Netherlands

The mechanical response of a polymer material, including the mode of failure and the time-scale on which it occurs, is strongly influenced by the processing conditions. This is particularly true for semicrystalline polymers in which structural features, such as the degree of crystallinity, crystal type, size and orientation, that strongly influence their mechanical properties, may vary drastically depending on subtle details of the manner in which the polymer is shaped into the final product. During processing of a material, often an oriented microstructure is formed, leading to anisotropic properties. To improve product performance, a fundamental and quantitative understanding of how anisotropic properties, including yield and failure kinetics, depend on the structure is required. A micromechanical model that describes the macroscopic response as a function of the morphological structure and constitutive properties of the constituents has the potential to form a predictive tool for the macroscopically anisotropic properties of a semicrystalline polymer with a processing-induced microstructure. This work focuses on the development a multiscale micromechanical model for the response and in particular the stress-dependence of the rate of plastic deformation, i.e. the yield kinetics, for oriented material. The model is based on a mean field framework, accounting for the crystalline phases, which are modelling by crystal plasticity and pre-stretched amorphous domains. Depending on the processing conditions, in addition to a preferential distribution of crystalline domains, the amorphous domains may become oriented as well. The anisotropy of these amorphous regions is incorporated in the micromechanical model and is found to be crucial for predicting the anisotropic properties of oriented semicrystalline HDPE.

Keywords: Semicrystalline Polymers, Micromechanics, Anisotropy

*Speaker

S2: Mechanics of composites - Experiments and models

Numerical Simulation Modeling Techniques for the Impact Behavior of Carbon Fiber/Epoxy Laminate Composite Plates

Furqan Ahmad * [1], Fethi Abbassi [2]

[1] Dhofar University – Oman
[2] Dhofar University – Oman

The low velocity impact responses of cross-ply CFRP composite plates are investigated experimentally and are simulated by using an FE code LS-DYNA. Experimental test was performed first and then two different modeling approaches are employed to model the composite plates. In the first modeling approach, solid elements are utilized for the composite layers, and in the second approach, shell elements are used. The numerical model using the shell elements shows good correlation with the experimental results while the impact damage in form of delamination is predicted more precisely using solid elements.

Keywords: Modeling approach, LS, DYNA, Impact damage, Solid and shell model.

*Speaker

Comparative study of the mechanical behavior of a clay-based materials of M'sila region reinforced by vegetal fibers (Date Palm)

Azzedine Benyahia * [1], Nouibat Brahim [1], Zid El Kheir Belkacem [1], Redjem Ali [1], Laib Nouri [1], Deghfel Nadir [2], Kouadri Zinat [1]

[1] Laboratoire Ville,environnement, société et développement durable (LVESDD) – University of Med Boudiaf M'sila 28000, Algeria

[2] Laboratoire chimie des matéraux inorganiques (LCMI) – University of Med Boudiaf M'sila 28000, Algeria

This work is part of the development of local materials such as clay and fibers palm in the south of Algeria. These materials are abounding, natural and renewable, they have mechanical properties that are very interesting important . Our objective is to study the fiber palm size effect on the mechanical characteristics of clay based materials. For this reason we mix the clay (chosen as base material) with different lengths of fibers palme (0.5, 1, 2, 3, 4 cm) to determine the optimum length used in the composite material. In the next step, the fiber was treated with 4% sodium hydroxide solution at different periods 3, 6, 24 and 48 hours, then we compare the mechanical properties of this new material with clay only, to prepose this material in the field of rural construction. The results show considerable improvement in the strength of the reinforced clay, with optimum palm fibre content of about 2 cm. However, further increase in fibre content did not significantly affect the strength. Stress-strain curves show inverse relation between peak stress and strain. It is therefore concluded that palm fiber cements soil particles and fiber together; thus, promotes stress distribution evenly and improves deformation resistance.

Keywords: Palm fibers, clay, tensile strength, compression, Strength, composite.

*Speaker

A Novel Protocol for Rapid Identification of Anisotropic Diffusion Properties of Composite Materials with Complex Texture

Marianne Beringhier [1], Marco Gigliotti * [2], Diego Maida [2,3]

[1] Institut Pprime (PPRIME) – Université de Poitiers, ENSMA, Centre National de la Recherche Scientifique : UPR3346 – Institut P: Recherche et Ingénierie en Matériaux, Mécanique et EnergétiqueSP2MI Téléport 2Boulevard Pierre et Marie CurieBP 3017986962 FUTUROSCOPE CEDEX, France

[2] Institut Pprime (PPRIME) – CNRS : UPR3346, Université de Poitiers, ENSMA – 1, avenue Clément Ader, BP 40109 F86961 FUTUROSCOPE CHASSENEUIL, France

[3] Department of Mechanical, Energy and Management Engineering, University of Calabria – via Pietro Bucci 87036 Arcavacata di Rende, Cs, Italy

Diffusivity of composite materials is usually measured by performing gravimetric sorption tests: for orthotropic materials having three distinct diffusivity coefficients (along the three orthogonal space direction), three distinct sorption curves are needed ([1, 2]). This is usually done by employing three thin samples cut along the three orthogonal direction in order to promote separate diffusion along the three directions. This protocol is generally time consuming, when the sorption curves are run up to saturation: moreover, when the directions of orthotropy are a priori unknown the choice of the sample is not straightforward. In this last case, the anisotropy of the diffusion should be taken into account in the identification protocol. The aim of this work is to define an identification protocol pertinent for materials when the directions of orthotropy are a priori unknown (composite materials with complex texture, ...), exploiting the short-time range of the sorption curves, with the minimum number of samples. To do so, first, an analytical expression of the short-time slope of the gravimetric curve for anisotropic materials is introduced and validated against experimental data ([3]). Then, the short-time slope expression is employed for identification in the full anisotropic case. From these results an identification protocol for the full anisotropic case can be proposed.

Keywords: diffusion properties, anisotropy, composite material, complex texture

*Speaker

Modeling dual-phase structures: a dream.3D-Abaqus coupling

Edison Bonifaz * [1]

[1] Universidad San Francisco de Quito (EQUATEUR) (USFQ) – Diego de Robles y Pampite, Cumbaya 170901, Ecuador

A 3D finite element model was developed to simulate the influence of secondary phases (precipitates or aggregates) on the inelastic stress-strain distribution of nickel-based alloys and concrete structures. In both situations, the digital microstructure code DREAM.3D was coupled to ABAQUS® finite element code through a MatLab® program. Representative Volume Elements (RVEs) of similar edge size but different inclusion (aggregate) size, morphology and distribution generated with DREAM.3D were tested with ABAQUS to investigate the relation between micro (and/or meso) and macro deformation and stress variables. The virtual specimens subjected to continuous monotonic strain loading conditions, were constrained with 3D boundary conditions. In the case of dual-phase polycrystalline nickel-based alloys, the difference in crystallographic orientation, which evolves in the process of straining, and the incompatibility of deformation between neighbouring grains were accounted for the evolution of geometrically necessary dislocation density, by the introduction of averaged Taylor factors, averaged young's modulus and single phase elastic limit through the strain hardening model documented in Bonifaz and Richards [1]. In the case of concrete structures consisting of aggregates and hydrated cement paste, individual experimental curves in compression and tension documented in Bonifaz, et.al [2] were considered in the nonlinear analysis. Results demonstrate a strong dependence of flow stress and plastic strain on phase type, inclusion (or aggregate) size, shape and distribution. The effect of plastic deformation gradients imposed by the microstructure is clearly observed.

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Keywords: Heterogeneous materials, Digital structures, Constitutive behaviour, Cement paste, Aggregates, Inclusions, Nickel, base alloys

*Speaker

Face sheet-to-core debonding analysis in sandwich panels under dynamic loading

Vyacheslav Burlayenko *† [1,2], Tomasz Sadowski [3], Svetlana Dimitrova [4]

[1] National Technical University 'Kharkiv Polytechnic Institute' (NTU KhPI) – 2 Kyrpychova Str., 61002, Kharkiv, Ukraine
[2] Lublin University of Technology (LUT) – 40 Nadbystrzycka, 20-618, Lublin, Poland, Poland
[3] Lublin University of Technology (LUT) – 40 Nadbystrzycka, 20-618, Lublin, Poland
[4] National Technical University 'Kharkiv Polytechnic Institute' (NTU KhPI) – 2 Kyrpychova, 61002, Kharkiv, Ukraine

The sandwich panels are widely used as structural members of aircrafts, and aero-space and transport vehicles, in primary due to their high stiffness and strength at a low specific mass. However, low fracture toughness of the face sheet-to-core interface in sandwich structural elements is the most important issue reducing the load bearing capacity of such structures. Interfacial stresses caused by dynamic loads during the service life may easy result in the debonding progression and, even, the eventual fracture of the sandwich structure. In order to improve fracture resistance of sandwich structures subjected to dynamic loading, it is essential to evaluate the strength and durability of the face sheet-to-core interface. Generally, the fracture resistance of composite sandwich structures is evaluated from the fracture tests prescribed by the ASTM standard procedures. In most such research the interface strength is discussed in terms of the singular stresses or energy release rate at the end of the interfacial crack in the fracture sandwich specimens under static loading, whereas dynamic loading conditions for three-layered composite structures have been considered in a limited number of works. The present research is concerned with predicting the dynamic fracture of sandwich panels due to deboning at the face sheet-to-core interface. In this regard, first, the dynamic stress intensity factors are extracted from the sandwich fracture specimens by using analytical approaches and numerical techniques for two-dimensional models. These fracture analyses allow us specifying appropriate material fracture properties and assessing the stress behaviour at the bi-material face sheet-to-core interface. The fracture models calibrated in such way further are used in dynamic debonding analysis of a three-dimensional sandwich panel. The finite element model of the debonded sandwich panel is created using the capacities available in the commercial finite element code ABAQUS. Simulations of debonding initiation and propagation are carried out by using the cohesive layer model, which is incorporated into the finite element mesh via cohesive elements. Contact and friction behaviours possible due to dynamic debonding progression are taking into account in the modelling procedure as well. The strain rate sensitivity of the fracture behaviour depending on the velocity of debonding growth is accounted for using a visco-elastic constitutive model of the cohesive material law. The model is incorporated into the ABAQUS code by programming the appropriate user-defined material subroutine. The fracture features of the sandwich panel obtained in the simulations are compared with those known in the literature to validate the developed model. Thereafter, various types of dynamic loads are considered in the simulations and their influence on the debonding resistance of the face sheet-to-core interface in the sandwich panel is studied. The results obtained are discussed in detail at the end.

Keywords: Sandwich panels, debonding, dynamic fracture analysis, finite element modelling

*Speaker
†Corresponding author: burlayenko@yahoo.com

Kinetic effects on themechanical properties of fibre reinforced thermoplasticlaminate under indentation and impact loadings

Lucien Cadieu *† [1], J-B Kopp [1], J. Jumel [1], J. Bega [1], C. Froustey [1]

[1] Institut de Mécanique et dÍngénierie de Bordeaux (I2M) – Université Sciences et Technologies - Bordeaux 1, Arts et Métiers ParisTech, Institut polytechnique de Bordeaux, Centre National de la Recherche Scientifique : UMR5295 – Université de BordeauxBât A4 RdC 351 cours de la libération33405 TALENCE Cedex, France

This study aims to highlight the time dependency on the mechanical properties of a thin bi-directional glass fibre reinforced polymethyl methacrylate (PMMA) laminate using indentation and impact loadings. The laminates present a 28% increase of stiffness as the loading rate increases under quasi-static indentation (QS). When comparing QS and low velocity impact (DYN) this increase rises up to 40%. The energy stored in the sample increases from 5 J in QS to 13 J for a 20 J DYN. The damaged areas ranging from 45mm2 to 275mm2 are estimated by transparency. This method shows that the majority of the damages occur at an indentation depth between 7 and 8 mm. Using a scanning electron microscope (SEM) other damage mechanisms such as micro-cracking, cracking (due to the coalescence of micro-cracks), matrix failure, bre failure, strand failure and delamination are identied. The damage mechanisms are not observable during the loading therefore they are observed once the test is over. This means the kinetic of damage can not be precisely analysed. By observing the damages present at different indentation depths it is possible to hypothesise which damages appear rst. Indeed if specic damages, such as widespread delamination, are present for indentations of 8 and 9mm but are absent at 7mm then widespread delamination occurs after all the damages present at 7 mm. Using this approach a macro-scale kinetic of damage is given for a thin bi-directional glass fibre reinforced PMMA laminate.

Keywords: GFRP Composites, Thermoplastic, indentation, low velocity impact

*Speaker
†Corresponding author: lucien.cadieu@u-bordeaux.fr

Characterization and multi-scale modeling of the transverse compression of thick RTM-processed uni-directional samples

Jérémy Chevalier * [1], Xavier Morelle [2], Pedro Camanho [3], Frédéric Lani [4], Thomas Pardoen [1]

[1] iMMC-UCLouvain – Belgium
[2] ESPCI Paris Tech – ESPCI ParisTech, ESPCI ParisTech – France
[3] Universidade do Porto – Portugal
[4] Any Shape – Belgium

Bottom-up multi-scale modeling approaches of composites involve a first scale-transition from the constituents at the microscopic scale to the behavior of the yarn and the ply at the mesoscopic scale. This contribution presents the results of a bottom-up approach which aims at a high fidelity prediction of the non-linear transverse deformation and failure behavior of the unidirectional plies for a composite processed by RTM. Hence, while the processing and characterization of RTM epoxy resin is not a challenge per se, the first scale transition is hindered by the fact that most so-called uni-directional laminates produced by RTM are actually only quasi-UD architectures. Hence, a low volume fraction of reinforcement or a secondary fibre is present in the in-plane transverse direction to ensure the stability of the material in dry conditions. The lack of experimental results on true unidirectional specimens, especially under compression, implies very little experimental validation of computational micromechanical analyses on UD RVEs, mostly assumed to be truly representative of the mechanical behavior of the composite at the scale of a ply. To overcome this limitation, a thick UD slab was manufactured by RTM and cubic samples were machined out of the UD slab and subjected to uniaxial transverse compression.

Finite element simulations carried out on representative volume elements (RVE) of the UD, based on a random generation algorithm, highlighted the inability of a classical constitutive model identified and validated at the macroscale to accurately predict both the time of failure and the non-linearity of the stress-strain response of the cubic specimens. The FE analyses contained the usual ingredients of micro-mechanical analyses: cohesive elements at the interfaces and a strain rate and pressure dependent elasto-visco-plastic constitutive model from [1]. Hence, in-situ compression tests and nanoindentation tests were performed to characterize the mechanical behavior of the resin in the composite. Both the comparison between DIC analyzes at the scale of the fibers and the nanoindentation results highlighted the discrepancies between the predictions of the constitutive model and the actual behavior of the matrix. A simple correction of the hardening law using the ratio between the insitu and the bulk hardnesses can lead to satisfactory predictions of the UD mechanical response. However, given the limitations and the lack of physics based parameters of classical constitutive models, a novel modeling approach based on the concept of shear transformation zones (STZ) is proposed. The framework of STZ is based on the modeling of single shear events whose probability of activation is dependent on the local thermo-mechanical history, and is provided by a Eyring-type equation. The STZ model is shown to be a promising tool to directly account for the high strain gradients around fibers and pressure dependence, without providing explicitly a priori the hardening law of the resin.

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*Speaker

of the deformation and failure of the highly crosslinked RTM6 epoxy resin. Mechanics of Time-Dependent Materials, 1-36.

Keywords: Unidirectional composite, micromechanical modeling, insitu characterization, shear transformation zone

Image-based impact (IBI) tests for high-rate behaviour of composites

Lloyd Fletcher [1], Jared Van Blitterswyk [1], Fabrice Pierron * [1]

[1] University of Southampton (Southampton, UK) – United Kingdom

In many applications, composite materials undergo high strain rate dynamic loading, for example: crash, impact and blast loading. For these cases, it is essential that the strain rate dependent material properties are accounted for in the design of composite structures. Computational power has exponentially increased in recent decades, allowing for extensive simulations of damage formation in composite structures. However, the usefulness of these simulations is dependent on the quality of the input constitutive models.

Current methods for testing the high strain rate properties of composites are based on limited information provided by point strain gauge measurements. The use of point sensors requires multiple assumptions that limit the effective strain rates obtainable. For instance, the gold standard, the so-called Kolsky or Split Hopkinson Pressure Bar (SHPB), relies on stringent assumptions like quasi-static equilibrium and uniform strain state in the specimen. For materials with a small strain to failure like unidirectional composites transverse to the fibre directions, failure occurs before this can be achieved and as a consequence, reliable modulus values above a few 100s of /s are just not available in the current literature.

With the advent of full-field imaging and high-speed cameras, it is possible to revisit high strain rate testing. This study presents a new method for testing the transverse tensile properties of unidirectional composites at high strain rates using ultra-high speed full-field measurements.

The proposed test method is based on the concept of an image-based impact (IBI) test. This type of test uses the reflection of a compressive stress wave to generate tensile stress in the specimen. Throughout the test, full-field displacement measurements are recorded using an ultra-high speed camera combined with the grid method. These measurements are used to calculate strain and acceleration fields over the specimen surface. The stress state in the specimen is inferred using the acceleration field as an embedded load cell. The material response is then obtained from the stress-and strain data. This paper describes the optimisation of the experimental configuration using explicit dynamics simulations and the first experimental validation of the technique. The image-based impact tests were performed on unidirectional carbon fibre specimens in the transverse direction, by imparting a compressive pulse using a projectile launched from a gas gun. Some results can be seen on http://photodyn.org/Presentations/Pierron_2017_CompTest_keynote/Pierron_2017_CompTest_keynote.html.

The main conclusions from the study were:

- Explicit dynamics simulations are a reliable tool for designing this IBI test giving suitable design predictions for the required test configuration.
- It is possible to cause transverse tensile failure in a composite material with a relatively low impact speed, about 30 to 35 m/s.

*Speaker

- Measurement quality with current ultra-high speed camera technology is sufficient to allow for both stiffness and strength identification in the same test.
- The average transverse elastic modulus of the tested composite material was identified as 7.9 GPa using the stress-gauge equation and 7.8 GPa using the optimised virtual fields at a peak average strain rate on the order of 2000 /s. This represents an 8% increase compared to the quasi-static value.
- The average transverse tensile strength was identified as 58 MPa at a strain rate approximately 2000 to 3000 /s. This represents a 57% increase compared to the quasi-static value.

Keywords: Ultra high speed imaging, Virtual Fields Method, High strain rate, IBI test

Multimaterial shell models for the analysis of triaxial braided composites

Carlos González * [1,2], Alejandro Carpintero [2], Miguel Herráez [2], Claudio Lopes [2]

[1] Polytechnic University of Madrid – Dpt. Material Science, ETS Caminos, Polytechnic University of Madrid, 28040 MADRID, Spain
[2] IMDEA Materials – c/Eric Kandel, 2, TecnoGetafe, 28906, Getafe, Madrid, Spain, Spain

In this paper, an efficient numerical methodology based on a multi material shell (MMS) approximation [1,2] is proposed for the simulation of the mechanical behaviour of triaxial braided composites, including the predictions of elastic and resistance properties as well as energy release rates. The model is based on a geometrical description of the textile architecture of the material at the Gauss point level of a standard shell including the corresponding yarn geometrical parameters. Simulations are carried out on single representative unit cells subjected to periodic boundary conditions, on multiple cell representative volume elements corresponding to the representative dimensions of a test specimen, and on embedded cells representative of the fracture progress zone. The numerical results are correlated with experimental data including stress-strain relations, damage mechanisms and crack progression, with remarkable results.
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Keywords: textile composites, fracture, mesomechanics

*Speaker

The new algorithms to study statistical behavior of failure in unidirectional fiber reinforced composites.

Ankit Gupta * [1], Sivasambu Mahesh [1], Shyam M. Keralavarma [1]

[1] Indian Institute of Technology Madras (IITM) – Department of Aerospace Engineering, Indian Institute of Technology Madras, Chennai 600 036, India, India

Monte Carlo simulations of fiber composites have been extensively used in the literature to yield insights into the failure modes and strength scalings with patch size. The simulations are useful indicators of the failure modes when the size of the critical failure event is substantially smaller than that of the patch. If the size scale of the critical event becomes comparable to, or exceeds the patch size, edge effects dominate the observed failure mode. It is therefore, useful to be able to efficiently simulate the failure of large composite patches. Computational limitations, however, have restricted simulation patches to a few thousand fibers in the literature. These limitations arise on account of the computational effort associated with determining (i) the stress overloads due to a single break in a large patch, (ii) the calculation of weights of a set of interacting breaks, and (iii) overloads on intact fibers by weighted superposition of the break influences. The focus of the present work is on developing algorithms for substantially speeding up these computations. The algorithm developed to address (i) exploits the circulant structure of the matrix describing the inter-fiber interactions in periodic unidirectional fiber reinforced composites. The asymptotic computational complexity of this algorithm equals that of the discrete Fourier transform: $O(N \log N)$, for composite patch composed of N fibers. This compares very favorably with the $O(N^3)$ classical algorithm in the literature. Computational effort associated with (ii) and (iii), are substantially reduced using a novel algorithm based on the quadtree data structure. In this method, interactions between nearby breaks are treated exactly. Clusters of distant breaks, on the other other hand, are lumped together into a single super-break. Interactions between super-breaks are then accounted for. This device reduces the total number of interactions that must be treated, and enables Monte Carlo simulations of larger patches than previously possible. Treecode based Monte Carlo simulation involves a small, but non-zero error that arises from lumping together distant breaks. Further, another algorithm is developed to speed up (ii) and (iii), based on the ideas used in treecode algorithm. The efficiency of this method derives from the computational simplicity of weighted superposition in Fourier space. The calculation is computationally exact, and much faster than earlier discussed treecode approach. The computational speed gain due to these algorithms is used to perform Monte Carlo simulations on the composites composed of as many as a million fibers. The data mined from these simulations are then used to develop more robust statistical model for the failure events underling the ultimate tensile strength in the unidirectional fiber reinforced composite.

Keywords: Composites, Fracture, Algorithm, Tree data structure, Discrete Fourier Transform, Numerical methods

*Speaker

Crack propagation in thin-ply composites: Experimental observations and multiscale modelling

Sébastien Kohler *† [1], John Botsis [1], Joël Cugnoni [1]

[1] Laboratory of applied mechanics and reliability analysis (LMAF), Ecole Polytechnique Fédérale de Lausanne (EPFL) – Switzerland

The enhanced mechanical properties of thin-ply composites in unnotched tensile tests, such as higher ultimate tensile strain, extended fatigue life and delayed onset of damage raised a significant interest in the engineering and materials communities alike. The high onset of damage in unnotched tensile tests of quasi-isotropic laminates [1] was especially interesting as the measurements performed by acoustic emission showed that for very thin plies, the LEFM based models, such as the in-situ strength model [2], were not in agreement with the experimental observations.
To understand the sources of these discrepancies, the free edges of the tested specimens were observed in-situ using a video microscope simultaneously with acoustic emission measurements. The appearance of the first transverse crack in the region of observation showed a clear non-linear scaling with decreasing ply thickness. The onset of damage defined by acoustic emission and the one defined by free edge observation differed both in their scaling's shape and magnitude, with the former always being observed at higher stresses than the latter. [3]

Microscopy observations of cross sections taken at the same position in the gauge length from both the free edge and the centre of partially loaded samples at different predefined stress levels were performed. They showed that the stresses at which the propagation of the free edge transverse cracks reached the centre of the specimen was in good agreement with the onset of damage defined by acoustic emission. This result was then confirmed by tomographic images taken from similar samples after a 24h infiltration of a contrasting agent. The free edge cracking that could be observed in the early stages of testing is thus shown to be better confined when the ply thickness is decreased, and the acoustic emission measurements accurately predicts significant damage reaching the centre of the specimen.

To model this phenomenon, a 2D multiscale embedded cell FE model based on real microstructures was developed. The fibre-matrix interface was modelled using a linear softening, energy based, cohesive model, and the matrix using a Drucker-Prager model with regularized damage. The constituents' and lamina properties were obtained from the material suppliers and experimental characterization. The problem was solved using a dynamic explicit solver (Abaqus Explicit) with mass scaling to represent the quasi-static response of the material.

Using plane-strain boundary conditions on this model to represent the behaviour of the bulk of the specimen, the interface toughness was recalibrated to match the acoustic emission onset of damage for the largest ply thickness modelled. The model thus defined was in very good agreement with the experimental acoustic emission measurements for smaller ply thicknesses. Using plane-stress boundary conditions on the same model as a first order approximation of the free edge behaviour, the numerical results were also in good agreement with the onset of free edge cracking observed experimentally.

This talk will focus on the sensitivity analysis of this model, as well as on the events of the damage sequence that it predicts when applied to composites with different constituents.

*Speaker
†Corresponding author: sebastien.kohler@epfl.ch

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Keywords: Thin, ply, Acoustic emission, Damage mechanisms, Optical microscopy, Multiscale modelling

Prediction of mechanical properties of glass fibre-reinforced polypropylene by means of computational micromechanics

Joseba Múgica *† [1], Miguel Herraez [1,2], Fernando Naya [3], Claudio Lopes [1], Carlos González [1]

[1] IMDEA Materiales – C/ Eric Kandel, 2, Tecnogetafe, 28906 Getafe, Madrid, Spain
[2] Institute IMDEA Materials [Madrid] (IMDEA Materials) – Tecnogetafe 28906 Getafe Madrid, Spain
[3] Laboratory of applied mechanics and reliability analysis (LMAF), Ecole Polytechnique Fédérale de Lausanne (EPFL) – Switzerland

The determination of ply properties of fibre-reinforced polymers (FRPs) is necessary to succeed in component design. However, traditional experimental characterisation methodology requires significant resource and time investments. As an alternative, there is coupled experimental-computational micromechanical approach. In this work, such an alternative is utilized to study the mechanical behaviour of a woven fabric composite constituted by glass fibre and polypropylene. The methodology proposed allows to determine both the longitudinal and the transverse yarn properties, under both tension and compression, as well as in-plane shear yarn properties. Firstly, the matrix and the fibre/matrix interface are characterised by means of micromechanical tests: nanoindentation for the matrix and fibre push-in for the interface. Subsequently, three different representative volume element (RVE) models are constructed to predict ply mechanical response under different loading conditions, including longitudinal tension, longitudinal compression, transverse tension, transverse compression as well as in-plane shear. From such responses, the yarn properties are deduced, being considered reasonable since they are consistent with data available in literature. Then, with these properties a yarn constitutive model is formulated. After this, the constitutive model is used within a ply unit cell model of the composite and is, finally, validated after demonstrating it is able to provide accurate predictions of ply behaviour.

Keywords: Micromechanics, Representative volume element

*Speaker
†Corresponding author: joseba.mugica@imdea.org

Influence of Fiber Waviness on Compressive Response of Fiber-Reinforced Composites using Micromechanical Approach

Mehdi Naderi *† [1], Nicole Apetre [1], Nagaraja Iyyer [1], Kishan Goel [2], Nam Phan [2]

[1] Technical Data Analysis, Inc. – 3190 Fairview Park Dr., Suit 650, Falls Church, VA, USA, United States
[2] US Naval Air Systems Command – United States

The influence of fiber waviness on the compressive response of fiber-reinforced composite is studied in this paper via micromechanical approach. Augmented finite element method (AFEM) is used to provide high-fidelity data on damage initiation and propagation along with micromechanical analysis. A python program is written to generate the micromechanical model as the input file for Abaqus model. We also discuss the three dimensional AFEM, developed as a Abaqus User Element (UEL). Zero-thickness cohesive elements are inserted on fiber/matrix interface for modelling fiber/matrix interface delamination. Both automatic damage initiation and propagation algorithm is implemented in AFEM to capture discontinuities. Random degree of waviness are considered in different sets of representative volume elements (RVEs). The results show how detrimental is the fiber misalignment to the structural integrity of composite components. It is also seen that the damage initiation and propagation locations are controlled by the degree and location of waviness.

Keywords: Fiber waviness, Micromechanics, Compression, Finite Element, Composite

*Speaker
†Corresponding author: mnaderi@tda-i.com

Micromechanical study of the origin of fiber bridging in mode I interlaminar and intralaminar fracture

Fernando Naya * [1], Georgios Pappas [1], Joël Cugnoni [1], John Botsis [1]

[1] Laboratory of applied mechanics and reliability analysis (LMAF), Ecole Polytechnique Fédérale de Lausanne (EPFL) – Switzerland

When a unidirectional (UD) carbon fiber reinforced polymer (CFRP) is loaded under mode I, fracture process in the steady-state is dominated by large scale fiber bridging (LSB) [1].
Although the energy release rate (ERR) during the initiation of fracture is the same for interlaminar and intralaminar failure, the development of fiber bridging and, therefore, the ERR during the steady state is quite different [1,2]. Maximum bridging tractions, bridging zone length and, specially, the morphology of fiber bundles are quite dissimilar for interlaminar and intralaminar fracture [1,2].

So far, identifying the morphology of these fiber bundles required the study of micrographs of the cross-section of the tested specimens. Therefore, a laborious experimental procedure is needed. In addition, the origin of the differences between interlaminar and intralaminar fracture remains unknown. The aim of this research is to obtain a physical explanation of these differences based on morphological studies, using real values of the mechanical properties of the constituents and realistic multiscale modeling.

Nowadays, numerical models based on computational micromechanics have stood out as powerful tools to predict fracture mechanisms and evaluate the influence of the material constituents and internal microstructure on the macroscopic material properties and response. Normally, the material microstructure is studied in detail and the results are used to generate a *Representative Volume Element* (RVE) of the composite material. However, understanding the mode I fracture process of a UD CFRP requires RVEs that are computationally unrealistic.

In order to deal with this problem, in this work, a new bottom-up multiscale model is proposed. The model uses large microstructures obtained by means of image reconstruction procedures. Material properties are assigned in a stochastic way relying on homogenized properties obtained by means of computational micromechanics based on the analysis of small periodic RVEs. The model is able to handle cross-sections of several millimeters capturing the influence of the ply microstructure in the interlaminar and intralaminar fracture process (Figure 1). The influence of several geometric parameters (ply and specimen thickness), together with the mechanical properties of the constituents, on the morphology of fiber bundles and fracture surface are investigated in the present work.

Keywords: Multiscale modeling, Intralaminar fracture, Interlaminar fracture, Micromechanics, Composite materials

*Speaker

Mode I delamination of a tufted through-thickness reinforced composite

Georgios Pappas *† [1], Simon Joncas [2], Véronique Michaud [3], John Botsis [1]

[1] Laboratory of applied mechanics and reliability analysis (LMAF), Ecole Polytechnique Fédérale de Lausanne (EPFL) – Switzerland
[2] Automated Manufacturing Department, École de technologie supérieure (ÉTS) – Canada
[3] Laboratory for Processing of Advanced Composites (LPAC), Ecole Polytechnique Fédérale de Lausanne (EPFL) – Switzerland

Through the thickness reinforcement (TTR) is employed to increase the resistance to fracture of layered composites. TTR mainly involves z-pinning for prepreg laminates, and stitching for dry-fiber textiles. Moreover, tufting has been successfully used in few industrial applications involving preforms and various liquid molding fabrication techniques. Numerous experimental and modeling studies exist in the literature, on the effect of z-pinning with some of which also deal with stitching. However, very few studies have dealt with tufting as TTR. This study presents experimental work and modeling techniques in mode I delamination fracture of a cross-ply, twill 2/2, E-glass/epoxy system with tufting TTR. A 5 mm squared (5-SQ) tufting pattern (4 tufts/cm2) is introduced on the fabric preforms prior infusion. The produced material is used to form symmetric double cantilever beam (DCB) specimens with a precrack introduced by means of a release film. In this study the effect of ply delamination with tow/ply bridging phenomena and the effect of tuft bridging phenomena are isolated. Moreover, apart from the behavior of normal tuft, the one of loop-less tufts is also investigated, with loops being removed after infusion by surface machining. In total five groups of DCB specimens are tested: 1) Neat E-glass/epoxy system (Nt). 2) Normal 5-SQ tufted. 3) Normal 5-SQ tufted with a full length release film (5F-SQ). 4) Milled down 5-SQ tufted (5-SQM). 5) Milled down 5-SQ tufted with a full length release film (5F-SQM).
All DCB specimens are tested using displacement controlled quasi-static, monotonic, mode I loading conditions and the corresponding load, displacement, rotation and crack advance data are employed to calculate the corresponding energy release rates (ERR) and R-curves. The traction-separation relation related to the ply delamination and the corresponding tow/ply bridging phenomena are identified using an inverse characterization scheme employing experimental strain measurements obtained by fiber Bragg grating (FBG) sensors. The force-separation relations, that describe the mode I failure response of a tuft, are acquired from uniaxial tuft pulling tests of fully pre-released specimens on the symmetric delamination plane, for both normal and loop-less ones.

The characterized traction-separation and force-separation relations are implemented in FE models using cohesive and discrete node connector elements, respectively, to predict the load-displacement response (Figure 1). Analysis of the normal tufted series shows that the ERR of the ply delamination response with the tow/ply bridging phenomena can be superimposed to the isolated one of the tufts to predict the behavior of the actual tufted DCB specimen (Figure 2). A very strong toughening effect is acquired from the 5-SQM series with an increase in the maximum ERR at the steady crack propagation state of about 60% compared to 5-SQ series (Figure 2). This toughening response is attributed to the change of tuft failure mechanism from mid-plane rupture (normal) to complete pull-out (loop-less) with the latter one dissipating almost twice the energy before complete failure. Moreover, tuft pull-out apparently triggers further tow/ply bridging phenomena adding another contribution to the aforementioned toughening effect.

*Speaker
†Corresponding author: georgios.pappas@epfl.ch

Keywords: Fracture resistance, Through thickness reinforcement (TTR), Tufting, Traction separation relations

Damage tolerant composites with discontinuous and hierarchical microstructures

Soraia Pimenta *† [1], Joel Henry [1]

[1] Department of Mechanical Engineering [Imperial College London] – South Kensington Campus London SW7 2AZ, United Kingdom, United Kingdom

Natural composites (e.g. nacre and bone) often display outstanding levels of damage tolerance, especially considering that they are mainly composed of brittle and stiff inclusions. It has been widely accepted that this damage tolerance in natural composites is the result of tailored microstructures featuring discontinuous inclusions distributed in a hierarchical arrangement [1]. This work explores the potential of translating these discontinuous and hierarchical features to the microstructure of carbon-fibre composites, in order to improve their damage tolerance; this is done through a combination of Finite Elements simulation and experimental testing of designed microstructures.

The microstructures investigated in this work are based on "brick-and-mortar" discontinuous composites [2], in which the "bricks" are creating by laser-cutting unidirectional carbon-epoxy thin-plies [3], and the "mortar" is the epoxy-based interface between the "bricks". It is shown (both via FE simulations and experimental testing) that such "brick-and-mortar" microstructures promote additional energy dissipation through damage of the interface. However, simple "brick-and-mortar" discontinuous microstructures – without any hierarchical features – suffer from damage localisation at the weak spots of a specimen, limiting the amount of diffuse damage accumulation and energy dissipation (even under uniform loading).

Hierarchical self-similar discontinuous composites were designed by assembling two scales of "brick-and-mortar" microstructures (in which a larger-scale brick is itself composed by smaller-scale bricks). In this case, "mortar" damage first appears at the interface between the larger "bricks", and then propagates stably within the smaller-bricks, creating a repeating pattern of diffuse damage in all large-bricks of a tensile specimen (observed both via simulations and experiments). Consequently, hierarchical self-similar discontinuous composites tested under uniaxial tension presented non-linear stress-strain curves.

The analysis of the diffuse damage patterns inside each large-brick suggested that some small-"brick" discontinuities in the hierarchical self-similar microstructure were not actively participating in damage accumulation and energy dissipation. Consequently, the self-similar constrain imposed to these microstructures was relaxed in a further design iteration, in which the small "bricks" used to assemble larger "bricks" were not all self-similar, but designed individually to maximise energy dissipation.

These non-self-similar hierarchical discontinuous microstructures were designed through Finite Elements simulations, and selected designs were tested experimentally under uniaxial tension. The specimens were tested under the scanning-electron microscope, which showed diffuse damage spread throughout the specimens, and significantly non-linear stress-strain responses. The optimal microstructures have also been subjected to tensile loading-unloading cycles, which showed that a significant proportion of the non-linear deformation observed in monotonic tests is permanent.

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*Speaker
†Corresponding author: soraia.pimenta@imperial.ac.uk

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Keywords: Carbon, fibre composites, Discontinuous composites, Hierarchical composites, Modelling, Experiments, Bio, inspired composites, Damage tolerance

Nacre-inspired CFRP with fractal-textured interfaces

Silvestre Pinho *† [1], Federico Narducci [1]

[1] Department of Aeronautics [Imperial College London] – Department of Aeronautics, South Kensington Campus, Imperial College London, SW7 2AZ London, UK, United Kingdom

Research on biological composites has provided many insights into how composite materials properties can be improved by micro-structural design. Some features of materials like bamboo, bone and shells, including structural hierarchy and crack arrest, can be adapted to synthetic composites in order to achieve increased toughness and defect tolerance.
In particular, nacre, with its characteristic staggered arrangement of hard ceramic platelets in a soft protein matrix, provides one of the most striking trade-offs between strength and toughness. Researchers have attempted to reproduce its discontinuous 'brick-and-mortar' micro-structure with various materials (including glass and ceramics), with the aim to achieve damage-tolerant behaviour in traditionally brittle materials.

Nacre-inspired crack deflection mechanisms can be exploited in Carbon-Fibre Reinforced Polymers (CFRPs), in order to avoid sudden failure in the most loaded part of the structure. In earlier work by the authors, this was achieved by means of a laser-engraved tiled architecture in the prepreg, with tiles of the order of 600 μm and with a hourglass shape, in order to increase energy dissipation during pull-out. Such composite is able to deflect cracks along a tortuous path; however, limited damage diffusion was observed in that case, suggesting the need for a tougher matrix at the tile/tile interface.

In this work, we design a carbon/epoxy composite with nacre-like micro-structure and PLA micro-textured interface. A film-casting technique is used to create thin (_˜12 μm) controlled patches of thermoplastic on the prepreg surface, with the aim to promote progressive unlocking and pull-out of subsequent layers of tiles, thus increasing the damage diffusion capability of the material. Different patterns of PLA patches are explored, with particular regard to fractal shapes, given their ability to dissipate energy at multiple scales and act as crack stoppers. The best performing pattern is eventually identified, based on its ability to diffuse damage and delay localisation of failure.

The nacre-inspired composite is then tested in four-point bend configuration (in an in-situ SEM environment), and the effect of interleaving a thin layer of thermoplastic is assessed by comparing the performance of the PLA-patterned nacre with the one with pure epoxy interface.
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Keywords: CFRP, bioinspired, nacre, interface

*Speaker
†Corresponding author: silvestre.pinho@imperial.ac.uk

Viscoelastic behaviour of nanocomposites reinforced with carbon nanostructures, PLA/CNT-COOH

Viviana Pinto [1], Rui Guedes [*†] [1,2]

[1] Institute of Science and Innovation in Mechanical and Industrial Engineering (INEGI) – Campus da FEUP Rua Dr. Roberto Frias, 400 4200-465 Porto, Portugal
[2] Faculdade de Engenharia da Universidade do Porto (FEUP) – Rua Dr. Roberto Frias, s/n 4200-465 Porto, Portugal

Biodegradable polymers like polylactic acid (PLA) have been proposed as a solution for anterior cruciate ligament (ACL) augmentation devices. These devices should allow proper tissue regeneration and tissue healing. Several studies pointed that the appropriate material for these devices should act as a mechanical support during ACL recovery, while simultaneously promote its regeneration. This is a huge challenge that requires biocompatibility and mechanical functionality [1]. PLA is a biodegradable polymer already approved by FDA (U S Food and Drug Administration) that presents higher tensile strength when compared to other polymers [2] and co-polymers with d-lactide (PLDA). Despite having a considerable short-term strength at higher loading rates, lifetime under static loading conditions is unsatisfactory, being prone to creep failure [3,4]. This feature is explained by the plastic flow created by molecular mobility induced by stress [3]. The enhancement of PLA mechanical resistance to fatigue offers a chance to circumvent this weakness, expecting to prevent laxity or premature rupture of the device [5]. For that purpose, PLA was reinforced with carbon nanoparticles, such as nanoplatelets of graphene (PLA/GNP) and carboxyl functionalized carbon nanotubes (PLA/MWCNT-COOH). These nanoparticules are expected to reduce permanent strain observed in neat PLA. Considering the nonlinear viscoelastic behavior of ligaments, it is crucial to understand viscoelastic properties of PLA, PLA/graphene (GNP) and PLA/-COOH functionalized carbon nanotubes (CNT-COOH) nanocomposites. Hence, a creep experimental and numerical study of PLA nanocomposites was accomplished.
Polymer nanocomposites were prepared, by melt blending followed by compression moulding, resorting to PLA (Mw_~50000, Ingeo™ 2003D, Natureworks LLC, EUA), nanoparticles of graphene (GNP - graphene nanoplatelets grade M5, 5 μm medium diameter and 6 to 8 nm thickness, from XG Sciences, Lansing™, MI, EUA), and functionalized multi-walled carbon nanotubes (NC3150, 9.5 nm average diameter and less than 1 μm average length, more than 95% carbon purity, Nanocyl™, Belgium). Specimens were cut in a rectangular format, with a total length of 10x80 mm. Nanocomposites were produced with several weight percentages compositions of reinforcements, namely PLA/GNP (98:2) and PLA/MWCNT-COOH (99.8:0.2; 99.7:0.3; 99.5:0.5; 99.3:0.7; 99:1).

Creep tests were performed under several tensile stress levels assigned as failure stress fractions, i.e. 10% (T1), 30% (T2), 50% (T3) and 70% (T4). The load ramp was set at 2.5N/s until reaching the desired stress level and then kept constant during 600 seconds. Thereafter the load was removed, during 600 seconds until load resetting. Specimen axial strain was logged as well as the time and the stress level. All tests were done at room temperature (20 °C) and at least three specimens were taken for each case.

As result, strain behavior was analyzed, considering permanent strain, recoverable strain and creep compliance. Also, observing the viscoelastic behaviour of PLA and its nanocomposites, numerical Findley's power law and Burgers model were employed to represent creep experimental data.

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*Speaker
†Corresponding author: rmguedes@fe.up.pt

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Keywords: viscoelasticity, Creep, carbon nanotubes, graphene, polylactic acid, biodegradable

Durability of mechanical performances of composite assemblies in a hygro-thermo-mechanical environment

Ivanna Pivdiablyk * [1], Patrick Rozycki [1], Laurent Gornet† [1], Frédéric Jacquemin [2], Stéphane Auger [3], Sophie Toillon-Rey Flandrin [3]

[1] Institut de Recherche en Génie Civil et Mécanique (GeM) – Ecole Centrale de Nantes, CNRS : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[2] Institut de Recherche en Génie Civil et Mécanique (GeM) – Ecole Centrale de Nantes, Université de Nantes, CNRS : UMR6183 – 58 rue Michel Ange, 44600 Saint-Nazaire, France
[3] Centre Technique des Industries Mécaniques (CETIM) – CEntre Technique des Industries Mécaniques - Cetim (FRANCE) – 74 Route de la Jonelière, 44308 Nantes, France

Threaded assemblies are mainly designed according to the standard VDI 2230 that facilitates the computations and enables a good understanding of involved parameters (such as flexibility of bolt and assembled parts, clamping force, loading position...). Hence VDI 2230 became a reference for mechanical assemblies; there are, however, major drawbacks, which significantly restrict proper design. For instance, these standards can be theoretically applied only to metals, and also they do not always take into account the effect of the temperature and humidity. Consequently, the impacts of environmental conditions on thermoplastic composite assemblies are of high interest.
The present project is made up of several steps, thus the first one is the experimental characterization of both thermoplastic composite material and bolted assemblies at various temperatures and relative humidity levels. The experimental data allows not only to identify the impact of the temperature and relative humidity level on the mechanical properties of the composite, but also the influence on the part flexibility, the stresses in the fixing area, and the creep resistance. In addition to these experiments, we also suggest some numerical simulations on composite Representative Volume Element in order to identify the out-of-plane properties of material which remain important for an assembly.

The first part of this paper deals with the experimental work. Preliminary tests with different drying and ageing conditions are performed before the material testing. The chosen temperature allows to accelerate desorption and absorption processes without modification of the mechanical behavior. Thereafter, tensile testing of aged specimens is conducted at varying temperature and moisture levels. This allows a proper identification of ultimate values, elastic and damage parameters of the composite material as functions of temperature and relative humidity. The previous experimental constants serve as input for numerical simulations on the composite RVE (its geometry has been identified with an electron scanning microscope) that represent the second part of the paper. Such approach facilitates the access to the out-of-plane properties because it is quite complex to define them experimentally. The last tests batch is aimed at determining mechanical properties of the bolted composite joint as functions of bolt preload, material thickness, moisture content and testing temperature.
Finally, we present the conclusions and developments which foresee the effects of environmental conditions on the behavior of composite assemblies.

Keywords: Composite assembly, experiments, mechanical properties, environmental conditions

*Speaker
†Corresponding author: laurent.gornet@ec-nantes.fr

Novel analytical approach for determining edge stresses in general composite laminates under tension

Jesus Maria Romera *† [1], Faustino Mujika [1]

[1] University of the Basque Country (UPV/EHU) – Spain

Free edge effect in composite laminates has been extensively studied because it reduces the strength of the laminate strips and the exact solution for this problem has not yet been attained. A recent analytical approach for quasi-isotropic symmetric laminates under tension has been extended to analyze any configuration of symmetric laminates. The assumed displacement field in the previous approach has been modified and a system of first-order linear differential equations with constant coefficients has been achieved. The system of equations has been solved by using the Euler Method. A novel closed-form analytical solution based on sinusoidal and exponential functions has been obtained. Through-the-width distributions of the out-of-plane interlaminar stresses have been tested with a Finite Element model based on the submodelling technique.

Keywords: SYMMETRIC COMPOSITE LAMINATES, EDGE EFECTS, ANALYTICAL APPOACH, FINITE ELEMENT METHOD, TENSILE LOAD

*Speaker
†Corresponding author: jesusmaria.romera@ehu.es

On the efficiency of the adaptive continuum shell element for the analysis of damage and delamination in layered composites

Joris Remmers * [1], Martin Fagerström [2]

[1] Eindhoven University of Technology (TUE) – Eindhoven University of Technology Den Dolech 2 5612 AZ Eindhoven, Netherlands
[2] Chalmers University of Technology (Chalmers) – Chalmers University of Technology SE-412 96 Gothenburg Sweden, Sweden

As a means to decrease the complexity and size of numerical models for the simulation of progressive failure in composite materials, an adaptive continuum shell element has been developed using the concept of Isogeometric Analysis [1]. The formulation, which is based on the work by Hosseini et al. [2], adopts T-spline basis functions for the discretisation of the shell mid-surface, whereas higher-order B-spline functions are used for the interpolation in the thickness direction. Layer interfaces and delaminations can be modelled as weak and strong discontinuities by knot insertions. If no discontinuities are assumed, all layers are lumped in a single element, yielding a fast and accurate formulation that can be used to analyse composite structures prior to failure. As a result, it is computationally efficient to start a simulation with this lumped approximation and enhance the element to correctly model layer interfaces and delaminations when stresses reach critical values.
In order to automatically enhance the element, various stress-based criteria using element local improved interlaminar stresses can be used. However, for such a stress based approach, the prediction of the through-thickness variation of out-of-plane stress components needs to be improved if a lumped approximation is used. For this purpose, the capability of a reconstruction technique based on the classical strategy of integrating the momentum balance equations can be used [3,4]. Due to the nature of the isogeometric analysis approximation and its higher order displacement smoothness over element edges, this reconstruction can be performed element-wise.

In this paper, we will investigate a variety of stress based criteria to obtain the most efficient strategy to enhance the adaptive continuum shell element. The performance of the models will be demonstrated in various cases, including the analysis of global buckling, ply failure and delamination.

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*Speaker

Keywords: Isogeometric Analysis, Continuum Shell, Delamination, Damage

A Computational Micromechanics Study of the Ballistic Performance of UHMW-PE Composites

R. Varun Raj *† [1], Ron Peerlings [1], Vikram Deshpande [2]

[1] Mechanics of Materials, Department of Mechanical Engineering [Eindhoven] – P.O box 513 5600 MB Eindhoven, Netherlands

[2] Department of Engineering [Cambridge] – Cambridge University, Department of Engineering, Trumpington Street, Cambridge CB2 1PZ, United Kingdom, United Kingdom

Composites reinforced with Ultrahigh Molecular Weight Polyethylene (UHMWPE) fibres such as Dyneema ® fibres - are widely used in impact and penetration resistant applications like blast resistant armors, spall liners, etc. These highly drawn fibres exhibit excellent specific strength and modulus. A strong rationale for their potential in ballistic applications is driven by work carried out by Cunnif in establishing a strong correlation between fibre properties and ballistic performance of the composite [1]. However, such an evaluation does not consider effects of other basic material properties and possible failure mechanisms/modes at play during ballistic loading [2, 3, 4]. This forms the motivation to undertake a more elaborate study, that can aid in gaining insights into operative failure mechanisms present under ballistic loading while establishing their dependence on model parameters like matrix shear strength, velocity of impact and fibre topology.
In this work, plane strain dynamic impact finite element simulations of a rigid cylindrical impactor onto an infinite UHMW-PE cross-ply beam were setup in Abaqus Explicit. The plies were constitutively modelled with transversely isotropic elasticity and crystal plasticity - in order to capture the mechanics governed by the fibre-matrix microstructure. The results from each simulation were used to track tensile fibre failure initiation within the plies. Upon failure initiation, the specific failure mode was identified. Overall parametric dependency was represented as an impact map. Fibre topology was incorporated into the model through modications of parameters in ply constitutive model and its effect on failure modes was studied using two separate impact maps - one for the fibre system (circular fibres embedded in a matrix) and one for the tape system (continuous microstructure, with no individual fibres discernible). Additionally, the effect of fibre strength, ply thickness, ply order and impactor size will also be reported.

Results of the simulations indicated improvement in resistance against failure under ballistic loads in tape systems compared with equivalent fibre systems. An additional operative failure mode was observed to be present for the tape systems which
is absent in the fibre system.

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*Speaker
†Corresponding author: r.varun.raj@tue.nl

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Keywords: UHMWPE, Impact, Ballistics, Fibre Topology, Crystal Plasticity

Modeling of water diffusion mechanism in PP/Date palm fiber composite materials

Sonia Boukettaya *† [1,2], Bendaly Hachmi *

[2], Chatti Sami *

[3], Ahmad Alawar *

[4]

[1] Ecole polytechnique de Sousse – Boulevard Khalifa Karoui, 4054 Sahloul- sousse, Tunisia
[2] Ecole nationale d'ingénieurs de sousse (LMS-ENISo) – B.P. 264, 4023 Sousse Erriadh, Tunisia
[3] Institut Supérieur des Sciences Appliquées et de Technologie de Sousse – Tunisia
[4] Polytechnic Abu Dhabi – United Arab Emirates

The aim of this work is to model the water diffusion mechanism of the PP/date palm fibers composite materials after their exposure at different immersion conditions. For short immersion periods, a model combining the fick law and the time temperature stress principle has been proposed to describe the water absorption mechanism. After a saturation time and at high immersion temperatures, it has been noted that the water diffusion mechanism leads to a physical degradation and a mass loss into the composite material. Microscopic observations have revealed the emergence and the development of the fiber/matrix debonding and the micro-cracks on the surface and along the composite materials. Thus, and in order to better describe the global water diffusion mechanism, anthor term describing the degradation phenomenon has been injected in our model. Then, a new general model has been also proposed in the present work. A good agreement between the theoretical and experimental data has been obtained.

Keywords: polypropylene, date palm fiber, composite, modeling, water diffusion, stress relaxation

*Speaker
†Corresponding author: sonia.boukettaya@polytecsousse.tn

S3: Mechanics of metals - Experiments and models

Control-point based hybrid discontinuous Galerkin method for geometrically nonlinear crystal plasticity

Atefeh Alipour * [1], Stephan Wulfinghoff [2], Stefanie Reese [2]

[1] Institute of Applied Mechanics, RWTH Aachen, Germany – Germany
[2] Institute of Applied Mechanics, RWTH Aachen, Germany – Germany

A new concept for hybrid discontinuous Galerkin methods is presented: control points. These are defined on the inter-element boundaries. The concept makes it possible to formulate element shape functions without nodes. Moreover, the theory is not restricted to certain element shapes. Furthermore, one can either formulate the discrete model such that the displacement is continuous or discontinuous at the control points. Classical continuous isoparametric elements are included as special case. As an additional new feature, a regularization technique for very high strain rate sensitivity exponents up to 1000 in finite single crystal viscoplasticity is presented and implemented into the new hybrid discontinuous Galerkin (DG) framework and the one by Wulfinghoff et al. (2017). To the knowledge of the authors, it is the first hybrid discontinuous Galerkin implementation of geometrically nonlinear plasticity, here in the context of single crystal plasticity. The regularization method in combination with the DG formulations allows to achieve a very simple implementation into existing finite element codes leading to a numerically efficient, robust and locking-free model. Two examples are investigated: the deformation of a planar double slip single crystal exhibiting localization in the form of shear bands and a 2D oligocrystal under uniaxial load.

Keywords: Crystal plasticity, Hybrid discontinuous Galerkin method, Quadrilateral element, control points

*Speaker

Thermo-mechanical simulation of ITER-like plasma facing components under thermal cycling tests.

Alan Durif * [1], Marianne Richou [1], Jean-Michel Bergheau [2], Guillaume Kermouche [3], Matthieu Lenci [4]

[1] Institut de Recherche sur la Fusion par confinement Magnetique (IRFM), CEA – Centre de recherche du Commissariat à l'Energie Atomique - CEA Cadarache (Saint Paul-lez-Durance, France) – F-13108 Saint-Paul-Lez-Durance, France
[2] Université de Lyon, ENISE LTDS UMR 5513 CNRS (ENISE LTDS) – Université de Lyon, ENISE LTDS – Ecole Nationale d'Ingénieurs de Saint-Etienne (ENISE), 58 rue Jean Parot, 42023 Saint-Etienne, France
[3] Centre Science des Matériaux et des Structures – École Nationale Supérieure des Mines - Saint-Étienne – 158 cours Fauriel 42023 SAINT-ETIENNE Cedex 02, France
[4] Centre Science des Matériaux et des Structures – Ecole Nationale Supérieure des Mines de St Etienne – 158 cours Fauriel 42023 SAINT-ETIENNE Cedex 02, France

In the future, the fusion reaction could become a viable way to generate electricity. To perform this reaction, reactors confine magnetically plasma in a vacuum chamber. However, plasma confinement is imperfect and due to the magnetic plasma configuration, energy losses are directed toward the main wall, mainly on the lower part of the vessel called divertor. For the ITER divertor, plasma facing components are made with tungsten as armor material, bonded on a coper alloy tube as heat sink structural material and cooled by water. Such tungsten armored plasma facing components are able to withstand high heat flux up to 20 MW/m2 and consequently satisfy ITER requirements. However, due to high heat flux, strong temperature gradients are generated on a thickness of 7mm leading to extreme temperature values from 2000∘C at the loaded surface to 500∘C near the cooling tube. 2000∘C is large enough to alter the tungsten microstructure by recrystallization causing mechanical properties losses and then damages such as macro cracks in the material. This damage process is not well understood yet and its understanding will be necessary to optimize the use of these components in tokamak environment. Up to now, numerical simulations were achieved to predict the life time of tungsten armored plasma facing components assuming pure linear elastic or linear elastic and ideal-plastic tungsten behavior [1].
In this paper, a numerical simulation to predict tungsten life time taking into account the actual mechanical behavior of tungsten is proposed. Indeed, compressive tests were performed at several temperatures from 500∘C to 1150∘C to study the mechanical behavior of stress-relieved and recrystallized tungsten. Stress-relieved tungsten tests reveal an elastoplastic behavior that is sensitive to strain rate over 900∘C. Concerning recrystallized tungsten, it shows an elastic-viscoplastic behavior on the entire explored temperature range which leads us to use an elastic-viscoplastic with isotropic hardening constitutive relation in the modeling. To estimate the life time of the tungsten block, the Manson-Coffin relationship [2] is used. Estimations of plastic strain and number of cycles to failure are performed from several typical thermo-mechanical solicitations. Tungsten recrystallization during transient is not simulated in this study since only steady state simulations were realized in a first approach. Various recrystallized layers thicknesses were modeled in order to highlight the effect of the static recrystallization phenomenon on the component life time. Using these mechanical properties and dedicated simulations, we estimated a higher number of cycles to failure compared to that obtained by considering the behavior of tungsten as linear elastic or linear elastic and ideal-plastic.

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*Speaker

Keywords: fusion reaction, plasma facing component, ITER, divertor, tungsten, damage, compressive test, mechanical behavior, plastic strain, recrystallization, simulation, cycles to failure

Observation and modeling of internal stresses around twin lamellae in beta-metastable Ti-alloy

Laurent Delannay * [1], Fengxiang Lin [2]

[1] iMMC - Université catholique de Louvain (UCLouvain) – av G Lemaitre 4 - 1348 Louvain-La-Neuve, Belgium
[2] Université catholique de Louvain, iMMC, av G Lemaitre 4, 1348 Louvain-la-Neuve, Belgium (UCLouvain) – Belgium

Plastic deformation by dislocation slip and twinning is investigated in a beta-metastable body centered cubic Ti-12Mo alloy. Experimental orientation maps show thin twin lamellae which are transmitted across grain boundaries with suitable lattice misorientations.
A three-dimensional crystal plasticity based finite element model (CPFEM) is used to predict internal stresses in the surrounding of deformation twins. It is found that twin transmission across grain boundaries relaxes the strong back-stresses at the twin tip more than dislocation slip does. CPFEM predictions also indicate that the forward-stresses, which promote twinning in the adjacent grain, depend not only on the crystal misorientation angle but also on the misorientation axis, and the inclination of the grain boundary plane.
CPFEM predictions tend to conform to HR-EBSD measurements of the lattice strains around a twin lamella.

Keywords: crystal plasticity, anisotropy, residual stresses, titanium

*Speaker

Microstructural Origins of Fatigue Crack Nucleation in Ni Aero-engine Alloys

Fionn Dunne * [1]

[1] Imperial College – London, United Kingdom

An integrated experimental, characterization and computational crystal plasticity study of cyclic plastic beam loading has been carried out for nickel single crystal (CMSX4) and oligocrystal (MAR002) alloys in order to assess quantitatively the mechanistic drivers for fatigue crack nucleation.
The experimentally validated modelling provides knowledge of key microstructural quantities (accumulated slip, stress and GND density [1]) at experimentally observed fatigue crack nucleation sites and it is shown that while each of these quantities is potentially important in crack nucleation, none of them is in its own right is sufficient to be predictive. However, the local (elastic) stored energy density, measured over a length scale determined by the density of GNDs, has been shown to predict crack nucleation sites in the single and oligocrystal tests. In addition, once primary nucleated cracks develop and are represented in the crystal model, the stored energy correctly identifies where secondary fatigue cracks are observed to nucleate in experiments [2]. This (Griffith-Stroh type) quantity also correctly differentiates and explains intergranular and transgranular fatigue crack nucleation.

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Keywords: Crystal slip, GND density, stored energy, fracture

*Speaker

An atomistic strategy to determine the activation energy for dislocation interaction with Guinier-Preston zones in Al-Cu alloys

Gustavo Esteban-Manzanares [1], Enrique Martínez [2], Javier Segurado [1,3], Javier Llorca [*1,4]

[1] IMDEA Materials Institute – Getafe, Madrid, Spain, Spain
[2] Los Alamos National Laboratory – Los Alamos, NM, United States
[3] Department of Materials Science, Polytechnic University of Madrid, Madrid – Spain
[4] Department of Materials Science. Polytechnic University of Madrid. Madrid, Spain – Spain

Al-Cu alloys are very efficiently strengthened during ageing at ambient temperature by means of Guinier-Preston (GP) zones. They are formed by monolayers disks of Cu atoms of a few nm in diameter on $\{100\}$ planes of the FCC Al lattice. The GP zones are overcome by the dislocations through a thermally-activated process and the standard strategy to determine the energy barrier is based harmonic transition state theory that assumes that the activation entropy can be approximated by the vibrational entropy. Under these conditions, the rate at which the dislocations overcome the GP zone is given by an Arrhenius equation with a pre-exponential factor and an activation energy, that can be obtained by means of molecular dynamics simulations and the nudged elastic band method, respectively.

It is well known that the nudged elastic band method is very sensitive to the initial and final configurations, which should be minimum energy configurations. They are normally obtained by means of molecular statics simulations but this strategy may not be accurate in the case of dislocation/precipitate interactions which –due to the large number of atoms involved– present a very rugged energy landscape. To overcome this limitation, a new strategy has been implemented to determine the initial and final configurations for the nudged elastic band. Molecular statics simulations are carried out by applying a shear strain to the simulation box that contains the dislocation and the GP zone. After the static equilibrium has been achieved, Molecular dynamics simulations are carried out at constant strain and high temperature using an NVT ensemble during ns. The different structures are stored each 0.2ns and and an energy minimization process is carried out in each one under molecular statics conditions. The minimum energy configuration attained is taken as the initial step, the applied shear strain is increased and the whole procedure is repeated. In this way, metastable energy configurations can be identified in very rough energy landscapes and the initial and final configurations for the nudged elastic band can be obtained.

Using this methodology, dislocations sheared the GP zones and the activation energy was determined as a function of the applied stress and temperature. This information was used to ascertain the influence of strain rate and temperature on the critical resolved shear stress for dislocation motion in Al-Cu alloys containing GP zones.

Keywords: Atomistic simulations, atomistic/continuum scale bridging, metallic alloys

*Speaker

Experimental and numerical multiscale analyses on the constitutive behavior of bimodal alloys

Baptiste Flipon *† [1], Fabrice Barbe [1], Clément Keller [1]

[1] Groupe de physique des matériaux (GPM UMR CNRS 6634) – CNRS : UMR6634, Université de Rouen, Institut National des Sciences Appliquées [INSA] - Rouen – Normandie Univ, INSA Rouen, UNIROUEN, CNRS, GPM, 76000 Rouen, France, France

Abstract. Improvement of mechanical strength in metallic alloys, such as AISI 316L, can be achieved by grain size refinement. Ultrafine Grain (UFG) alloys present a higher yield stress and ultimate strength than their Coarse Grain (CG) counterpart. Grain size reduction also induces a decrease in material ductility [1,2] which can be detrimental regarding forming processes.
A compromise between strength and ductility can be found by using bimodal grain size distribution alloys. In the latter, two distinct grain size populations, an UFG one and a CG one contribute respectively to material mechanical strength and material ductility [3]. Beside grain sizes, CG volume fraction and their spatial distribution inside the UFG matrix (*e.g.* isolated or clustered CG) are two main factors influencing the mechanical response [4]. The study of both macroscopic and local mechanical responses aims at achieving a better understanding of plastic strain mechanisms in bimodal alloys.

Experimental elaboration, tensile tests and microstructural observations are coupled with full-field crystal plasticity simulations. Elaboration of bimodal microstructures based on powder metallurgy and spark plasma sintering enable a proper control of UFG and CG volume fractions. Tensile tests and microstructural observations are realized on the obtained bimodal alloys which present different grain size distributions. These results are used as inputs for both virtual microstructure generation and finite element computations. Polycrystalline aggregates are generated using Neper software [5] with a Laguerre-Voronoi based algorithm. Full field crystal plasticity enables to investigate a large range of bimodal grain size distributions and to study the effects of morphological characteristics (for example CG clustering) on both macroscopic and local mechanical responses. Phenomenological [6] and physically-based [7] crystal plasticity models implemented in Z-set software [8] are used to investigate stress and strain fields. Stress concentration and strain localization are particularly analyzed. Results with strain gradient plasticity model [9] are also soon to be expected. This dialogue between experience and simulation aims at a global better understanding of mechanical response and deformation mechanisms in bimodal grain size distribution alloys.

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*Speaker
†Corresponding author: baptiste.flipon@insa-rouen.fr

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Keywords: bimodal microstructure, powder metallurgy, spark plasma sintering, crystal plasticity

Relaxation Mechanisms in a Nanocrystalline Gold Thin Film on a Compliant Substrate

Pierre Godard * [1], Renault Pierre-Olivier [2], Damien Faurie [3], Dominique Thiaudière [4]

[1] CNRS, Université de Poitiers, SP2MI (Institut P') – Université de Franche-Comté – Téléport 2, 11 bd Maire et Pierre Curie, BP 3079, 86962 Futuroscope Chasseneuil Cedex, France
[2] Institut Pprime (PPRIME) – CNRS : UPR3346, Université de Poitiers, ENSMA – France
[3] LSPM – Université Paris-Nord - Paris XIII – France
[4] Synchrotron SOLEIL (SSOLEIL) – CNRS : UMRUR1 – L'Orme des Merisiers Saint-Aubin - BP 48 91192 GIF-sur-YVETTE CEDEX, France

This presentation will focus on some of our last results obtained thanks to the unique biaxial testing machine available at the DiffAbs beamline of the synchrotron Soleil. Thin films are deposited on compliant substrates, Kapton^{TM}in our case. The elastic deformation is monitored in-situ through X-ray diffraction. Several Bragg reflections for several grain families are observed simultaneously with a two-dimensional detector. Moreover, the macroscopic strain ϵ is precisely measured thanks to an optical camera and a digital image correlation analysis. Knowing the macroscopic strain and the elastic strain allows to deduce the plastic deformation occurring in the metallic film.
We work in particular on metallic thin films deposited on compliant substrates. These composites find useful applications in flexible electronic circuits, biocaptors, artificial muscles or skin, etc.

In this talk, we will first show that the strain is completely transferred from the polymeric substrate to the metallic thin film. Then we will concentrate on relaxation experiments. A 500 nm thick nanocrystalline gold thin film was equibiaxially stretched. We applied strain jumps and let the sample relax. It is observed that after a strain jump, the macroscopic strain in the polymeric substrate-metallic thin films remains constant, whereas the elastic strain in the film decreases. That is, a part of the elastic strain is reduced through plastic events. Activation volumes are characterized thanks to the relaxation amplitude and rate. These activation volumes are interesting in that they are signatures of the plasticity mechanisms: atomic diffusion, dislocation nucleation, dislocation interactions etc. Moreover, the Bragg peak shape evolution presents complementary information. We show that the evolution of the coherent domain size is greatly dependent on the crystalline orientation: the isotropic texture component (mainly small grains at the substrate-film interface) shows a continuously increasing strain heterogeneities whereas the main texture component (columnar grains, 50 to 100 nm in diameter, with their (111) planes parallel to the specimen surface) presents a change in plasticity mechanism. The data gathered lead to the following scenario: there is a stress-assisted annealing at the very beginning of the test, then from ϵ 0.25% dislocations are continuously emitted and the density of point defects decreases, and starting from ϵ 1.1% the density of mobile dislocations decreases. To our knowledge, the evolution of the activation volumes and the change of Bragg peaks shape are correlated for the first time in nanocrystalline metals.

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Keywords: nanocrystals, gold thin films, polymeric substrate, relaxation, activation volume, synchrotron X, ray diffraction

*Speaker

Effect of pre-existing dislocations on the strength of gold at very small scales - using EBSD data to characterize local dislocation densities prior to nanoindentation

Paula Guglielmi * [1], Markus Ziehmer [1], Erica Lilleodden [1]

[1] Helmholtz Center Geesthacht (HZG) – Max-Planck-Straße 1 21502 Geesthacht, Germany

A new and non-destructive method based on Electron Backscattered Diffraction (EBSD) is proposed and used to characterize site-specific dislocation densities prior to nanoindentation. In this method, a new scalar misorientation parameter called the Characteristic Misorientation Angle (CMA) is derived from uncorrelated misorientation data obtained from site-specific areas selected on bulk gold samples with different amounts of pre-straining. We show that CMA is virtually independent of the scan step size and is more sensitive to plastic deformation than the more conventional parameters Grain Average Misorientation (GAM) and Grain Orientation Spread (GOS). A coupled effect of local plastic strain and area size is observed on the measured values of CMA, based on which values of local GND density are determined. The strength of the characterized areas is subsequently measured by spherical nanoindentation and is defined as the hardness at the first pop-in observed on the load-displacement curves. Results show that the site-specific strength of gold decreases with increasing initial dislocation density. While previous studies have suggested the same trend, the present work offers a new approach to more quantitatively correlate local dislocation densities to the onset of plasticity, without the need for destructive TEM investigations or micro-sample fabrication.

Keywords: EBSD, local dislocation densities, nanoindentation, local strength

*Speaker

Plastic deformation and surface roughening in contact shearing: A finite strain discrete dislocation study

Nilgoon Irani *† [1], Lucia Nicola [2,3]

[1] Delft University of Technology (TUD) – Netherlands
[2] University of Padua – Italy
[3] Delft University of Technology – Netherlands

During plastic deformation, metal surfaces tend to roughen and this directly influences the surface quality of manufactured parts and their tribological performance. Two-dimensional discrete dislocation plasticity (DDP) simulations of contact [1, 2] have shown severe surface roughening due to dislocations gliding out of the metal and leaving pronounced crystallographic steps on the surface. The surface roughening has a significant impact on the evolution of the traction profiles at contact, and therefore, on its shearing response. However, these simulations were performed using the small strain DDP formulation of van der Giessen and Needleman [3]. Hence, the effects of finite lattice rotations and shape changes due to slip are neglected, although both effects are expected to play an important role in roughening. To incorporate these effects, we employ the finite strain DDP formulation of Irani et al. [4] to study the shearing response of a single crystal loaded by means of a flat platen in adhesive contact with its surface.

Simulations are performed for platens of different sizes. The finite strain simulations typically show a reduced shear flow compared to the small strain simulations, especially for platens that are small enough to give a hardening response. The difference between the finite and small strain DDP predictions of shear flow is reduced when large platens or a high dislocation source density is considered as both assumptions result in sizeable dislocation nucleation. Subsequently, the impact of these results on size-dependent plasticity is highlighted. Finally, the effect of platen size, crystallographic orientation and plastic hardening slope on the resultant surface profile is studied. It is shown that the finite strain simulations typically show less distinct crystallographic steps. Besides, the level of roughening, i.e. the depth of the valley in the rear of the contact and the height of the bump in its front is highly affected by the crystallographic orientation and plastic hardening slope.

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Keywords: Contact shearing, Surface roughening, Dislocations, Finite strains, Size effects

*Speaker
†Corresponding author: n.irani@tudelft.nl

Constitutive modelling of creep in nickel-based single crystal superalloys

Aalok Kumar Jha * [1], Chandra Shekhar Upadhyay† [1]

[1] Indian Institute of Technology,Kanpur (IITK) – Indian Institute of Technology Kanpur,Kanpur -208016, India

The first stage turbine blades of aeroengines are made up of single crystal nickel based superalloys and operate at very high temperature in a hostile environment. Thermodynamic consistent and microstructure sensitive accurate modelling of creep is still a challenging and key issue for the life prediction of the blade. Initial rafting of γ'(due to misfit stress, applied load and temperature); evolution of dislocation density in two phases; hardening due to dislocation forest and cross slip; plastic and viscoplastic flow in γ channels at relatively low and high temperature respectively; the shearing of hard phase by dislocation from γ phase around 950C; dissolution and reprecipitation of γ'(fluctuation of volume fraction of γ/γ') at very high temperature (due to thermal shocks); anisotropic kinematic behaviour and morphological and microstructral evolution are modelled through introduction of internal variables by employing potentials for free energy (inelastic stored energy) and dissipation. Evolution equations of these internal variables are proposed which reflect the physical changes in material with load, temperature and time.

Keywords: Creep, Single crystal, Superalloy, Constitutive equations

*Speaker
†Corresponding author: shekhar@iitk.ac.in

Multi-scale modelling of plasticity and damage of martensite in advanced steels

Varvara Kouznetsova * [1], Francesco Maresca [2], Marc Geers [3]

[1] Eindhoven University of Technology (TU/e) – Netherlands
[2] Ecole Polytechnique Fédérale de Lausanne (EPFL) – Switzerland
[3] Department of Mechanical Engineering (TUE) – P.O box 513 5600 MB Eindhoven, Netherlands

Advanced high strength steels (AHSS) exhibit excellent combination of strength and ductility and for this reason are widely used in various industries, in particular automotive. The high strength of AHHS is, to a large extend, due to the presence of the martensite as one of the constituent phases. Nevertheless, the mechanical behaviour of the martensite has up to date not been fully understood. Martensite is often considered to be a strong, but brittle phase. In the last several decades, however, multiple evidences have been presented in the literature demonstrating the deformation of martensite to large strains and traces of ductile fracture. At the same time, the development and significant improvement of high resolution electron microscopy techniques allowed to reveal and identify the fine scale hierarchical structure of the martensite. The relation between the two experimental observations has however not been established in the literature.
In his contribution, a possible relation between the ductile mechanical behaviour of the martensite and its substructure is investigated through a systematic multi-scale modelling approach. To this end, thin layers (tens to hundred nanometers thickness) of austenite phase, retained between the laths of the martensite phase, have been hypothesized to be responsible for the apparently ductile behaviour of the martensite.

The hypothesis on the role of the thin films of austenite is first investigated by modelling the martensite aggregate as a bicrystal by means of crystal plasticity. Results reveal that the austenite acts like a "greasy" plane on which the stiffer martensite laths can slide. The shearing mechanism is intrinsically related to the orientation relationship, which ensures that slip planes of the austenite are approximately parallel to the lath habit planes. It is demonstrated that that this "greasy" mechanism can indeed explain the experimentally observed deformation behaviour of martensite crystals from the literature; it is shown that if the presence of interlath austenite is neglected, the observed experimental flow curves cannot be captured. Next, to enable the simulations at the scale of multi-phase microstructures, this fine scale "greasy" mechanism has been incorporated in a computationally efficient two-scale framework, through the development of a reduced crystal plasticity model for materials with constrained slip activity. Using this model, the effect of the "greasy" plane mechanism on the behaviour of multi-phase AHSS has been investigated. It has been shown that even negligible volume fraction of the interlath retained austenite can have a huge impact on both the local as well as global response of these materials. Finally, a model for damage and fracture of martensite related to the "greasy" plane mechanism has been proposed. The model is validated on experimental results from the literature, and it can in the future be applied to the microstructural design of AHSS, containing martensite phase as well as other laminated microstructures.

Keywords: advanced steels, lath martensite, retained austenite, crystal plasticity

*Speaker

Modelling of Fatigue Crack Initiation in Metals under Hydrogen Environment using Coupled Framework of Hydrogen Transport Model and Non-Local Crystal Plasticity Model

Rakesh Kumar [1], Dhiraj K. Mahajan *† [1]

[1] IIT Ropar (IITRPR) – Ropar Mechanics of Materials Laboratory, Department of Mechanical Engineering, Indian Institute of Technology Ropar, Rupnagar-140001, Punjab, India

To meet the essential C02 emission targets by exploiting ultra-high strength steels for the automotive industry and for high-pressure hydrogen gas transportation under hydrogen-based economy, a thorough understanding of hydrogen-metal interaction that can lead to hydrogen embrittlement is required. Extensive studies on hydrogen embrittlement of metals, under monotonic loading, have revealed a multitude of material specific mechanisms (HELP, HEDE etc.) correlating hydrogen concentration to the degradation of local fracture/mechanical properties. However, in case of fatigue failure of metals under hydrogen environment, in addition to the above mechanisms, microstructural features such as grain size, type of grain boundary (special/random; low angle/high angle), the fraction of special grain boundaries and their network can play a significant role. In this regard, a coupled framework of non-local crystal plasticity model and hydrogen transport model is developed to model the fatigue crack initiation in polycrystalline metals under hydrogen environment. This framework considers dislocations as primary trapping sites for hydrogen. Representative volume elements (RVE) with controlled grain size/orientation are used to analyse the fatigue crack initiation behaviour in hydrogen charged polycrystalline nickel specimens. Within the polycrystalline modelling domain of nickel, non-local crystal plasticity model leads to segregation of total dislocation density into statistically stored dislocations (SSDs) and geometric necessary dislocations (GNDs) based on the microstructural features such as the type of grain boundaries, grain size/orientation and triple junction. Hydrogen transport model simultaneously performs the non-steady state diffusion in such polycrystalline samples while taking care of the pressure gradient jumps at the grain boundaries and equilibrium between lattice and trapped hydrogen concentration. For hydrogen charged specimens, competing mechanisms of critical accumulated plastic strain and critical hydrogen concentration then provide the potential sites for fatigue crack initiation. Such a simulation framework can give greater insight into the role of microstructure, cyclic frequency, stress-ratio and other experimental parameters on fatigue crack initiation and propagation behaviour of hydrogen charged metal specimens while comparing well with the experiments [1].

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Keywords: Nonlocal crystal plasticity, hydrogen transport model, fatigue crack initiation, critical accumulated plastic strain, critical hydrogen concentration

*Speaker

†Corresponding author: dhiraj.mahajan@iitrpr.ac.in

Investigation of the composite screw dislocation source activation in α-iron with irradiation defects dispersion by dislocation dynamics

Yang Li *† [1], Christian Robertson [1], Laurent Dupuy [1]

[1] CEA, DEN, SRMA – CEA – Gif-sur-Yvette 91191, France

α-iron steels are widely used as structural nuclear materials, thereby subjected to radiation-induced ageing mechanisms including hardening and embrittlement [1-2]. These evolutions are usually ascribed to the formation of dispersed defect cluster populations, in the form of sessile dislocation loops [3]. Beyond a critical dose, plastic straining becomes heterogeneous and can give rise to defect-depleted channels, where the defect-loops are progressively removed by interaction with the mobile dislocations [4]. It is thought that channel-induced deformation can facilitate brittle fracture initiation, and is therefore regarded as a crucial damaging mechanism. In defect-depleted shear bands indeed, mobile dislocations emitted from random sources eventually intersect a defect cluster, arresting the incoming dislocation line [5]. In this case, relatively long dislocation arms are present on both sides of the interacting defect. A screw-type arm can then change its glide plane through thermally activated cross-slip mechanism and resume gliding in its new crystallographic plane [6]. This most typical and poorly understood configuration is here called a "composite" dislocation source, which will be examined by using DD simulations (Numodis).

We investigate the movement of dislocations gliding in the presence of [1-11] and [111] sessile loops, with a view to predict interaction mechanisms and strengths representative of post-irradiation plastic straining conditions. It is found that realistic finite length sources bear significant differences with respect to the more usual, periodic boundary condition case study [7-8] (e.g. infinitely long dislocations, without pinning points). Namely, interaction with a [1-11] loop gives rise to the formation of a strong junction which is then by-passed by an Orowan-like mechanism. The corresponding interaction strength is then relatively high, with respect to periodic boundary conditions [8]. Interaction with a [111] loop gives rise to a helical jog that closes itself and yields the same interaction strength expression if subtracting the activation stress, with respect to periodic boundary conditions.

The case of composite screw dislocation source is investigated next. The sources include two distinct (Lcs , Lp) long segments, gliding in the primary and cross-slip systems, respectively. The effect of various loading conditions (τcs , τp) on the composite source is examined in terms of interaction mechanisms and plastic strain evolutions with time. It is observed that the dislocation arm gliding in the primary slip plane, if initially blocked by the defect, can later be liberated by the cross-slipped segment. The effective obstacle strength associated with this mechanism is in any case significantly lower than the interaction strength associated with the coplanar dislocation sources. Cross-slip mechanism can then greatly facilitate dislocation source activation in post-irradiated materials, depending on the local configuration and loading conditions.

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*Speaker

†Corresponding author: yang.li@cea.fr

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Keywords: composite screw dislocation source, cross slip segment, dislocation dynamics simulation

Derivation of microstructure dependent flow curves of two steel gears suitable for cutting simulations

Gottfried Laschet * [1], Mustapha Abouridouane [2], Viktor Kripak [3], Jens Dierdorf [4]

[1] ACCESS e.V. – Intzestraße 5, D-52072 Aachen, Germany
[2] Lab. of Machine Tools and Production Engineering (WZL) – Steinbachstrasse 19, D-52074 Aachen, Germany
[3] Department of Ferrous Metallurgy (IEHK) – Intzerstrasse 1, D-52072 Aachen, Germany
[4] Institute of Metal Forming (ibf) – Intzestrasse 10, D-52072 Aachen, Germany

Within this work, a multiscale approach is presented investigating the effect of the ferrite-pearlite microstructure after annealing on the subsequent machining process of a steel gear. The case-hardening steel 18CrNiMo7-6 and a cost efficient alternative, where Ni is substituted by Mn and Mo and Nb is added to carburise at higher temperatures, are retained in this study. In order to analyse the influence of their ferrite/pearlite microstructure on the cutting process, a multi-scale approach is presented here. Based on an advanced microstructure characterisation, three different scales are introduced: the nano-scale with the pearlite, built of ferrite-cementite bi-lamellas, the micro-scale, which corresponds to a RVE of the ferrite/pearlite microstructure and the macro-scale. In order to derive the effective flow behaviour of pearlite, uniaxial tensile and shear tests of the bi-lamella of ferrite and cementite are performed at the nanoscale. The flow behaviour of the ferrite phase is described there by the Gutierrez law [1]. As some model parameters like the initial dislocation density are delicate to measure, a sensitivity analysis of their impact on the effective pearlite properties is performed. The ferrite matrix containing either small soft MnS (18CrNiMo7-6) or hard NbC (substitute) inclusions is homogenised also at the nanoscale [2]. At the microscale, 3D RVE's of both steel microstructures are generated containing ferrite as matrix, pearlite and few large CeS inclusions. Effective flow curves for both steel grades are determined at room temperature. These curves are used to derive microstructure dependent strain hardening parameters of Johnson-Cook model variants. Modified hardening descriptions of Ludwik or Voce type have been introduced to set the initial yield stress to the ferrite matrix one, to describe the strong hardening increase at small strains and to describe accurately the alloy hardening at very large strains (up to 500%), crucial for cutting simulations. To evaluate and compare the machinability of both alloys, orthogonal cutting simulations with the different Johnson-Cook model variants were performed in a coupled Eulerian-Lagrangian framework. Machinability predictions are validated by comparing with cutting experiments proving thus the adopted multiscale approach. Moreover, they show that the variant combining a Voce saturation term with a linear hardening term outperforms the other modified Johnson-Cook model variants.

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Keywords: Multiscale modeling, Johnson, Cook material law, orthogonal cutting, microstructure characterization

*Speaker

Observation of deforming polycrystalline microstructures using a combination of 3D X-ray diffraction and imaging techniques

Wolfgang Ludwig * [1,2], Nicola Vigano [3], Henry Proudhon [4], Nicolas Gueninchault [5], Yoann Guilhem [6]

[1] Matériaux, ingénierie et sciences (MATEIS) – CNRS : UMR5510, Institut National des Sciences Appliquées (INSA) - Lyon, Institut National des Sciences Appliquées [INSA] - Lyon – Bâtiment Blaise Pascal 7, avenue Jean Capelle 69621 VILLEURBANNE CEDEX, France
[2] European Synchrotron Radiation Facility (ESRF) – ESRF – 6 rue Jules Horowitz BP220 38043 GRENOBLE CEDEX, France
[3] Centrum voor Wiskunde en Informatica (CWI) – Kruislaan 413 P.O. Box 94079 1090 GB Amsterdam, Netherlands
[4] Centre des Matériaux (MAT) – MINES ParisTech - École nationale supérieure des mines de Paris, PSL Research University, Centre National de la Recherche Scientifique : UMR7633 – Centre des matériaux P. M. Fourt RN 447 - BP 87 91003 EVRY CEDEX, France
[5] Centre des Matériaux (MAT) – CNRS : UMR7633, MINES ParisTech - École nationale supérieure des mines de Paris – Centre des matériaux P. M. Fourt RN 447 - BP 87 91003 EVRY CEDEX, France
[6] Laboratoire de Mécanique et Technologie (LMT) – École normale supérieure (ENS) - Cachan, CNRS : UMR8535 – Bât. Léonard de Vinci 61 Av du président Wilson 94235 CACHAN CEDEX, France

State of the art near-field X-ray diffraction imaging techniques can map the 3D orientation field in polycrystalline sample volumes at micrometer spatial resolution and with a repetition rate of order of one hour. Far-field measurements yield grain resolved elastic strain tensors from the same sample volume. X-ray phase contrast tomography, carried out on the same instrument enables tracking of microstructural detail like secondary phases, inclusions, porosities and cracks. Repeated observation of deforming microstructures using a combination of these imaging modalities yield rich datasets which can serve as input for image based modeling efforts. In this talk we will review the current possibilities and limitations of the combined 3D grain mapping and imaging capabilities available at the materials science beamline ID11 at ESRF. Application examples include the observation of fatigue damage in a duplex steel, the sequential activation of slip systems during incipient plasticity in Al-Li alloy and the activation of mechanical twins in pure Ti and Mg alloys.

Keywords: synchrotron, X, ray, diffraction, phase contrast, mechanical twins, orientation microscopy

*Speaker

Thermodynamically-consistent chemo-mechanical phase-field simulation of Widmanst´atten ferrite.

Kubendran Amos Prince Gideon * [1], Ephraim Schoof [2], Schneider Daniel [1], Nestler Britta [1]

[1] Institute of Applied Materials - Computational Materials Science (IAM-CMS) Karlsruhe Institute of Technology – Germany

[2] Institute of Materials and Processes (IMP) Karlsruhe University of Applied Science – Germany

Despite the extensive usage and research of steels, a comprehensive understanding on the phase transformations involved during the austenite decomposition is yet to be acheived. Formation of plate-like ferrite structures, referred to as Widmanstätten ferrite, is one such transformation where contending views still prevail. Owing to the hostile influence of these Widmanstätten structure on the ductility of steels, a comprehensive understanding of this transformation is sought for from an engineering perspective. Most simulation studies while adopting the diffusive aspect of this transformation, considerably overlook the role of invariant-plane strain. Futhermore, theoretical studies that consider mechanical strains fail to comply entirely with the analytical and experimental observations, particularly in cases of low-undercooling wherein chemical-driving force is not suffiencient enough to overcome the mechanical strain.

Substantiated by the experimental observation and formation of surface relief, it is postulated that at temperatures close to Widmanstätten-start temperature (Ws), the ferrite plates grow co- operatively in a self-accommodating fashion, thereby reducing the strain energy associated with the transformation. Thermodynamically-consistent chemo-mechanical phase-field model presented in the talk, facilitates the simulation of this cooperative growth of self-accommodating plates at low-undercooling conditions. The incorporation of CALPHAD-based chem- ical driving force ensures the quantative nature of the simulations. Additionally, theoretically consistent growth of single plate at low temperatures and the corresponding distribution of concentration owing to the Gibbs-Thomson effect is captured by the present model.

Keywords: widmanst´atten ferrite, chemo, mechanical simulation, CALPHAD, phase, field modelling

*Speaker

Coupling experiments and simulation to understand local deformation mechanism in Ni micro-wire

Ravi Raj Purohit Purushottam Raj Purohit * [1], Céline Gerard [1], Loic Signor [1], Abhinav Arya [2], Girish Bojjawar [2], Satyam Suwas [2], Atul H. Chokshi [2], Ludovic Thilly [1]

[1] Institut Pprime (PPRIME) – CNRS : UPR3346, Université de Poitiers, ISAE-ESMA – Département de Physique et Mécanique des Matériaux, SP2MI, Téléport 2, Boulevard Marie et Pierre Curie, BP 30179, 86962 Chasseneuil-Futuroscope Cedex, France
[2] Indian Institute of Science (IISc) – Bangalore 560 012, India

Severely cold drawn Ni micro-wires exhibit significant size effects, where their tensile strength approaches the theoretical strength with a reduction of diameter from 120 μm down to 20 μm, by electropolishing [1]. Thus in-situ deformation (monotonous and cyclic tensile tests) study of Ni micro-wires under synchrotron radiation has been carried out to achieve a fundamental understanding of the observed size effect. Subsequently, finite element (FE) simulations have been performed to get a better understanding of the local deformation mechanisms.
On the experimental side, X-ray diffraction peaks are followed during deformation providing the possibility to follow the evolution of microstructure (including dislocation storage) and to detect elastic-plastic transition. The measurements were carried out on several micro-wires with diameter ranging from 100 μm down to 40 μm: a first batch of wires has been thinned down by electropolishing, while a second batch has been cold drawn. Comparison between these two series allows for discriminating the contribution of internal microstructure (texture and grain size) and external size on the observed mechanical properties.

On the modeling side, realistic 3D microstructure were generated using several large EBSD maps (characterizing grain shape and orientation distribution of the micro-wires). Texture information obtained by high-energy X-ray diffraction pole figures validates the representativeness of texture information coming from EBSD maps. Then, the obtained microstructures were used to perform crystal plasticity FE simulations within framework of small perturbations assumption.
The influence of different microstructural parameters (crystallographic and morphological texture, grain size and shape) on the mechanical properties of micro-wires will be investigated with FE simulations and the average behavior of different grain families (,) will be compared with experiments.

Keywords: crystal plasticity finite element simulation, insitu x ray diffraction, size effect, cold drawn microwire

*Speaker

A configurational approach to modeling propagating strain bands: application to the Portevin-Le Châtelier effect in aluminum alloys

Baptiste Reyne *† [1,2], Pierre-Yves Manach [3], Nicolas Moës [4]

[1] Institut de Recherche Dupuy de Lôme (IRDL - CNRS FRE 3744) – Université de Bretagne Sud, Centre National de la Recherche Scientifique : FRE3774 – Centre de Recherche Rue de Saint Maudé, 56100 Lorient, France
[2] Institut de Recherche en Génie Civil et Mécanique (GeM) – Ecole Centrale de Nantes, Centre National de la Recherche Scientifique : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[3] Institut de recherche Dupuy de Lôme (IRDL) – Université Bretagne Sud, Centre National de la Recherche Scientifique - CNRS : FRE3774 – Centre de Recherche Rue de Saint Maudé, 56100 Lorient, France
[4] Institut de Recherche en Génie Civil et Mécanique (GeM) – Ecole Centrale de Nantes, Université de Nantes, CNRS : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France

Propagating strain bands are met in a wide variety of materials such as metals [Antholovitch, 2014], soils [Olsson, 2000], snows [Barraclough, 2017] or polymers [Allison, 1967]. They are characterized by a strain localization at yield that propagates through the whole medium; this process can repeat until fracture. In aluminum alloys, they are associated with so called plastic instabilities (repetitive load drops) and characterize together the Portevin-Le Châtelier effect [Portevin, 1923].

The classical approach to their macroscopic modeling has been extensively developed for the last five decades and stands within the crystal plasticity framework. The Kubin-Estrin-McCormick model [Kubin, 1985; McCormick, 1988] simulates a serrated hardening based on microscopic considerations: an interaction between crystal dislocations and mobile solute atoms referred to as dynamic strain aging [Cottrell, 1949]. However, it leads to heavy computations and unsatisfying predictions of the bands nucleation and propagation [Mazière, 2010].

This work is based on a somewhat inverse approach: to build a constitutive model that directly governs the evolution of the interface and to superimpose it on an elastic behavior that steers the rest of the domain. To picture this, one could imagine a layer of plastic strain being spread over an elastic medium like a coat of paint is applied on a frame.
Such a model is non-classical since the location of the band's front is an immaterial interface. Following the configurational mechanics [Maugin, 2013] point of view, the bands are considered to be full blown mechanical objects: their consequence is modeled as a strain discontinuity and their velocity is chosen as a thermodynamic state variable. The conjugate quantity is derived from the second principle of thermodynamics and a constitutive model based on dislocation dynamics considerations is proposed.

Following analytical deductions from compatibility and balance laws applied to our description, experimental observations strengthen our hypotheses and clarify the dynamics of strain bands. Tensile tests are performed at various imposed velocities on small samples to increase the spatial precision and isolate the motion of single bands. Digital image correlation coupled with a high time resolution enables a measurement of in-plane kinematic fields and the accurate characterization of the bands nucleation, propagation and coalescence [Yilmaz, 2011].
We show that serrated flow is the consequence of a non-smooth front propagation; therefore only the envelope of the serrated hardening curve makes sense when we choose to see the band growth as a smooth function. This growth depends strictly on the imposed kinematics and the carried strain jump. The orientation of the interfaces

*Speaker
†Corresponding author: baptiste.reyne@ec-nantes.fr

maximizes energy dissipation and the corresponding discontinuities are oriented tangentially as a consequence of an isochoric flow.

The constitutive model relevance is then confirmed: it involves a configurational hardening linking stress to strain jump and an evolution law connecting the rates of change of the interface position and its energy conjugate. Finally, a dedicated numerical strategy is presented. Level set functions [Sethian, 1999] are used to describe the bands location and the efficiency of the formulation is evaluated on several tensile cases simulations.

Keywords: Portevin Le Châtelier effect, localization, strain bands, configurational mechanics

In-grain lattice rotation heterogeneities in deformed aluminium: synchrotron X-ray diffraction experiments and finite element simulations

Quey Romain * [1], Loïc Renversade [1]

[1] Ecole Nationale Supérieure des Mines de Saint-Etienne – Ecole Nationale Supérieure des Mines de St Etienne – France

The crystal lattice orientations and rotations of about 500 grains of an aluminium polycrystal deformed in tension were analysed using in situ synchrotron X-ray diffraction techniques and finite element simulations. Experimentally, the initial grain structure of the polycrystal was measured by diffraction contrast tomography (DCT), and the lattice rotations of the grains during deformation were followed by 3D X-ray diffraction microscopy (3DXRD), at strains of 1.0, 1.5, 2.0, 2.5 and 4.5%. First, the average grain orientations were determined from the positions of the diffraction peaks through standard indexing techniques. Second, a new method was developed to extract information on the in-grain orientation distributions from the spreading of the diffraction peaks obtained in 3DXRD. The method assumes a simplified shape of the orientation distribution and optimizes its parameters to get the best possible correspondance between the experimental diffraction patterns and the diffraction patterns simulated from the model orientation distribution using a virtual diffractometer. The polycrystal deformation was then simulated using the crystal-plasticity finite element method, taking the DCT microstructure as input. The grains were finely discretized into hundreds of elements to enable in-grain lattice rotation heterogeneities to develop. The experimental and numerical in-grain lattice rotations were then analysed based on the properties of the instantaneous orientation distributions, in terms of trends over all grains and correlation to the grain average orientations. Experimentally, it was found that the in-grain orientation distributions develop preferentially along the macroscopic tensile direction at strains lower than 2% and along a direction normal to the tensile direction at larger strains. The finite element simulation provides a good agreement on the largest-strain behaviour.

Keywords: crystal plasticity, microtexture, syncrotron, finite elements

*Speaker

Work hardening and recovery behavior of fully lamellar TiAl alloys investigated by a defect density based crystal plasticity model

Jan Eike Schnabel * [1], Swantje Bargmann [2]

[1] Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht – Germany
[2] Chair of Solid Mechanics, University of Wuppertal – Germany

Due to intense research activity, the available fully lamellar TiAl alloys outperform most competing materials in high temperature lightweight applications up to temperatures around 750∘C – 800∘C. Thus, they are increasingly used as structural materials for, e.g., turbine blades in aircraft engines.

With their increasing industrial use, investigation of the work hardening and recovery behavior of fully lamellar TiAl becomes of high practical relevance. Profound knowledge on the evolution of a material's strength with deformation and annealing is not only crucial for forming applications it also helps to assess the effectiveness of processes that specifically aim to benefit from the introduced work hardening like, e.g., shot peening.

Due to the intrinsically different lengths scales that coexist in fully lamellar microstructures, it is, however, difficult to attribute the complex hardening interactions of evolving dislocations and twins to the macroscopic materials behavior by experiments. Since the analysis of defect structures usually involves destructive methods like TEM (transmission electron microscopy), experimental investigations are naturally limited to study a specific deformation state. Thus it is challenging to reveal, e.g., transitions between predominant deformation systems as they might result from hardening interactions.

In the present contribution, the work hardening and recovery behavior in fully lamellar TiAl alloys is studied by a defect density based crystal plasticity model that was presented earlier. This model allows to study the evolution of the relative activity of deformation systems which can be attributed to their hardening interactions and is useful to explain specifics in the macroscopic stress strain response. From simulations with systematically altered microstructures, it is possible to investigate the influence of the different microstructural interfaces that coexist in fully lamellar TiAl on the plasticity on micro and macro scale. Based on the findings from static recovery experiments, the model is finally applied to analyze trends in the recovery behavior.

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Keywords: Crystal Plasticity, TiAl, Fully Lamellar Microstructure, Work Hardening, Recovery

*Speaker

Martensite Fracture in Dual Phase Steel - a computational study of the influence of grain morphology

Luv Sharma *† [1], Ron Peerlings [1], Marc Geers [1], Fady Archie [2], Pratheek Shanthraj [2], Franz Roters [2]

[1] Eindhoven University of Technology (TU/e) – Netherlands
[2] Max Planck Institute for Iron Research (MPIE) – Germany

Martensite fracture is considered as a major mode of failure in Dual Phase steels, as evidenced in recent experimental studies [$Archie2016$; $Archie2017$]. Narrow sections of the martensite islands, which typically coincide with prior austenite grain boundaries (PAGBs) are found to be preferable sites for damage initiation. Specifically, the concave regions of martensite-ferrite phase boundaries may play the role of stress concentrators, causing crack nucleation in the martensite regions. Sometimes, cracks are found to nucleate away from these phase boundaries along the PAGB. PAGBs provide a region of crystallographic mismatch, residual stresses and chemical segregation. These factor may result in driving forces for crack nucleation or degradation of intrinsic strength of these boundaries. The subsequent propagation of these cracks is influenced by the plastic activity within the martensite phase.
In this work, we try to understand these phenomena using a computational methodology. Idealised geometries for martensite islands in a ferritic matrix are considered. FFT based micromechanical simulations are performed in order to study the stress profiles along the internal boundaries within martensite. The dependence of these stress profiles on the curvature of the phase boundary is also explored. In order to separate the effects of phase contrast and crystallography, isotropic and anisotropic (crystal plasticity [$Roters2010$]) constitutive models are used. The methodology to model damage nucleation and propagation at such internal interfaces is also discussed and as an example application to a cluster of grains is shown.

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Keywords: DP Steels, Martensite, Damage, Interfaces

*Speaker
†Corresponding author: l.sharma@tue.nl

Multilevel modelling: kinematic and constitutive relations at high displacement gradients

Alexey Shveykin * [1], Peter Trusov [1]

[1] Perm National Research Polytechnic University – Russia

The formulation of geometrically nonlinear boundary value problems is required for modelling of materials thermomechanical processing, main issues in it are the description of the nonlinear kinematics and the formulation of constitutive relations. The preference should be given to the formulation of the boundary value problem in terms of current configuration using the rate form representation of the constitutive relations, because such formulation is convenient for implementation by numerical methods: it allows a step-wise computation with re-determination of the computational domain (including contact surfaces).
Crystalline metals and alloys at different scale levels always have anisotropic properties in a certain extent, in different directions properties can be differ significantly. In addition, under intense plastic deformation even initial isotropic polycrystalline materials (at the representative macrovolume level) are also becoming anisotropic due to the occurrence of texture. In frameworks of multilevel approach at the crystallites level for metals symmetry elements (planes and axes of symmetry) can be determined, and the moving coordinate system, which defines the quasi-rigid motion, will be connected with them. This idea has been proposed previously in [1], but without specifying relations for spin and with another constitutive equations. The new motion decomposition to rigid and deformation parts is proposed – multiplicative representation of deformation gradient with explicit separation of the moving coordinate system motion [2]. The mesolevel spin is connected with the crystallographic direction and the crystallographic plane. The mesolevel elastoviscoplastic constitutive relations in lattice unloaded configuration were formulated with the proposed motion decomposition [2]. The results of computations using the developed model for complex cyclic elastic loading of f.c.c. and h.c.p. crystallites indicate that the no energy dissipation and no hysteresis of stresses are met. The results of copper polycrystalline large inelastic deformations simulation using the proposed model are in a satisfactory consistence with the experimental data.

In case of small elastic deformations (this is typical for metals) the proposed constitutive relations in lattice unloaded configuration are close to the crystal plasticity constitutive relations in rate form in terms of the current configuration with correspondence corotational rate (with spin defined above), so the last can be used in simulation of technological thermomechanical processing of metals and alloys.

Proposed multilevel models contain the description of main mechanisms of inelastic deformation: intragranular dislocation sliding, grain boundary sliding, twinning, breaking and fragmentation of grains, rotation of the crystallites lattice taking into account the inconsistency of dislocation motion in the neighboring crystallites. The simulation results of plastic metal working processes are obtained with developed the software package. They include description of internal structure evolution: form, dimension and orientation of crystallographic axes of polycrystal structural units (grains, subgrains, fragments), effective macroscopic elastic and plastic properties of polycrystalline materials.

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Keywords: large inelastic deformations, corotational derivatives, multilevel models

An advanced numerical framework for the comparison of synchrotron X-ray diffraction experiments and numerical simulations - application to grain-scale stresses in an elastically-deformed NiTi shape memory alloy

Aurelien Villani *† [1], Ludek Heller‡ [2], Petr Sittner [2], Pejman Shayanfard [2], Romain Quey [1]

[1] École des Mines de Saint-Étienne – Institut Mines-Télécom [Paris] – 158, Cours Fauriel - 42023 Saint Étienne cedex 2, France

[2] Institute of Physics of the Czech Academy of Sciences – Na Slovance 2, 182 21 Prague, CZECH REPUBLIC, Czech Republic

In the past 15 years, synchrotron X-ray diffraction methods have been developed to probe the deformation behaviour of individual grains of polycrystalline aggregates subjected to in situ loading. These methods provide unprecedented insight into the mechanics of polycrystals, and the results can be compared to full-field numerical simulations of the polycrystal deformation. If successful, such a comparison would both validate the model and offer access to additional information, as some properties which are no accessible experimentally may be well available in the simulation.
Among existing X-ray diffraction methods, 3DXRD is dedicated to the measurement of grain-averaged values: the lattice orientation, elastic strain (and stress), position and volume. Although valuable, the information remains incomplete as the intra-grain stress variations or details on the grain morphology are not available, which may be problematic for several reasons. First, stress "hot spots" may locally exceed the grain-averaged values. In the context of shape memory alloys, stress hot spots trigger transformation deformation processes accompanied with irreversible deformation processes that lead eventually to fatigue damage under cyclic loading. Second, even if the experimental grain centers and volumes can be used to instantiate a polycrystal model, this model can only be partially representative of the real microstructure.

In this work, we provide a complete methodology for the comparison between 3DXRD experiments and full-field numerical simulations. The principle is to optimize the polycrystal's properties to improve the agreement between the experimental and numerical results. This approach has been previously used, to a certain extent, to study inter- and intra-granular stresses arising from a simple tensile loading of a NiTi wire [1]. Note that the present study is focused on the grain-scale stress state in the elastic regime, prior to any stress-induced martensitic transformation. The optimized microstructure will finally be used to analyze grain-scale stresses during stress-induced martensitic transformation in NiTi wires. From a methodology point of view, the present work includes several novelties. First, the polycrystal is represented as a Laguerre tessellation whose seed attributes are varied during optimization about their nominal values, which accounts for the experimental data being both partial and subjected to uncertainties [2]. Second, an FFT-based algorithm is used to simulate the polycrystal deformation, by solving the Lippmann-Schwinger equation based on strain or polarization [3]. Such an algorithm is adapted to the current problem for two reasons. On the one hand, we take advantage of a fast iterative solver

*Speaker
†Corresponding author: aurelien.villani@emse.fr
‡Corresponding author: heller@fzu.cz

to set, at each optimization step, the initial strain field as the final one of the previous iteration (for which slightly different polycrystal properties were used), which is a key point to make the process computationally-tractable. On the second hand, as the FFT simulation is based on a regular grid of voxels, local polycrystal morphology modifications can be simply and rapidly handled by grain voxel reassignment. Finally, we define an appropriate objective function for the comparison between the experimental and numerical grain-averaged stresses.

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Keywords: FFT, X, ray diffraction, stresses, numerical optimization, full, field simulations

An atomistic description of dislocation mobility in the pure-glide regime

Jonas Verschueren * [1], Benat Gurrutxaga-Lerma [2], Daniel Balint [3], Adrian Sutton [4], Daniele Dini [3]

[1] Department of Materials, Imperial College London – United Kingdom
[2] University of Cambridge – United Kingdom
[3] Department of Mechanical Engineering, Imperial College London – United Kingdom
[4] Department of Physics [Imperial College London] – Department of Physics, South Kensington Campus, Imperial College London, SW7 2AZ London UK, United Kingdom

Our understanding of dislocation mobility - quantifying the relationship between the force on a dislocation and its resulting velocity - is largely based on experiment. However, the validity of mobility laws extracted from this work breaks down for fast travelling dislocations moving with speeds comparable to the speed of sound in the medium. Debate on the topic of dislocation mobility in the pure glide regime has been ongoing for over half a century. At the heart of the discussion lies the problem that in this regime, the usual approximations by which elasticity theory is linearised are violated and the quasi-static approximation no longer holds.

In the last 20 years, large-scale non-equilibrium molecular dynamics simulations have been used to produce qualitative mobility laws for fast travelling dislocations. Despite the breadth of physical phenomena that are captured in these simulations, they have failed to provide the community with a general understanding of dislocation mobility in this regime. We will show how lattice-dynamics models of uniformly moving dislocations may provide an accurate description of the dislocation - phonon interactions in metals. These interactions are widely believed to play a crucial part in physical descriptions of dislocation mobility. Quantitative comparisons between the lattice dynamics model and equivalent molecular dynamics simulations will be made. Furthermore, the effect of the dislocation core width on its mobility will be presented. Finally, the consequences of these results for a more general theory on dislocation mobility in the pure glide regime will be discussed.

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Keywords: dislocation mobility, pure, glide, dislocation, phonon interaction, lattice dynamics

*Speaker

Modelling of severe plastic deformation of polycrystals taking into account grain structure and its evolution

Pavel Volegov *† [1], Michael Telkanov [1], Vladimir Ozernykh [1]

[1] Perm National Research Polytechnic University (PNRPU) – 29 Komsomolsky prospekt, Perm, Perm krai, Russia, 614990, Russia

Changes in the physical and mechanical properties of the specimen during severe plastic deformation is a consequence of a substantial restructuring of the micro- and mesostructure of the material, mainly due to a significant evolution of the dislocation (defective) material structure. Describing such processes is impossible if not studying and establishing mathematical models that explicitly take into account the physical root causes of the microstructure evolution under large deformations. The foregoing explains the considerable attention in crystal plasticity, which is paid to the modification of hardening laws, submodels of lattice rotations and damage accumulation.
We used the two-level modified model of inelastic deformation of polycrystalline materials with introducing intermediate quasi-scale level (grain) – the aggregates of slightly misoriented fragments separated by low-angle boundaries to describe the grain fragmentation and splitting processes. In this case, a separate fragment with a homogeneous crystal lattice orientation becomes the low-scale element. The model associated with the incompatibility of plastic shears is used to describe the rotations. This model has clear physical causes of lattice rotations of structural elements, and it can also be applied to any subset of connected elements. Some numerical experiments of modeling the initial stage of fragmentation is carried out; the estimation of energy associated with rotations is given. As a result of the study it can be concluded that the consideration of the rotational hardening effect on the texture will ensure a more accurate description of metals properties after their treatment.

The research also deals with the so-called intergranular damage accumulation mechanism, which is characterized by the formation and development of defects near grain boundaries. It is shown that the appearance of the grain boundary dislocation's internal stress field can lead to the locking of slip system in the direction "to the boundary," which in turn leads to the formation of clusters of dislocations near the boundary. Under certain conditions, confluence of the cluster head dislocations and formation of a microcrack can occur. We proposed a method for taking into account internal stresses using back-stresses in the dislocation shear rate along slip systems. The critical values of effective stresses, which can lead to the appearance of microcracks near the boundary, are calculated, evolutional equations for the density of such defects are obtained. In addition, the average grain size and grain size distribution is explicitly taken into account; it has been found that a material with a finer grain has increased strength characteristics, but is more prone to microcracks near grain boundaries or phases.

It is shown that the material damage (as a measure of the density of microdamages) in the process of inelastic deformation can both increase and decrease. In the course of the work it was found that blocking the slip system in some cases leads to the activation of new, so-called secondary slip systems, as a result dislocations "bypass" the barrier formed on the slip system, due to which the material damage is reduced.
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*Speaker
†Corresponding author: crocinc@mail.ru

Keywords: crystal plasticity, mathematical model, severe plastic deformation, grain boundary, hardening, damage accumulation

Constitutive modeling and numerical simulation of impacts during Surface Mechanical Attrition Treatment of TWIP/TRIP steels

Zhenglin Chen * [1], Zhidan Sun [1], Benoît Panicaud† [1]

[1] Université de Champagne, CNRS, Institut Charles Delaunay (ICD) /LASMIS – Université de Technologie de Troyes – 12 rue Marie Curie, 10004 Troyes, France

Surface Mechanical Attrition Treatment (SMAT) is a mechanical surface treatment process that generates higher level of compressive residual stress coupled with stronger plastic deformation in the near surface region of structures than conventional shot peening. SMAT is based on multidirectional mechanical impacts between balls and the surface of material. The particularity of this technique lies in the fact that it can transform the top surface layer of material from coarse grains to nano-sized grains due to severe plastic slips. A good understanding of deformation mechanisms of material during SMAT, including grain refinement, is important in terms of material processing optimization. In this work, a dislocation density-based model including the kinetics of twinning and martensitic transformation is developed to study the strain hardening behavior of twining induced plasticity (TWIP) and transformation induced plasticity (TRIP) steels, in which mechanical twining and martensitic transformation play significant roles during plastic deformation of these materials. The material parameters for the constitutive model are obtained by an inverse analysis from the volume fraction evolution of twinning and martensitic transformation as well as the stress-strain curve. Based on the proposed model, the mean free path, the volume fractions, the dislocation density are calculated to analyze the effect of mechanical twining and martensitic transformation on the mechanical behavior of TWIP/TRIP steels. Comparison between modeling results and experimental data shows that the proposed model can well predict the macroscopic behavior and the volume fraction of twinning and martensitic transformation, which demonstrates that the material parameters obtained can accurately describe the properties of the material. Afterwards, the model is implemented in a subroutine of Abaqus Explicit for the 3D simulation of a single shot impact to investigate the impact process of material during SMAT, in which twinning and martensitic transformation can occur in addition to plastic slips. The simulation results show that the volume fraction of twinning and martensitic transformation, the dislocation density in both austenitic and martensitic phases and the compressive residual stress in the near surface region are determined by ball diameter, ball velocity, incident impact angle, etc. during SMAT due to the occurrence of twinning and martensitic transformation in TWIP/TRIP steels.

Keywords: SMAT, Dislocation density based model, Twinning, Martensitic transformation, Finite element method

*Speaker
†Corresponding author: benoit.panicaud@utt.fr

Prediction of Scatter in Fatigue Life Using a Microstructure Sensitive Local Energy Method

Duncan Maclachlan * [1], Fionn Dunne [2]

[1] Rolls-Royce plc – Moor Lane ML-80, Derby, PO Box 31, DE24 8BJ, United Kingdom
[2] Imperial College London – Chair in Micromechanics, Faculty of Eng. Dept. of Materials, London SW7 2AZ, United Kingdom

In the aerospace industry very strict rules are put on the declaration of safe cyclic lives (numbers of flights) for critical engine components. Typical examples of these are rotating compressor and turbine discs and fan blades, the failure of which would severely compromise aircraft safety. Due to the demanding operating conditions of these components, there is frequently very little margin on life remaining after safety factors are accounted for. As such it is very important to determine the maximum safe life a component can withstand. Safe life declaration is performed primarily by read-across from mechanical testing of specimen, sub-element or full-scale component rig testing. There are two significant problems using a life declaration strategy based on mechanical testing. The first of these is the complexity and cost, of accurately representing real engine operating conditions in a test environment. The combination of load regimes, in particular those such as non-proportional loading and thermo-mechanical fatigue, make fully representative testing very difficult. The second obstacle is the ever present scatter and distribution in fatigue life which demands a number of identical tests be performed such that the variation can be quantified and a maximum safe life calculated. The challenges in using mechanical testing to calculate safe lives of critical components operating in complex load regimes are described.
Presented with these challenges, and with the objective of supporting mechanical test by (a). simulating behaviour under complex loading, and (b). calculating scatter based on representative microstructure, it is important to develop models of the mechanisms of fatigue crack initiation. A crystal plasticity model has been developed which accurately calculates creep and plasticity under a wide range of validated operating conditions, including primary, secondary and tertiary creep, stress relaxation and monotonic as well as cyclic plasticity. The crystal plasticity model is used in conjunction with a local stored energy parameter [1,2] that has been shown to predict both the location and number of cycles to crack nucleation under controlled testing conditions. The local energy parameter identifies local areas or 'hotspots' in a microstructure that, due to adverse combinations of stress state and interactions with neighbouring grains, causes large localised cyclic plastic deformation. By simulating many different microstructures we can determine the frequency and severity of these hotspots and calculate the expected distribution or scatter in fatigue life. In this work the combination of a crystal plasticity model and local plastic energy parameter, [1,2] are developed further and validated against a wide range of fatigue data for RR1000, a powder Ni based superalloy used for the highest temperature rotating discs, and RS5, a coarse grain cast Ni alloy used for static structural components. In particular the range of data available for these alloys allows validation of the ability of the stored energy criterion to predict scatter in fatigue life.

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*Speaker

Keywords: crystal plasticity, fatigue, creep, scatter

In-situ TEM Study of Migration of Interfaces between Austenite and Ferrite in a Duplex Stainless Steel

Frédéric Mompiou * [1], Juan Du [2], Wenzheng Zhang [2]

[1] Centre d'élaboration de matériaux et d'études structurales (CEMES) – CNRS : UPR8011 – 29 Rue Jeanne Marvig - BP 4347 31055 TOULOUSE CEDEX 4, France
[2] Key Laboratory of Advanced Materials (MOE), School of Materials Science and Engineering, Tsinghua University – Beijing, 100084, P R China, China

Fcc/bcc phase transformation is common in many technically important alloys, such as steels and copper alloys. Extensive experimental investigations have been made and various geometry models have been proposed for understanding the crystallographic morphology of transformation products. However, the existing geometry models mainly deal with the morphology of transformed precipitates. It remains unclear how the morphology develops during a phase transformation, and especially what is the role of dislocations in strain accommodation processes. An in-depth understanding of anisotropic nature of interface migration is essential for correct interpretation of the morphology evolution of precipitates.
In the present work, a commercial duplex stainless steel with the composition of Fe-24.9wt.%Cr-7.0wt.%Ni-3.1wt.%Mo was used to study migration of the interfaces between austenite and ferrite. In situ experiments were carried out by using transmission electron microscope (TEM) equipped with a heating holder. The phase transformation from ferrite to austenite occurs either by migration of existing interfaces or by nucleation and growth of fresh austenite. The new austenite precipitates all exhibit a lath morphology with long axis almost lying parallel to the TEM foil. The interface migration process can be described by two modes, normal motion and ledge motion.

The emission of dislocations from the tip of a newly transformed austenite lath, with a near Pitsch orientation relationship with the ferrite matrix, was observed at 760∘C. The dynamics of dislocation loops with [111]b/2 Burgers vector were carefully analyzed. An estimation of stress concentration at the tip was made using dislocations as stress probes.
These real-time observations verify directly for the first time that dislocation activity assists the growth of austenite precipitates, and provide quantitative data for revealing the stress field generated by interface migration.

Keywords: in, situ TEM, phase transformation, duplex steel, dislocation nucleation

*Speaker

S4: Mechanics of ceramics - Experiments and models

Models for ceramic powder forming

Davide Bigoni * [1]

[1] University of Trento (UniTN) – Via Mesiano 77 38123 Trento, Italy

Elastoplastic models are presented to describe the forming of ceramic powders [1]. The models are developed on the basis of micromechanical considerations [2]. The calibration of the constitutive models with experiments on cold powder compaction is presented together with a description of the principal problems connected to the computer implementation of the models. The final validation of the modelling is developed through comparisons with "ad-hoc" experiments, showing a good agreement. Experiments have been performerd through the development of a tomographic reconstruction techniques for density analysis of green bodies [3].

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Keywords: Constitutive modelling, ceramics, elastoplasticity

*Speaker

Finding representative material parameters for complex constitutive models used in ceramic powder compaction

Vladimir Buljak * [1], Shwetank Pandey [1], Severine Romero [2], Achraf Kallel [2]

[1] University of Belgrade, Faculty of mechanical engineering – Serbia
[2] Vesuvius - Material modeling anc characterization – Belgium

Refractory materials are commonly produced through a two-step process: mechanical compaction of ceramic powder as a first phase, followed by sintering at high temperature, to produce final product. Such production path usually introduces a density gradient, which is strongly affecting local shrinking during the sintering phase. It is therefore essential to produce reliable numerical models of the compaction process to provide support to the production, better optimization of part's and tools' geometry, and ultimately reduce defects in final products. One of the most challenging tasks within numerical modeling of powder compaction phase is constitutive description of the material involved within the process. To this purpose frequently phenomenological constitutive models, like those used in soil mechanics are employed. While attempting to capture most of the physics involved, these models are usually governed by fairly large number of parameters. Such circumstance makes the calibration process rather demanding, as some of the parameters require high pressure experiments. Within the usual praxis, quantification of diverse parameters is performed through various destructive tests, performed on a green body (a solid body resulting from a compaction test), with tendency to directly relate experimentally measured quantities to the parameter of interest. This procedure however, has limited applicability for the present case, since some of the parameters have vague physical interpretation, or are difficult to measure. As an alternative and potentially advantageous strategy for this calibration, a procedure centered on inverse analysis methodology can be used. The inverse analysis sinergically combines experiments with numerical simulations and mathematical programming apt for the minimization of suitable discrepancy function, which quantifies the difference between measured and computed experimental quantities. While offering important benefits of performing material mechanical characterization on the basis of data collected only from the compaction test, the selection of experimental quantities becomes crucial as it may lead to the ill-posed inverse problem. Proper selection of experiments can be made on the basis of sensitivity analysis performed to ascertain reasonable sensitivity of measurable quantities to the sought parameters. Within this communication, some innovative methodological procedures based on inverse analysis methodology will be presented regarding the problem of calibration of constitutive models used for powder compaction. A reference will be made to the modified Drucker-Prager CAP model with field dependence, introduced to incorporate elasto-plastic coupling, and two types of hardening. Presented results will evidence the importance of designing an experimental protocol when calibrating complex constitutive models governed by an elevated number of parameters. Such systematic approach leads to the identification of material representative parameters instead of particular solutions fitting only single experiment.

Keywords: Powder compaction, constitutive models, calibration, inverse analysis

*Speaker

Damage in silica glass due to laser shock : Experiments and simulations

Corentin Dereure * [1], Jean-Pierre Guin [1], Ibrahim Guven [2], Didier Loison [1], Jean-Christophe Sangleboeuf [1], Laurent Berthe [3], Benjamin Jodar [1], Emilien Lescoute [4], Mariette Nivard [1], Hervé Orain [1]

[1] Institut de Physique de Rennes (IPR) – Universite de Rennes 1, Centre National de la Recherche Scientifique : UMR6251 – Bâtiment 11A , B, C, E – 10B263 av. Général Leclerc35042 Rennes cedex FRANCE, France
[2] Virginia Commonwealth University (VCU) – 907 Floyd Ave, Richmond, VA 23284a, USA, United States
[3] Procedes et Ingenierie en Mécanique et Matériaux [Paris] (PIMM) – Arts et Métiers ParisTech, Conservatoire National des Arts et Métiers (CNAM), CNRS : UMR8006, Conservatoire National des Arts et Métiers [CNAM] – 151 boulevard de l'hôpital, 75013 Paris, France
[4] DAM Ile-de-France (CEA-DIF) – CEA – France

Silica (SiO2) is one of the most common materials on earth. It is usually encountered in one of its many crystalline forms, but a vitreous form can be obtained by rapid quenching of the molten material. The glass hence obtained is used in many aspects of the everyday life, but is also the main material for some highly critical structures such as space shuttle windows and solar panels. Silica glass has been extensively studied under quasi-static loading conditions, which is distinctly different than those of laser shock involving both high pressures and strain rates. Fracture initiation and propagation under laser shock is the main focus of the current study.
The shock loading condition was generated by a high intensity laser[1]. Recovered samples were observed and their damage was quantified by different techniques (optical, X-Ray tomography). They ranged from no damage at all to a completely damaged sample on both front and rear faces. Micro-CT showed that the most damaged samples also have several types of internal failure.

Peridynamic simulations [2] were used to first study how well it qualitatively compare to experimentation and to obtain more insight on the damage initiation and propagation in silica samples. This method is a non-local formulation that uses integrals instead of tensors, thus removing the singularities caused by geometric discontinuities. The system is discretised into material points, each one interacting with those in its vicinity through bonds. A damage parameter may be defined by the accumulation of broken bonds on a material point. It ranges from 0 (undamaged material point) to unity (completely separated from the rest of the domain), thus allowing for a quantification of the damage in the structure.

The laser-shock experiments were simulated by using a peridynamic grid matching the size of the shocked silica samples. The loading conditions were determined by one-dimensional laser-matter simulations using the ESTHER code (developed by the CEA). They were applied to material points on the front face of the mesh corresponding to the experimental laser irradiated zone. Two specific cases were considered : High Flux (HF) and Low Flux (LF). These cases represent clear differences in both loading conditions and the observed failure modes. In the current study the HF case was used to refine the peridynamic material parameters allowing for a satisfactory description of the experimentally observed damage on both the front and rear faces. This setup was then used in LF case and damage predictions were compared to those of the recovered sample to test the accuracy of the method.

Although the comparison between experimental measurements and peridynamic predictions is encouraging, considering the lack of current data on such studies, results are also discussed in terms of qualitative or quantitative

*Speaker

matching in order to set the limitations of the numerical approach [3].

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Keywords: Silica glass, laser shock, peridynamic, damage, fracture

Increase of fracture energy by microstructure design of refractory materials. Investigations by coupling wedge splitting tests with adapted DIC technique.

Marc Huger *† [1], Imad Khlifi [1], Octavian Pop [2], Pascal Doumalin [3], Jean-Christophe Dupre [3]

[1] Institut de Recherche sur les Céramiques (IRCER) – Centre National de la Recherche Scientifique : UMR7315 – Centre Européen de la Céramique, 12 Rue Atlantis, 87068 LIMOGES CEDEX, France
[2] Laboratoire de Génie Civil, Diagnostic et Durabilité (GC2D) – Université de Limoges : EA3178 – Centre Universitaire de Génie CivilBoulevard Jacques Derche, 19300 Egletons, France
[3] Institut Pprime (PPRIME) – Centre National de la Recherche Scientifique : UPR3346 – Institut P? Recherche et Ingénierie en Matériaux, Mécanique et EnergétiqueSP2MI Téléport 2Boulevard Pierre et Marie CurieBP 3017986962 FUTUROSCOPE CEDEX, France

In steelmaking, glassmaking or cement making industries, the ability to sustain severe thermal shocks is of prime importance in order to increase the lifetime of refractory linings and to avoid their premature failure. For such purpose, the choice of materials to be used in these linings should be well done by end users and the design of their microstructure should be well optimised by refractory producers. Refractory materials usually exhibit a heterogeneous microstructure consisting in coarse aggregates surrounded by fine grains that form an aggregate/matrix composite. This heterogeneous microstructure often leads to a complex mechanical behaviour during loading that could be optimised by a suitable choice of aggregates, especially in term of thermal expansion mismatch with the matrix. In fact, the tailored network of microcracks which can result from this thermal expansion mismatch after the sintering process, could be advantageously used to improve the thermal shock resistance of materials. Indeed, it is well known that such a network of microcracks induces a significant decrease in elastic properties. However, additionally, it can also strongly affect the thermal expansion at low temperature, and modify the stress-strain behaviour in tension with an enhanced strain to rupture by improving the fracture energy. Thus, these targeted characteristics are generally obtained by the development of a specific microstructure network based on well-chosen constituents of the materials. Among the refractory materials used in rotary kilns for cement making industries, magnesia-spinel and manesia-hercynite materials exhibit a great interest, thanks to a pertinent difference between the thermal expansion of their magnesia matrix and that of the spinel or hercynite inclusions. From these considerations, the present study aims to highlight the relationship between the microstructure of different magnesia materials and their fracture behaviour investigated through wedge splitting tests (WST). This type of mechanical test is well known for its ability to produce reliable data (especially fracture energy) during crack propagation. In order to assess the fracture process and process zone presence, WST has been coupled with Digital Image Correlation (DIC). This optical technique allows the monitoring of displacement fields and the calculation of strain fields during crack advancement. In accordance with DIC principle, the material transformation is usually assumed homogeneous inside each subset which finally lead to poorly defined cracks. In order to overcome this limitation, an improved DIC technique has been developed. This new approach allows each DIC subset to split in two parts with different kinematics. By this way, it is possible to automatically find the fracture paths and follow the crack geometries (length, opening) within the process zone during loading with a much higher spatial resolution than the one obtained by standard DIC. This new approach is especially useful to highlight the "crack branching" phenomenon involved in the enhancement of fracture energy in case of materials containing pre-existing microcracks.

*Speaker
†Corresponding author: marc.huger@unilim.fr

Keywords: Ceramic refractories, Fracture mechanics, Digital Image Correlation, Heterogenous Microstructure

Numerical simulation of the UO2 viscoplasticity at the polycrystal scale : microscopic validation

Luc Portelette * [1], Bruno Michel [1], Etienne Castelier [1], Marcelle Ibrahim [1], Mariem Ben Saada [2], Xavière Iltis [2], Philippe Garcia [2]

[1] French Alternative Energies and Atomic Energy Commission, Fuel Study Department, Fuel Simulation Laboratory (CEA/DEN/DEC/SESC/LSC) – Centre de recherche du Commissariat à l'Energie Atomique - CEA Cadarache (Saint Paul-lez-Durance, France) – France
[2] French Alternative Energies and Atomic Energy Commission, Fuel Study Department, Fuel Behavior Laboratory (CEA/DEN/DEC/SFER/LCU) – Centre de recherche du Commissariat à l'Energie Atomique - CEA Cadarache (Saint Paul-lez-Durance, France) – France

A model based on dislocation glide in a single crystal has been developed in order to simulate uranium dioxide (UO2) viscoplastic behavior during reactor operation of PWRs (pressurized water reactors). This model is then implemented through a 3D finite element formulation to simulate the polycrystal behavior in the volume element application (VER) of the PLEIADES nuclear fuel behavior software environment [1]. With this full field computation, the strain incompatibility induced by the disorientation at grain boundaries is computed along with associated stress and strain heterogeneities. In order to assess the grain size effect, the geometrically necessary dislocation densities are also computed from the viscoplastic strain field. The main objective of this study is to propose a validation methodology at the microscopic scale, in order to check that the computed stress-strain heterogeneity is in good agreement with experimental results. The experimental data used for this validation are based on 2D SEM-EBSD characterizations of polished sections of UO2 pellets, with as-fabricated grains in the 10 μm size range, following to uniaxial compressive creep tests [2]. EBSD provides quantitative micronscale information relating to the crystal lattice orientation, which is strongly correlated to the local viscoplastic strain induced during the mechanical test. Regarding simulation results, the crystal lattice orientation is derived from the elastic rotation computed through a finite strain formulation of the elastoviscoplastic transformation.
First a qualitative comparison between experiment and simulation is proposed which enables us to analyze the spatial variation of orientations within the original grains. Simulation results show that polycrystal viscoplasticity induces a non-uniform crystal lattice orientation as is observed from EBSD measurements. However the experimental spatial variation is discontinuous, as sub-grain boundaries appear, whereas our model describes a continuous variation in grain orientation. Statistical comparisons are provided of the orientation changes within the grains. In order to avoid grain size sensitivity and 2D-3D corrections, a variogram function is defined. According to these first results, it appears that the spatial statistical distribution is consistent with experimental results. However, the magnitude of the orientation variation is greater in the simulation, which suggests that the strain incompatibility is overestimated. Applying this methodology provides a more robust means of both analyzing basic deformation mechanisms and identifying the appropriate intragranular model to describe viscoplastic strains in uranium dioxide polycrystal.

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*Speaker

Keywords: UO2, uranium dioxide, ceramic, viscoplasticity, model, polycristal, variogram, disorientation

Modeling of the elastic and fracture behavior of nacre-like alumina using a discrete approach

Kaoutar Radi *† [1], Christophe Martin‡ [1], David Jauffrès§ [1]

[1] Laboratoire Science et Ingénierie des Matériaux et Procédés (SIMaP) – Centre National de la Recherche Scientifique - CNRS, Université Grenoble Alpes, Institut Polytechnique de Grenoble - Grenoble Institute of Technology – 1130, rue de la Piscine, 38402 Saint-Martin-d'Hères, France

Ceramics exhibit a unique combination of high stiffness and strength in materials, which makes them a most suitable choice for high stress and/or high temperature applications. However, their brittleness limits their use for a wide range of applications. Therefore, the appeal of damage-resistant ceramics is driving intense research activity. Interestingly, several damage-resistant materials that include ceramics are commonly used for structural purposes in nature. Mother-of-pearl (nacre) is the perfect example of nature's design of damage-resistant materials. Due to its complex hierarchical "brick and mortar" structure, nacre can achieve high strength and toughness simultaneously. In this context, a new bio-inspired material, nacre-like alumina, was designed and processed from brittle constituents arranged as brick and mortar (Bouville et al. 2014). Although the new ceramic shows significant improvements compared to conventional ceramics, the intrinsic and extrinsic toughening mechanisms are still poorly understood. A better insight on the reinforcement mechanisms and on the relationships between microstructure and properties together with microstructural optimization are paramount for this new class of ceramics.

Most of the models used to simulate the mechanical behavior of such materials are mostly elastic or elasto-plastic and do not include damage, therefore they only account for intrinsic reinforcements. Consequently, the increase of the fracture resistance as the crack propagates due to crack bridging is not taken in consideration. The modelling efforts performed so far have shown that the key parameters are the aspect ratio of bricks (tablets), the thickness of the mortar (interface) and their relative strength. Using Discrete Elements Method (DEM), we developed a pseudo-2D numerical model to study the influence of these microstructural key parameters on the elastic and fracture behavior of nacre-like alumina. The model is calibrated both in elasticity and fracture for the tablets and the interface, which are modeled by a packing of spherical discrete particles. The model is validated against the analytical model of Barthelat (Barthelat. 2014) on a 2D periodic unit cell of an idealized geometry of the brick and mortar structure. In order to preserve the tablets sliding energy dissipation mechanism and thus ultimately the toughness of the composite, tablets should remain intact. Depending on the overlap region, the tablets volume fraction and the strength of the interface, we are able to retrieve two failure modes, interface failure and tablets failure. Consequently, the parameters which will prevent tablets failure and control the failure mode can be determined. Building on this validated periodic unit cell model, an example of a realistic 2D microstructure encompassing a few hundred platelets was created to investigate crack propagation and extrinsic reinforcement mechanisms such as crack bridging.

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*Speaker

†Corresponding author: kaoutar.radi@simap.grenoble-inp.fr

‡Corresponding author: christophe.martin@grenoble-inp.fr

§Corresponding author: David.jauffres@simap.grenoble-inp.fr

Keywords: Modeling fracture, Ceramics, Discrete approach, Bioinpired materials.

Which representative volume element to account for rupture?

Nhat Ta * [1], Desiree Ciria [2], Guilhem Dezanneau [2], Veronique Aubin * † [3]

[1] Laboratoire de Mécanique des Sols, Structures et Matériaux (MSSMat) – CNRS : UMR8579, CentraleSupélec – 3 rue Joliot-Curie F-91 190 Gif sur Yvette, France
[2] Structures, Propriétés et Modélisation des Solides (SPMS) – CNRS : UMR8580, CentraleSupélec – France
[3] Laboratoire de mécanique des sols, structures et matériaux (MSSMat) – CNRS : UMR8579, CentraleSupélec – 3 rue Joliot-Curie F-91 190 Gif sur Yvette, France

Solid oxide fuel cells (SOFCs) offer a promising alternative to classical technologies for the generation of electricity by clean, efficient and environmental-friendly means. Nevertheless, the use of SOFCs is limited by their unsatisfactory durability and reliability due to the high operating temperatures and thermal cycling characteristic of these devices. One solution consists in lowering the operating temperature and then increase the durability. A potential electrolyte material for intermediate-temperature solid oxide fuel cells is lanthanum silicate [1].
The durability of fuel cell structures depends on their capability to withstand thermal fatigue during in service loading and residual stresses due to the cell manufacturing process. Thermal and residual stresses are mainly caused by the anisotropy of the thermal expansion coefficient and of elastic properties. The understanding and prediction of local stresses is then of great interest.

The notion of representative volume element (RVE) plays a key role in mechanics and physics of heterogeneous materials with the aim of predicting effective properties. The RVE allows to establish bounds but also estimations of the effective properties. A quantitative definition of RVE size has been proposed by [2] and illustrated for elastic and thermal properties of a two-phase composite. The authors showed notably that the RVE size depends on the property expected. However, the rupture of a polycrystalline ceramic does not result from of the mean stress state, as elastic property does, but is linked to the tail of distribution of stress states. A method is thus proposed in this paper to define the RVE accounting for failure.

The residual stress state in polycrystalline lanthanum silicate cells has been studied using a finite element approach. The methodology is applied to a specific random microstructure, a 3 dimensional Voronoi mosaic. Lanthanum silicate single crystals have anisotropic thermal expansion and elasticity parameters. Finite element simulations of volumes of varied sizes are performed under thermo-mechanical loading. The volumes are subjected to kinematic, static or periodic boundary conditions. It is shown that a failure criterion can be determined for large volumes and a small number of realizations. For smaller volumes, the same information can be reached providing that a sufficiently large number of realizations are carried out. Failure criterion is written using a stochastical approach.

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*Speaker
†Corresponding author: veronique.aubin@centralesupelec.fr

Keywords: thermo, mechanical loading, failure, micro, macro approach

S5: Additive Manufacturing

Multiscale mechanical observations of 316L specimens obtained by a direct laser deposition technology: influence of writing parameters

Yanis Balit *† [1], Andrei Constantinescu‡ [1], Eric Charkaluk§ [1]

[1] Laboratoire de mécanique des solides - École Polytechnique - CNRS – Ecole Polytechnique Université Paris Saclay – France

The aim of this paper is the analysis of the additive manufacturing parameters of the direct laser deposition (DLD) technology. More exactly, three of the main parameters such as the laser power, deposition speed and the powder flow will be investigated. The combination of those parameters associated with the strategy of deposition have a direct impact on the microstructure and thus, on the mechanical properties.

For DLD, Ocelík et al. [1] highlighted that the impact of the machine parameters can identified by the geometric analysis of a single track cut and Wang et al [2] showed that the deposition strategy has a direct impact on the tensile performance for a stainless steel 304L.

In this paper we shall focus on a similar topic for a 316 L stainless steel fabricated by the DLD technology using a *BeAM Mobile* machine. The novelty of the present analysis stems from microscale testing developed in-situ suing a scanning electron microscope (SEM). We there characterize both macroscopic microscopic mechanical parameters.

Result and discussion: The results show that the writing parameters and the strategy deposition have an influence on (i) size and (ii) orientation of the microstructure, as well as the (iii) residual stresses.

Constitutive law: In situ tensile tests on samples extracted from 3d manufactured wall with different parameters were performed. The deformation was captured by different scales of DIC and EBSD at every step of the tensile test.

Microstructure: the SEM and EBSD images show that the microstructure is mainly composed of columnar grains. Moreover, the solidification front followed the strategy deposition. The first result seems to show a texture of the microstructure. Finally, some of the deformation mechanisms are analysed during the tensile tests.

Residual stresses: The existence of residual stresses can conduct to local buckling of the walls and a predictive model will be coopered with experiments.

This study opens new perspectives in the measurement of the prestrain dependent properties of viscoelastic materials. The new measurements will challenge the theoretical constitutive models to take these results into account in order to represent a complete three-dimensional behaviour as needed in structural computations.

Acknowledgement: this work was funded by the Direction Génerale de l'Armement (France) and SNCF (France)

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*Speaker
†Corresponding author: yanis.balit@polytechnique.edu
‡Corresponding author: andrei.constantinescu@polytechnique.edu
§Corresponding author: eric.charkaluk@polytechnique.edu

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Keywords: additive manufacturing, laser cladding, writing parameters, microstructure, residual stresses

Fatigue damaging mechanisms of Ti-6Al-4V samples produced by Selective Laser Melting and Electron Beam Melting

Victor Chastand *† [1], Philippe Quaegebeur [2], Wilson Maia [1], Eric Charkaluk [3]

[1] Thales Industry Group (Thales) – THALES – 19/21 avenue Morane Saulnier, France
[2] Laboratoire de Mécanique de Lille - FRE 3723 (LML) – Centre National de la Recherche Scientifique : UMR8107, Arts et Métiers ParisTech, Ecole Centrale de Lille, Université de Lille, Sciences et Technologies – Bâtiment M6 Bvd Paul Langevin 59655 VILLENEUVE D ASCQ CEDEX, France
[3] Laboratoire de mécanique des solides (LMS) – Polytechnique - X, MINES ParisTech - École nationale supérieure des mines de Paris, Centre National de la Recherche Scientifique : UMR7649 – Route de Saclay 91128 PALAISEAU CEDEX, France

Additive manufacturing is a technology which can offer real benefits for new products. Taking advantage of this layer by layer production technology, new design parts can be manufactured and give the opportunity to reduce it weight, assembly time or integration time. Yet, mechanical properties of such parts must be well known in order to contribute to industrialize the process and use it for future part production.
Titanium Ti-6Al-4V is a common material used in the aeronautic and aerospace industries because of it high resistance compared with it low density. Several demonstrators showed that parts can be produced by additive manufacturing in Ti-6Al-4V, with mechanical properties equivalent to casting process. Effects of defects still have to be analyzed in order to select the right control methodologies and criteria for control strategies.

In this presentation, fatigue tests results performed on samples produced by SLM and EBM will be exposed to compare several properties: process, manufacturing direction, surface finishing and heat treatment. Results were analyzed in relation with the observation of each fracture surfaces. Damaging mechanisms could be proposed, taking into account the different types of defects observed.
Some micro tomography tensile *in situ* tests results will be presented in order to observe the fracture propagation in such samples and start to confirm the proposed damaging mechanisms.

Keywords: additive manufacturing, titanium Ti, 6Al, 4V, fatigue, damaging mechanism

*Speaker
†Corresponding author: victor.chastand@thalesgroup.com

Micromechanical behavior and thermal stability of a dual-phase α+α' titanium alloy produced by additive manufacturing

Stéphane Godet * [1,2], Guilhem Martin [3], Thibaut Dessolier [4], Frédéric Prima [5], Sébastien Allain [6], Fan Sun [5], Charlotte De Formanoir [1]

[1] 4MAT, Materials Engineering, Characterization, Processing and Recycling, Université Libre de Bruxelles – 50 Avenue FD Roosevelt, CP194/03, B-1050 Brussels, Belgium
[2] Université Livre de Bruxelles – Belgium
[3] Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, F-38000 Grenoble, France – Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, F-38000 Grenoble, France. – France
[4] Univ. Grenoble Alpes, – Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, F-38000 Grenoble, France. – France
[5] PSL Research University, Chimie ParisTech – CNRS, Institut de Recherche de Chimie Paris, 75005, Paris, France – PSL Research University, Chimie ParisTech – CNRS, Institut de Recherche de Chimie Paris, 75005, Paris, France – France
[6] Institut Jean Lamour, UMR 7198 CNRS - Université de Lorraine, Parc de Saurupt - CS 50840, 54011, Nancy Cedex, France – Institut Jean Lamour, UMR 7198 CNRS - Université de Lorraine, Parc de Saurupt - CS 50840, 54011, Nancy Cedex, France – France

In order to improve the mechanical properties of additively manufactured Ti-6Al-4V parts, specific heat-treatments should be developed without performing traditional hot deformation. An innovative heat-treatment consisting of a sub-transus thermal hold at 920◦C followed by water quenching generates a dual-phase α+α' microstructure with a high work-hardening capacity inducing a desirable increase in both strength and ductility. The present study investigates the micromechanical behavior of this particular dual phase α+α' microstructure. The thermal stability of the metastable α' martensite is assessed. To that end, annealing of the α+α' microstructure was performed and the resulting microstructural evolution was analyzed, along with its impact on the tensile properties. A deeper understanding of the micromechanics of the multiphase microstructures was achieved through the determination of the microscale strain partitioning between both phases. This was done by performing DIC measurements based on SEM images acquired during in-situ tensile testing. . A model based on the iso-work assumption and describing the macroscopic tensile behavior of the material depending on the individual mechanical behavior of each phase was also developed. This model enables to provide insights into the underlying deformation mechanisms.

Keywords: additive manufacturing, electron beam melting, post treatments, heat treatments, mechanical properties, work hardening

*Speaker

In-situ synthesis of Aluminum/nano-quasicrystalline Al-Fe-Cr composite by using selective laser melting

Nan Kang * [1]

[1] Mechanics surfaces and materials processing (MSMP) – Arts et Métiers ParisTech – Centre Arts et Métiers ParisTech 2 cours des Arts et Métiers 13 617 Aix en Provence, France

As a novel, high accuracy additive manufacturing process, selective laser melting (SLM) has attracted more and more attentions and well developed in the past decades. The component part with complex-formed was initially designed in 3D with a computer aided designed (CAD) technique. After that, the part is directly built layer by layer with a high power laser beam from the powder bed feedstock. Due to the small diameter of laser beam (< 50 μm) and low thickness of powder layer (< 100 μm), SLM process shows a great potential to produce the components with high accuracy. Al-based quasicrystalline materials (QC) are generally known for their high strength, high corrosion/wear resistance, low cost and density. In this research, Al-Fe-Cr QC as reinforcement in Al-based metal matrix composite was in-situ manufactured by using SLM. According to our previous work about SLM processed QC, a parametrical optimization of SLM process was performed with focus on laser powder and scanning speed. An almost dense sample (over 99%) was obtained from powder mixture with a homogenous microstructure. X-ray diffraction as well as microstructural investigations indicated that phase transition from decagonal QC Al65Cu25 Fe10Cr5 to icosahedral QC Al91Fe4Cr5 appears as energy density increases. The possible formation mechanism of metal-quasicrystal nanostructure was discussed on account of the result of transmission electron microscopy. And then, a normalizing process (heat treatment) was employed to improve the structural homogeneity and stability of SLM processed part. Tensile test was performed to determine the effect of normalizing process (heat treatment) on the mechanical strength and ductility. It indicated that recrystallization and growth of Al grains could be prevented by QC particle until the molten of Al matrix. Meanwhile, the growth of nano-QC particle leads an improvement of Young modulus and decline of ductility. Additionally, the sample obtained at relatively low laser power presents a mixed microstructure (partially melted QC, micro-QC and nano-QC) and high wear resistance. The instrumented indentation tests indicate that the partially melted QC particle present higher hardness than that of the other structure in the composite. Moreover, the wear mechanism changes from oxidation to delamination as the laser power increases. In conclusion, these results prove that this composite could be a new kind of metallic material with high strength and thermal stability and low density, which could be potential used in aerospace industries.

Keywords: Selective laser melting, Quasicrystal, Microstructure, Heat treatment, Wear, Tensile.

*Speaker

Definition on a REV based on fused deposition modelling process parameters

Guillaume Le Verge * [1]

[1] Institut de Recherche Dupuy de Lôme – IRDL – France

One of the most promising additive manufacturing processes is the fused deposition modelling (FDM) process. FDM technology is based on a filament of thermoplastic material which is driven at a controlled rate into a liquefier that is heated to a prescribed temperature associated with the material being used. The filament is heated to above its melting point and then extruded through a nozzle while the head scans a building stage along a programmed tool-path. Although much effort has been devoted to optimizing the process, it was shown that proper head control can lead to structural integrity of high quality. The objective of this work is to investigate and improve mechanical properties and dimensional accuracy. FDM process involves a multitude of machine operating and material parameters, which have a strong influence on the ply adhesion and on the mechanical strength of the printed part. Therefore, we propose a delaminated test to assess the impacts of the deposition speed, the head temperature and the deposition orientation on the inter-laminar adhesion. At last, we present an analysis based on a finite element method, that considers a representative elementary volume (REV) to characterize mechanical properties of the filament and printing parameters. The purpose of this model is to predict the mechanical behavior of the structure by taking into account the manufacturing process.

Keywords: fused deposition modelling, homogenisation, process parameters, adhesion, mechanical

*Speaker

Microstructural and Nano-Hardness in 316L+WC Composite Coatings Processed by Laser Cladding

Tommaso Maurizi Enrici * [1], Elena Mancini† [1,2], Julien Magnien‡ [3], Jérôme Tchuindjang§ [1], Anne Mertens¶ [1]

[1] University of Liège, A&M Department, MMS Unit (MMS) – Quartier Polytech 1, Allée de la Découverte 13A, B 4000 Liège, Belgium
[2] University of Padua, Department of Industrial Engineering – Via Marzolo 9, 35131 Padova (Italy), Italy
[3] Sirris Group – Rue Bois St-Jean, 12, B 4102 Seraing (Belgium), Belgium

Austenitic stainless steels (e.g. SS316L) are widely used due to their corrosion resistance and good toughness. However, their applications are still limited by their relatively poor tribological properties at high temperature. Surface damage occurs in areas under contact loadings. A composite coating in those zones appears as an interesting solution, combining the matrix material with hard reinforcements such as carbides. Among the possible reinforcements, WC is a popular candidate due to its hardness and its theoretical high melting temperature of 2600∘C.
Additive manufacturing, and in particular laser cladding, is a suitable technique for the manufacturing of composite coatings, allowing for a large variability in raw materials. In laser cladding, a stream of a powder, or a mixture of different powders, is fed into a focused laser beam while being scanned across a substrate, thus leaving behind a coating or object. Laser cladding process involves ultra-fast cooling rates during the solidification stage and the subsequent solid state transformations, thus giving rise to out-of-equilibrium phases.

This work considers a metal matrix composite composed by 316L stainless steel and reinforcements of tungsten carbides (WC) particles (16 and 28 in vol.%)1. The dissolution and interfacial reactions of WC reinforcements during casting is a well-known challenge in the production of metal matrix composites2. Indeed, because of carbide dissolution during solidification and re-precipitation, several layers composed by different out-of-equilibrium phases are formed around the partially dissolving carbide. The microstructure away from the particles is not affected by the carbide presence and is more homogeneous. The effects of the high cooling rates on the WC particles and the resulting microstructure are evaluated. A special attention was given to the dissolution of the reinforcements by reactions with the metallic matrix and to the different phases that could form depending on the local composition. In order to obtain more insights into the relative contributions of the various strengthening mechanisms at play in the composites (i.e. composite effect, precipitation and solid solution strengthening), macro-hardness tests have been performed and correlated with scanning electron microscopy (SEM), and nano-indentations that have been carried out to completely characterize the out-of-equilibrium phases formed around the original reinforcements.

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*Speaker
†Corresponding author: elena.mancini@studenti.unipd.it
‡Corresponding author: julien.magnien@sirris.be
§Corresponding author: j.tchuindjang@ulg.ac.be
¶Corresponding author: anne.mertens@ulg.ac.be

Keywords: SS316L, WC, Laser Cladding, DTA, EBSD

Influence of the local thermal history and microstructure on the wear behaviour of laser clad high speed thick coatings

Anne Mertens * [1], Neda Hashemi [1], Jérôme Tchuindjang [1], Olivier Dedry [1], Henri-Michel Montrieux [1], Ruben Jardin [2], Hoang Tran [2], Raoul Carrus [3], Anne Habraken [2]

[1] University of Liège, A&M Department, MMS Unit (MMS) – Quartier Polytech 1, Allée de la Découverte 13A, B 4000 Liège, Belgium
[2] University of Liège, ArGEnCo Department, MSM Unit (MSM) – Quartier Polytech 1, Allée de la Découverte 13A, B4000 Liège, Belgium
[3] Sirris Research Centre – Rue Bois St-Jean 12, B 4102 Seraing, Belgium

Fe-Cr-C-based alloys known as High Speed Steels (HSS) have been found useful in a wide variety of applications as machining and cutting, hot stamping and hot strip mills, thanks to their complex microstructure containing very hard carbides (V-rich MC, Mo- or W-rich M2C, Cr-rich M7C3 or M3C). Direct laser deposition, also known as laser cladding, has recently emerged as a very promising technique for the production and repair of thick coatings made from these alloys. Indeed, the very high cooling and solidification rates imposed by laser cladding result in strongly refined out-of-equilibrium microstructures and potentially enhanced wear resistance. However, the progressive accumulation of heat in the deposit during fabrication leads to variations of the thermal history as a function of position inside the build, resulting in turn into local variations of microstructure and wear properties.
Consequently, this work aims to investigate the influence of the local thermal history and microstructures on the wear behaviour of three HSS grades with varying contents of V, Mo and W in order to vary the type, size, morphology and amounts of the hard carbides. In a first step, 2D finite element simulations compute the thermal field during the direct laser deposition of 20 mm thick HSS deposits (a similar FE approach has already been published by the present group on Ti alloy Ti6Al4V [1]). The validated thermal history yields a deeper understanding of the microstructure generated as a function of the position inside the deposits. In a second step, the wear behaviour of the deposits is characterised at two different depths (i.e. at 2 mm from the free surface or at 2/3 of the total height) and for two constant test temperatures (i.e. room temperature [2] and 300∘C) using a pin-on-disc tribometer. In analysing the results of these tests, a particular attention was given to the role of the various carbides – including their type, morphology, hardness and failure mode – in determining the wear mechanisms of laser clad HSS deposits at the two tested temperatures.

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Keywords: Additive mnaufacturing, Laser cladding, High speed steels, Microstructures, Thermal model, Wear

*Speaker

Modelling the flow of a fiber filled polymer induced by a FDM 3D printer

Dihya Mezi *† [1], Gilles Ausias‡ [1], Julien Férec§ [1]

[1] Institut de Recherche Dupuy de Lôme (IRDL) – IRDL : Institutde Recherche Dupuy de Lôme – Rue St Maudé-56100 Lorient, France

The fiber orientation in 3D printing parts directly influences the mechanical performance of a composite. Therefore, it is important to control the final orientation pattern retained in the part following solidification. Hence, a numerical modelling is proposed to investigate the flow field of a short fiber filled thermoplastic through the nozzle and just after the die exit. It involves to consider the die swell phenomenon. As a first attempt, this works simulates axisymmetric FDM extrudate swell extending from the nozzle exit by adjusting the radial location of the free surface by minimizing the integrated free surface stress. Results quantify the effect of nozzle geometry and extrudate swell on fibre orientation in the extruded polymer. A second approach, which adds a thermal physics, considers the impact of the moving plate on the average final fibre orientation state of the extruded polymer bead. It also allows to investigate the heat diffusion through the deposited layers and the consolidation process.

Keywords: numerical modelling, rheology, thermal, FDM 3D printer, fiber composite thermoplastic material

*Speaker
†Corresponding author: dihya.mezi@univ-ubs.fr
‡Corresponding author: gilles.ausias@univ-ubs.fr
§Corresponding author: julien.ferec@univ-ubs.fr

Microstructural evolution and mechanical properties of Inconel 625 processed by Laser Metal Deposition and by Selective Laser Melting

Josiane Nguejio * [1], Fabien Szmytka† [2]

[1] Institute for Mechanical Sciences and Industrial Applications - UMR EDF/CNRS/CEA/ENSTA ParisTech (IMSIA) – IMSIA, UMR 9219, CNRS, CEA, EDF, UNIVERSITY OF PARIS-SACLAY – ENSTA ParisTech 9219, 828 Boulevard des Maréchaux 91762 Palaiseau, France

[2] Institute for Mechanical Sciences and Industrial Applications – UMR EDF/CNRS/CEA/ENSTA ParisTech (IMSIA) – IMSIA, UMR 9219, CNRS, CEA, EDF, UNIVERSITY OF PARIS-SACLAY – 828 Boulevard des Maréchaux 91762 Palaiseau Cedex, France

Inconel 625 is a nickel-based superalloy, strengthened mainly by the solid-solution hardening effect of certain elements, such as niobium (Nb) and molybdenum (Mo) in nickel-chromium matrix. Due to its specific characteristics which include good yield strength, creep resistance, fatigue properties and strong resistance to high temperature corrosion, this material is widely used in the aerospace, defense or energy industries [1, 2]. However, many of the Inconel 625 components have complex shapes which are very expensive and difficult to machine by traditional processes. Additive manufacturing (AM) technologies are therefore a suitable alternative to create complexes geometries and reduce the costs. AM technologies also have other advantages related to the design freedom, the process control and the parts performance.
In this study, an investigation procedure including scanning electron microscopy observations, differential thermal analysis and microhardness tests was carried out on wrought Inconel 625 to study the effect of long time exposure (up to 7h) at temperature (between 600 and 1100◦C) on the mechanical properties and to properly estimate the range of possible microstructures. Inconel 625 cylinders were then produced by laser metal deposition (LMD) from a commercial powder. First, the powders are characterized in order to study the shape, size and porosity for grains. Then, a 3D printing process parameters optimization is performed to determine the best combination of parameters (laser power, powder flow rate, printing head speed, etc.) leading to the most advantageous microstructure for producing Inconel 625 parts. Microstructure and tensile properties are then investigated and compared to the reference material. On the other hand, parts of Inconel 625 printed by selective laser melting (SLM) are also characterize . Measurements of both "metal printing" processes will then be compared to know which findings are consistent with those for wrought Inconel 625.

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Keywords: Laser, Powder, Inconel 625, Microstructure, Mechanical properties

*Speaker
†Corresponding author: fabien.szmytka@ensta-paristech.fr

Fatigue mechanisms of Ti-6Al-4V cellular structures fabricated by Electron Beam Melting

Théo Persenot * [1], Jean-Yves Buffière [2], Rémy Dendievel [3], Eric Maire [2], Guilhem Martin [4]

[1] Matériaux, ingénierie et sciences [Villeurbanne] (MATEIS) – Institut National des Sciences Appliquées de Lyon, Centre National de la Recherche Scientifique : UMR5510, Université Claude Bernard Lyon 1 – Bâtiment Saint-Exupéry 25, avenue Jean Capelle 69621 VILLEURBANNE CEDEX, France

[2] Matériaux, ingénierie et sciences (MATEIS) – CNRS : UMR5510, Institut National des Sciences Appliquées (INSA) - Lyon, Institut National des Sciences Appliquées [INSA] - Lyon – Bâtiment Blaise Pascal 7, avenue Jean Capelle 69621 VILLEURBANNE CEDEX, France

[3] Science et Ingénierie des Matériaux et Procédés (SIMAP) – Université Joseph Fourier - Grenoble I, CNRS : UMR5266, Institut National Polytechnique de Grenoble - INPG, Institut National Polytechnique de Grenoble (INPG) – 1130 rue de la Piscine, BP 75 38402 Saint Martin D'Hères, France

[4] Science et Ingénierie des Matériaux et Procédés (SIMaP/GPM2) – Université Joseph Fourier - Grenoble 1, Institut Polytechnique de Grenoble - Grenoble Institute of Technology : UMR5266, Institut National Polytechnique de Grenoble, Centre National de la Recherche Scientifique : UMR5266, Université Grenoble Alpes : UMR5266 – 101 rue de la Physique, BP 75 38402 Saint Martin D'Hères, France

Reducing the energy consumption is a crucial issue for most industries, in particular in the field of transport. In the aerospace industry, this can be achieved through weight reduction. In this context, cellular structures turn out to be one of the most efficient solution. The main obstacle to the use of cellular structures is their complex geometry which makes them difficult to produce. This problem tends to be released with the development of additive manufacturing. However, the introduction of cellular structures fabricated by additive manufacturing will remain limited as long as the fatigue performances of such structures are not understood.

The objectif of this work is to study the fatigue performance of a Ti-6Al-4V cellular structure produced by EBM. Fatigue mechanisms have been first identified from cyclic tests (constant stress amplitude R=0,1) performed on dog bones cylindrical specimens with a diameter comparable to that of the elementary strut of the lattices which will be produced eventually. The samples main microstructural features are a dual alpha/beta phase microstructure, a porosity with a non-homogeneous spatial distribution along the diameter and a significant surface roughness. SEM and tomographic observations of the fracture surfaces reveal that crack initiation always occurs at the surface from thin and relatively deep (up to 240μm) notch-like defect inherited from the fabrication process. The fatigue performance of as-built samples is therefore relatively low. Chemical etching has been used to reduce the specimens roughness; the notch-like defects responsible for fatigue crack initiation can be suppressed if the etching duration is long enough, significantly improving the fatigue performance. Hot Isostatic Pressing has also been used to suppress internal porosity although this type of defects appears to be less critical for fatigue. Other post-treatments are being investigated and compared with the previous ones (abrasive flow machining, mechanical surface finishing, ...).

Finally, similar fatigue tests have been performed on cellular structures. The results are discussed based on the mechanisms identified previously on single struts. The impact of the structure is also studied.

Keywords: Electron Beam Melting, X, ray tomography, TA6V, Cellular structures, Powder recycling, Chemical etching, HIP, Fatigue tests

*Speaker

On the mechanical behaviour of SLM AlSi10Mg and its improvement by friction stir processing

Guillermo Santos * [1], Jean-Yves Buffière [2], Eric Maire [3], Jerome Adrien [2], Chola Elangeswaran [4], Antonio Cutolo [4], Brecht Van Hooreweder [4], Frédéric Lani [5], Pascal Jacques [6], Aude Simar [1]

[1] Université catholique de Louvain (UCL) – Belgium
[2] Matériaux, ingénierie et sciences (MATEIS) – CNRS : UMR5510, Institut National des Sciences Appliquées (INSA) - Lyon, Institut National des Sciences Appliquées [INSA] - Lyon – Bâtiment Blaise Pascal 7, avenue Jean Capelle 69621 VILLEURBANNE CEDEX, France
[3] Matériaux, ingénierie et sciences (MATEIS) – CNRS : UMR5510, Institut National des Sciences Appliquées (INSA) - Lyon – Bâtiment Blaise Pascal 7, avenue Jean Capelle 69621 VILLEURBANNE CEDEX, France
[4] Additive Manufacturing, Department of mechanical engineering, KULeuven (PMA) – Celestijnenlaan 300B, 3001 Heverlee, Belgium
[5] Any Shape – Belgium
[6] Université catholique de Louvain (UCL) – Place de l'Université 1 - 1348 Louvain-La-Neuve, Belgium

Great expectations have been placed in the additive manufacturing (AM) technologies, coming from countless different sectors and fields. Potential applications are very diverse, in part due to the flexibility the technique offers.
When aiming at high performance mechanical properties for structural applications, metals are frequently the best if not the only available option. In the transport industries AM of lightweight metal alloys is therefore attractive for structural parts manufacturing. Nevertheless, there are some aspects of mechanical behaviour of AM metal parts that are hindering their industrial implementation. Anisotropy and heterogeneities, porosity, surface quality, reproducibility, etc. are problems that frequently occur regardless of the AM technique or the metal alloy used. Other issues can be more serious depending on the method, like residual stresses, which are more significant in selective laser melting (SLM), the most popular metal AM technique, than in e.g. electron beam melting (EBM).

In applications where good mechanical properties, especially good fatigue resistance, are sought, the anisotropy and heterogeneities, porosity, surface quality and residual stresses issues can become critical. A representative example could be SLM AlSi10Mg, the most used AM Al-alloy. Despite its static mechanical strength well above the cast reference owing to its very fine microstructure typical of SLM high cooling rates, both ductility and fatigue resistance are fairly low and exhibit anisotropy. These issues are directly linked to microstructural defects (inhomogeneities, porosities and Fe-rich intermetallics, some of them significantly larger than the α-Al+Si-rich eutectic microstructure).

Considering the phenomena behind this underperformance, a good way to improve mechanical behaviour of SLM AlSi10Mg parts could be to perform friction stir processing as a post-processing technique. This method derives from friction stir welding and consists in introducing a rotating tool composed of a shoulder with a pin at the tip into the part to treat, traversing the desired area of the part in order to produce at the same time severe plastic deformation, a forging and a thermomechanical effect on the material. The benefits of FSP in cast parts are proven and include microstructure refinement, homogenization and porosity elimination, resulting in significantly enhanced ductility and fatigue resistance.

The application of FSP on SLM AlSi10Mg plates has yielded homogenization, porosity elimination, Fe-rich

*Speaker

intermetallic particles breakage and redistribution, all the while little affecting the initial fine microstructure. This has been analysed through imaging techniques, including SEM and X-ray (laboratory and synchrotron) microtomography, the latter allowing for 3D porosity studies.
Static mechanical testing has shown the significant 400% ductility improvement brought about by FSP. Fatigue testing has also yielded promising fatigue life behaviour improvement after FSP. In situ tensile and ex situ fatigue testing performed in the synchrotron X-ray facilities of the ESRF (Grenoble) have allowed to study monotonic and cyclic damage mechanisms in the bulk of AlSi10Mg samples to understand the changes introduced by FSP and their impact on the mechanical behaviour.

Keywords: Additive manufacturing, Selective laser melting, Friction Stir Processing, Mechanical behaviour, Fatigue resistance

Predicted microstructures in repair technology of Ti-6Al-4V

Hoang Tran [1], Jérôme Tchoufang Tchuindjang [1], Hakan Paydas [1], Ruben Jardin [1], Raoul Carrus [2], Anne Mertens [1], Anne Habraken *† [1]

[1] University of Liege (ULiege) – Allée de la Découverte 1 Bât B52 teams MMS and MSM 4000 Liège, Belgium
[2] Sirris (Sirris) – Liège Science Park Rue Bois Saint-Jean 12 4102Seraing, Belgium

Laser cladding is a metal deposition technique often used to repair components [1]. Solidification following melting and partial remelting of pre-existing layers is coupled with heat treatment of the solidified material due to the repeated heating and cooling cycles during building. The effect of the building strategy on the metallurgical characteristics of the material for a decreasing track length (DTL) or a constant track length (CTL) strategy is analysed.Optical Microscopy (OM), Stereo Microscopy (SM), and Scanning Electron Microscopy (SEM) were used in order to study the microstructure. The generation of the microstructure results from the material thermal history.
The updated Lagrangian FE code Lagamine developed by ArGEnCo Department of the University of Liège to model forming processes is applied here on the laser cladding process [2]. The 3D-mesh is refined in the deposit and the top of the substrate in order to accurately model heat fluxes while the bottom of the substrate is meshed as coarse as possible. To generate an optimal mesh, transition refinement elements were used. In this powder injection technique, the continuous addition of material on the substrate is modelled by the element birth technique also called "switch" within Lagamine code.

The predicted thermal field is found close from the measurements of type-K thermocouples introduced inside the substrate. Such results were computed for both building strategies: decreasing track length (DTL) and constant track length (CTL) strategy. The predicted temperature histories confirm that a more uniform temperature history is applied to the deposit by the CTL choice than the DTL one. The presence in DTL case of heterogeneity within the hardness measurements and the phases observed by metallography [1] can be explained by the computed temperature distributions. A detailed analysis linking microstructure and thermal history is provided.

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Keywords: Laser cladding process, Titanium alloy, TA6V, Finite Element Modelling, Repair

*Speaker
†Corresponding author: Anne.Habraken@ulg.ac.be

A Numerical model for roughness effect on the mutliaxial HCF behavior of additively manufactured (SLM-EBM) Ti-6Al-4V parts

Bastien Vayssette *† [1], Nicolas Saintier [1], Charles Brugger‡ [1], Mohamed Elmay [1]

[1] Institut de Mécanique et d'Ingénierie de Bordeaux (I2M) – Arts et Métiers ParisTech – I2M - Site : Arts et Métiers ParisTech, Esplanade des arts et métiers 33405 TALENCE Cedex, France

Selective Laser Melting (SLM) and Electron Beam Melting (EBM) are powder bed fusion processes which allow to build parts by successive addition of layers directly from 3D-CAD models. Among the advantages are the high degree of freedom of design and the small loss of material, which explain the increase of Ti-6Al-4V parts obtained by these processes.

However Ti-6Al-4V parts produced by SLM and EBM contain defects (surface roughness, porosity) which decrease significantly the High Cycle Fatigue (HCF) life. In order to minimize porosities and residual stresses, post-processing like Hot Isostatic Pressing (HIP) and Stress Relieving are often conducted. The modification of the surface roughness by machining is very costly and not always possible, especially for parts with complex design. The aim of this work is to evaluate and propose a numerical model to account for the effect of the surface roughness and microstructure of Ti-6Al-4V parts produced by SLM and EBM on the multiaxial HCF behavior.

Five configurations were tested in tension-compression and torsion (R=-1 ; f=120Hz): Hot-Rolled (reference) ; SLM HIP machined ; SLM HIP " As-Built " ; EBM HIP machined ; EBM HIP " As-Built ". For every condition, microstructures characterization, observations of the fracture surface of the specimens and surface analysis were carried out respectively by Optical Microscope (OM), Scanning Electron Microscope (SEM), 3D optical profilometer and X-ray tomograph. The results of the fatigue testing show a significant decrease of the HCF life due to the surface roughness.

Along with experimental testing, numerical simulations using FEM were conducted using surface scans obtained by profilometry and volume scans obtained by tomography. Based on a precise description of the surface topology and extreme values statistics, a methodology is proposed in order to take into account the effect of the surface roughness on the HCF life.

Keywords: HCF, SLM, EBM, Surface Roughness, Ti, 6Al, 4V, FEM, Fatigue

*Speaker
†Corresponding author: bastien.vayssette@ensam.eu
‡Corresponding author: charles.brugger@ensam.eu

A numerical study on the multiphysical additive manufacturing process for ceramics

Steyn Westbeek * [1], Joris Remmers [1], Hans Van Dommelen [1], Marc Geers [1]

[1] Eindhoven University of Technology (TU/e) – P.O. box 513, 5600 MB, Eindhoven, Netherlands

Fabrication of ceramics through an additive manufacturing (AM) process opens up new possibilities in comparison to conventional ceramic manufacturing techniques, considering the high geometrical flexibility that is feasible even in small series production.
The process chain considered here is highly similar to the injection molding of ceramics using a polymer binder [1], whereas in this case the part geometry is constructed through vat photopolymerization or stereolithography. In conventional vat photopolymerization a photo-active monomer resin layer is sequentially deposited and selectively illuminated according to the part's cross section.
By dispersing ceramic powder into the resin the intermediate 'green' phase ceramic can be printed.
To obtain the final dense part a subsequent debinding and sintering step are required.

Although the current state-of-the-art facilitates printing of fine features accurately, several challenges prevent the manufacturability of larger technical ceramics.
The main challenges are: increasing the monolithic part density, increasing feasible product sizes and wall thickness and avoiding the formation of cracks [2].
In order to overcome these challenges a better understanding of the ceramic vat photopolymerization process is considered key.

In this contribution a coupled finite element framework is proposed which relates process parameters, e.g. light source characteristics, and material properties, e.g. ceramic filling fraction, to the development of residual stresses. As the the wavelength of the light and the dimensions of the inclusions are of comparable size in AM for ceramics, Maxwell's wave description is used to model the UV-illumination.
The frequency-domain light propagation simulation is directly linked to a time-domain chemical-thermo-mechanical model.
The numerical results illustrate the relevance of the ceramic inclusions in all the considered physical phenomena, ranging from the illumination, the conversion reaction, the generation of heat to the final stress state.

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Keywords: additive manufacturing, ceramics, vat photopolymerization, coupled multiphysics, process modeling

*Speaker

S6: Ductile damage and fracture

Prediction of fracture strain for AHSS sheets using different fracture models

Vivek Barnwal [†‡ 1], Shin Yeong Lee [1], Jin-Hwan Kim [1], Frédéric Barlat [1]

[1] Graduate Institute of Ferrous Technology, Pohang University of Science and Technology (POSTECH) – 77 Cheongam-ro, Nam-gu, Pohang, Gyeongbuk 37673, South Korea

AHSS sheets are increasingly used in automobile industries owing to their excellent mechanical and shock absorption properties. The exact prediction of formability is a major challenge for wider acceptability of these steels, which are known for their complex fracture behavior at different states of stress. Therefore, the accurate prediction of fracture is crucial to estimate the formability of AHSS sheets. The occurrence of fracture for these steels is often characterized by the presence of shear during plastic deformation. Though various fracture models have been proposed, the presence of shear still poses an interesting challenge in prediction of fracture strain for these steels. Most of the available models utilize stress triaxiality and/or lode angle parameter as two key variables to predict the fracture. Some of these models require a set of experiments (apart from uniaxial tensile test) leading to different states of stress and an appropriate optimization technique to calibrate all the key parameters. Hence, accurate prediction of fracture strains remains an interesting challenge especially at complex states of stress. The present work is aimed at predicting the fracture strain for DP980 and TRIP1180 steel sheet samples, with 1.2 mm and 1.4 mm of sheet thickness respectively, at low stress triaxiality using available fracture models. The key parameters for these fracture models are primarily calibrated from uniaxial tensile test experiments. Moreover, whenever required, additional experiments leading to different states of stress are performed to determine the complete set of parameters for fracture models used in present study. The uniaxial tensile tests are conducted at three different directions (0○, 45○ and 90○ from rolling direction) of the sheet. These tests are carried out as per ASTM E8 standard at 0.001 per second strain rate and room temperature. The critical fracture strain for all the experiments are calculated using digital image correlation (DIC) technique. The fracture strains predicted using different fracture models are compared with experimentally determined fracture strains. A comparative and detailed discussion is made on the extent of accuracy and user-friendliness of the fracture models considered in present study. This study also discusses the need to enhance/modify the available models in order to accurately predict the fracture strain under complex state of stress.

Keywords: AHSS alloys, Fracture models, Fracture strain

[†]Speaker
[‡]Corresponding author: vivekbarnwal@postech.ac.kr

Analysis of material failure under shear-dominated loading

Amine Benzerga * [1], Mohammad Torki [2]

[1] Texas A&M University – United States
[2] Texas A&M University (TAMU) – United States

The phenomenology of failure under shear dominated loadings begins to be understood on the basis of cell model calculations and *in situ* experiments. The process involves void nucleation at, say second-phase particles, followed by significant void distortion, including rotation and partial closure, as well as void-induced strain concentration in intervoid ligaments. Void nucleation aside, attempts at modeling failure in shear have employed isotropic models, which do not account for the induced anisotropy inherent to the process of shear failure. Here, we employ a two-surface void-shape dependent porous metal plasticity model to capture (i) void-induced inhomogeneous deformation at sub-cell level; (ii) void distortion preceding failure; and (iii) final void linkup. A mechanism of failure is uncovered in simple shear, which is found to prevail over a range of tension to shear stress ratios in the shear-dominated regime. Furthermore, the capabilities of the model at capturing transitions to tension-dominated loading are highlighted. Comparisons are made with available finite element cell model studies.

Keywords: voids, anisotropy, coalescence, shear, localization

*Speaker

Hardening of porous single crystals: an approximate description using sequential limit-analysis

Renald Brenner *† [1], Joseph Paux [1], Djimédo Kondo [1]

[1] Institut Jean Le Rond d'Alembert, UMR CNRS 7190 – Université Pierre et Marie Curie [UPMC] - Paris VI – France

This work adresses the constitutive response of voided single crystals subjected to plastic deformation. In this context, it is well-known that porosity evolution is the dominating factor in the fracture process. Voids are either intially present in the material or result from the debonding of precipitate phases. In the case of single crystal material, a particular attention has to be paid to the plastic anisotropy of the matrix phase (i.e geometry of the slip systems and ratios of the critical resolved shear stresses).
Although the importance of the crystalline anisotropy to describe the local stress field in the vicinity of intragranular voids has been clearly evidenced both experimentally and numerically, relatively few works on the constitutive response of 3D plastic single crystals containing voids have been undertaken until recently [see, among others,1,2]. Building on the study of Paux et al. [3] on the yield surface of porous single crystals, we propose a constitutive plastic law accounting for the hardening of the material. It is derived by solving successive limit-analysis problems, for different hardening state [4]. The approximate model is compared with finite-element results from the literature on porous BCC single crystals.

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Keywords: plasticity, single crystal, porosity

*Speaker
†Corresponding author: Renald.brenner@upmc.fr

Micromechanical modeling of porous ductile solids with isotropic and linear kinematic hardenable matrix under cyclic loading

Long Cheng * [1], Kostas Danas [2], Andrei Constantinescu [2], Djimedo Kondo [3]

[1] Université de Lorraine (UL) – GeoRessources, UMR 7359 CNRS-UL – France
[2] Université Paris-Saclay – Ecole Polytechnique - X – France
[3] université pierre et marie curie – Institut Jean le Rond d'Alembert – France

We propose a semi-analytical micromechanical model to study the elasto-plastic response of porous materials subjected to cyclic loading with isotropic and linear kinematic hardening at finite strains. To this end, we use an approximate but numerically efficient decoupled homogenization strategy between the elastic and plastic parts. The resulting effective back stress in the porous solid, similar to the macroscopic stress and plastic strain, has non-zero hydrostatic terms and depends on the porosity, the void shape and orientation as a result of the homogenization process. Subsequently, a complete set of equations is defined to describe the evolution of the microstructure, i.e., void volume fraction (porosity), (ellipsoidal) void shape and orientation both in the elastic and the plastic regimes. The obtained model is then numerically implemented in a general purpose user-material subroutine. Full field finite element simulations of multi-void periodic unit cells are used to assess the predictions of the proposed model. The latter is found to be in good qualitative and quantitative agreement with the finite element results for most of the loading types, hardening parameters and porosities considered in this study.

The combined analytical and numerical study shows that elasticity is an important mech- anism for porosity ratcheting in addition to strain hardening. Specifically, in order to recover the main qualitative features of porosity ratcheting, it is shown to be critical to take into account the evolution of the microstructure not only during the plastic loading, as is the usual hypothesis, but also during elastic loading. Finally, the effect of isotropic and linear kinematic hardening is found to be highly non-monotonic and non-trivial upon porosity ratcheting for most cases considered here.

The proposed analytical model was also used to investigate three different cyclic loading types with several values of the isotropic and linear kinematic hardening parameters. The three loading types considered involve a standard tension/compression cycle with equal amplitude positive and negative axial strain, a tension loading-elastic unloading with a non- zero positive average stress state, as well as a cyclic load where a positive prestress is added first and then cycling around this point is carried out. For the amplitudes considered here, the tension/compression load is found to lead to the largest porosity ratcheting effect while the positive prestress load to the smallest one. The relative effect of isotropic and kinematic hardening in those three loading states is found to be very different. In the last two loading types the kinematic hardening appears to have a weaker effect than in the first one.

Keywords: Cyclic loading, Porous ductile material, Porosity ratcheting, Non, linear homogenization, Strain hardening, Elasto, plasticity

*Speaker

A modified Gurson model accounting for Lode-dependent void growth

Lars Edvard Dæhli * [1], David Morin [1], Tore Børvik [1], Odd Sture Hopperstad *

[1]

[1] Norwegian University of Science and Technology (NTNU), Faculty of Engineering, Department of Structural Engineering, Centre for Advanced Structural Analysis (CASA) – Norway

Unit cell simulations have shown that the third invariant of the stress deviator has a marked effect on the evolution of the porosity. In this study, a modified Gurson model is proposed to account for this effect based on unit cell simulations and strain localization analyses. A cubic unit cell with a spherical void located at the centre was modelled by finite elements assuming an elastic-plastic matrix material governed by J2 flow theory. The unit cell simulations show a monotonic decrease in the void growth when changing the stress state from generalized axisymmetric tension via generalized shear to generalized axisymmetric compression for moderate and high levels of stress triaxiality. The Gurson model is then modified by including a term in the void evolution rule that accounts for Lode dependence in a similar manner as proposed by Nahshon and Hutchinson (2008). The modified Gurson model is assessed qualitatively through comparison with the unit cell simulations and strain localization analyses using imperfection band approach. It is found that the modified Gurson model compares well with the unit cell results. Further, the imperfection band analyses show that the modified Gurson model give a greater difference between the failure strains in generalized axisymmetric tension and compression than the original Gurson model and the shear-modified Gurson model of Nahshon and Hutchinson (2008). The Lode-dependent void evolution rule gives ductility predictions in better agreement with previously reported studies based on unit cell simulations for the set of material parameters employed in this study.

Keywords: Unit cell analyses, Void growth, Lode dependency, Gurson model, Strain localization analyses

*Speaker

Strain localization as an indicator for ductile fracture in metals

Odd Sture Hopperstad * [1], David Morin [1], Lars Edvard Dæhli [1], Tore Børvik [1], Ahmed Benallal [2]

[1] Norwegian University of Science and Technology (NTNU), Faculty of Engineering, Department of Structural Engineering, Structural Impact Laboratory (SIMLab, NTNU) – Norway
[2] Laboratoire de mécanique et technologie (LMT), Ecole Normale Supérieure (ENS), Paris-Saclay/CNRS/Université Paris-Saclay (LMT/ENS Cachan) – lmt – France

In this paper, we investigate the possibility of using strain localization as an indicator for initiation of ductile fracture in metals. The imperfection band approach of the strain localization theory proposed by Rice [1] is adopted in the analyses. A planar imperfection band is assumed in an otherwise homogeneous and homogeneously deformed material element and the conditions for localization inside the band are sought for under a wide range of band orientations and stress states. Metal plasticity is assumed outside the band, while the band material is modelled with porous plasticity. The imperfection is taken as either an initial porosity or a volume fraction of void nucleating particles. The results from the strain localization analyses are compared with results from unit cell simulations, using von Mises plasticity and metal plasticity with a high-exponent yield surface, and existing experimental data for steel and aluminium alloys. It is concluded that strain localization, when carefully calibrated, gives consistent estimates of the onset of ductile fracture in a wide range of loading conditions. Finally, an example is presented in which the imperfection band approach is used within a multi-scale modelling sequence to establish a computational failure model for large-scale simulation of a structural component without experimental calibration. [1] J. R. Rice, "The Localization of Plastic Deformation", in Theoretical and Applied Mechanics (Proceedings of the 14th International Congress on Theoretical and Applied Mechanics, Delft, 1976, ed. W.T. Koiter), Vol. 1, North Holland Publishing Co., 1976, 207-220.

Keywords: ductile fracture, strain localization, metals

*Speaker

Coalescence yield criteria for materials with small-scale voids

Jérémy Hure *† [1], Kim Nielsen [2], Valentin Gallican [3]

[1] CEA Saclay (CEA) – Commissariat à l'énergie atomique et aux énergies alternatives – France
[2] Technical University of Denmark (DTU) – Kongens Lyngby, Denmark
[3] Université Pierre et Marie Curie - Paris 6 (UPMC) – Université Pierre et Marie Curie - Paris 6 – France

Ductile fracture of metal alloys involves nucleation, growth and coalescence of voids. Macroscopic yield criteria have been derived over the last decades - since the work of Gurson based on homogenization and limit analysis - to describe porous materials in the growth regime corresponding to diffuse plastic flow around voids. Macroscopic yield criteria have also been proposed in the coalescence regime – corresponding to localized plasticity between voids - following the work of Thomason. Most of these homogenized models consider matrix material around voids obeying von Mises – isotropic – or Hill – anisotropic – yield criteria, thus assuming implicitly large-scale voids, at least larger than microstructural lengthscales related to grain size, dislocation density, and interfacial effect. However, theoretical considerations and numerical simulations have shown that these effects should be accounted for as void size decreases. More recently, yield criteria in the growth regime have been developed for small-scale voids by accounting for various phenomena relevant at lower scales. The effect of crystallographic orientation have been incorporated into homogenized models by considering crystal plasticity constitutive equations. Additional hardening due to the presence of interfacial energy at the void / matrix interface or because of a matrix material obeying strain-gradient plasticity have also been considered. In order to have complete ductile fracture models relevant for materials with small-scale voids, yield criteria for the coalescence regime are still required. Therefore, two analytical coalescence models are derived through homogenization and limit analysis. The first one accounts for interface stresses at the void / matrix interface that lead to an additional dissipation. Such model is relevant for nanoporous materials where the contribution of interfacial energy is not expected to be negligible. Both isotropic - through von Mises criterion – and anisotropic – through Hill criterion – interface and matrix material are considered, as well as the presence of shear loading conditions. The second model assumes that the matrix material obeys Fleck-Willis strain-gradient plasticity, and considers axisymmetric loading condition. For both models, the analytical coalescence criteria involve dimensionless parameters that relate a microstructural size to the void radius, thus exhibiting size effects. Numerical limit analysis is finally performed in order to assess the validity of the proposed criteria, and a good overall agreement is observed.

Keywords: Ductile fracture, Coalescence, Size effects

*Speaker
†Corresponding author: jeremy.hure@cea.fr

Damage mechanisms and fracture toughness of dual-phase steels exhibiting a platelet-like microstructure

Karim Ismail * [1], Laurence Brassart [2], Astrid Perlade [3], Pascal Jacques [1], Thomas Pardoen [1]

[1] iMMC-UCLouvain – Belgium
[2] Materials Science and Engineering, Monash University – Australia
[3] ArcelorMittal – Arcelor Mittal - Research and Development (FRANCE) – France

Dual-phase steels have long been used in the automotive industry for their excellent mechanical properties in terms of strength and ductility balance combined to a low processing cost. The good compromise between strength and ductility results from the very different properties of the constituent phases, namely ductile ferrite and hard martensite.
In contrast with the plastic flow properties, the fracture toughness of dual-phase steels (quantified by KIc or JIc) has been far less investigated. Common values of the fracture toughness are around 100 kJ.m-2 or lower. However, a minimum level of fracture toughness is required to prevent the propagation during forming operations of small edge damage or cracked zones induced by cutting. Therefore, unravelling the relationship between fracture toughness, microstructure and damage mechanisms is essential to develop advanced steels with superior forming ability. Furthermore, reaching superior fracture toughness could open to other potential applications.

Dual-phase steels are usually processed following an intercritical annealing which generally leads to equiaxed martensite particles. An alternative heat treatment, consisting of a double annealing as first proposed N.J. Kim and G. Thomas [1], brings about martensite particles in the form of platelets. A recent study on bulk samples of such steels shows that this microstructure can potentially lead to a very high fracture toughness, while retaining good properties in terms of strength and ductility [2].

In this work, rather oriented towards thin sheets, the Essential Work of Fracture (EWF) method [3] is used to quantify the work per unit area spent in the fracture process zone by separating it from the total work expended for material failure. EWF values in excess of 300 kJ.m-2 have been found on platelet-like microstructure steels confirming their interesting resistance to the propagation of a crack. Equiaxed microstructures are investigated as well and the impact of martensite volume fracture is assessed. Moreover the work of necking is separated from the work of damage using an extension of the EWF method [4].

As a first step towards the general objective of investigating the fundamental damage mechanisms governing the fracture toughness of dual-phase steels, a model for the plastic behaviour and for the damage mechanisms related to the microstructure has been developed. A finite element based unit cell approach is used to address the plastic behaviour with a particular focus on the effect of morphology and orientation, as well as of martensite volume fraction and of carbon content.

The data extracted from the elastoplastic analysis are fed into a cellular automaton approach of the damage evolution [5] with the aim of taking into account the effect of microstructural heterogeneities on fracture strain. Being able to incorporate a large number of different particles distributed differently in the microstructure in addition to a distribution of critical stress for nucleation, this model introduces a statistical description of the

*Speaker

material while using relatively simple damage evolution laws.

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Keywords: dual, phase steels, damage behavior, cellular automaton, essential work of fracture

Bifurcation Analysis of Unit Cell to Determine Macroscopic Localization

Hemanth Janarthanam * [1], Pd Dr. Ingo Schmidt [1], Dr. Silke Sommer [1]

[1] Fraunhofer-Institut für Werkstoffmechanik IWM (Fraunhofer IWM) – Wöhlerstraße 11, 79108 Freiburg im Breisgau, Germany, Germany

FE-Unit cell models have been widely used to understand the behavior of low porosity metals at large deformations and to determine the onset of localization. Determination of localization is a topic of active research and various localization indicators have been proposed in the literature. Based on the theoretical framework of plastic localization developed by *Rice (1976)*, here, a computational framework to determine the bifurcation of finite strain porous elastoplastic solid to planar bands is introduced. A fully periodic 3D-unit cell with a spherical void at center is investigated using the introduced framework. The unit cell is proportionally loaded by a coordinate transformation method, as proposed by *Faleskog (1998)*. The macroscopic stress state is characterized by stress triaxility and lode angle parameter. Here, stress triaxility in the range of $2/3 \leq T \leq 2$ and lode angle parameter between $-1 \leq L \leq 1$ for HCT600X is investigated. The elastic tangent tensor is computationally determined using a linear perturbation analysis at the stress free intermediate configuration and the elastoplastic tangent is further computed using the numerical technique as introduced by *Ingo Schmidt (2011)*.
Vanishing determinant of spatial acoustic tensor (Q) is used as a macroscopic strain localization indicator where the acoustic tensor is investigated for different directions in 3 dimensional space. The strain at localization obtained from this method is then compared to other localization indicators used in the literature for unit cell analyses. The influence of using a constant elastic tensor on localization strain as used in Gurson type porous plasticity models is also investigated. Apart from the macroscopic localization strain, this method also gives the direction of localization plane. The results show that the Lode angle parameter has a considerable influence on the localization strain.

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Keywords: Unit Cell Analysis, Localization Indicatior, Birfurcation Analysis

*Speaker

A reduced micromorphic single crystal plasticity model to study localization and void growth in ductile metals

Chao Ling [1], Samuel Forest * [2], Jacques Besson [2], Benoît Tanguy * [1], Félix Latourte [3]

[1] DEN–Service d'Etudes des Matériaux Irradiés, CEA, Université Paris–Saclay – CEA Saclay – 91191 Gif-sur-Yvette cedex, France
[2] MINES ParisTech, PSL Research University, MAT – Centre des matériaux, CNRS UMR 7633 – MINES ParisTech - École nationale supérieure des mines de Paris – BP 87 91003 Evry, France
[3] EDF R&D, MMC, Site des Renardières (EDF) – EDF, R – 77818 Moret-sur-Loing cedex, France

A micromorphic single crystal plasticity model is formulated at finite deformations as an extension of Mandel's classical theory based on a multiplicative decomposition of the deformation gradient. It involves a single microslip degree of freedom in addition to the usual displacement components. One of the proposed formulation which relies on a Lagrangian microslip gradient and leads to a Laplace term in the isotropic hardening law, is implemented in a 3D finite element code. The model is applied first to strain localization phenomena in a single crystal in tension undergoing single slip. The regularization power of the model is illustrated by mesh-independent simulations of the competition between kink and slip bands. The model is then used to investigate void growth and coalescence in FCC single crystals. Cylindrical and spherical voids are considered successively. The simulations show, for the first time in the case of spherical voids embedded in a single crystal matrix, that smaller voids grow slower than bigger ones, and that the onset of void coalescence is delayed for smaller voids.

Keywords: Micromorphic model, Strain gradient plasticity, Ductile single crystal, Strain localization, Slip band, Kink band, Regularization, Void growth, Size effect

*Speaker

Unfolding the effect of residual ferrite on damage and fracture resistance in a martensitic stainless steel for automotive application

Alvise Miotti Bettanini * [1], Laurent Delannay [1], Pascal Jacques [1], Thomas Pardoen [1], Coralie Parrens [2], Jean-Denis Mithieux [2]

[1] Université catholique de Louvain (UCLouvain) – Place de l'Université 1 - 1348 Louvain-La-Neuve, Belgium
[2] Aperam Research Center (APERAM) – Aperam Research Center – BP 15, 62230 Isbergues, France, France

In order to comply with new regulations on safety and pollution, the automotive industry is constantly seeking for new alloys to reduce the weight of chassis, while increasing strength and ductility. Martensitic stainless steels (MSS) exhibit good strength, acceptable ductility and corrosion resistance, which make these alloys a valid solution for automotive applications. MSS for hot-stamping are heat treated in the austenitic range for few minutes and then quenched to room temperature. Other than martensite, residual ferrite is usually present after this process. The ductile damage mechanism of a martensitic stainless steel with 15 vol.% of residual ferrite and Cr-carbide particles is investigated using a combined multiscale experimental and modelling approach. A preliminary study reveals that Cr-rich carbides are preferential damage nucleation sites. Hence, three different heat treatments are applied to partially dissolve these particles while keeping the same ratio of ferrite versus martensite volume fraction. Surprisingly, ductility decreases with decreasing volume fraction of Cr-carbides. Nanoindentation mapping indicates that the strength contrast between ferrite and martensite increases with Cr-carbide dissolution. According to finite element simulations of strain partitioning inside the dual phase microstructure, the stress triaxiality in ferrite increases with the mechanical strength contrast. This promotes nucleation and growth of primary voids, which reduces the fracture strain. In addition, a statistical study of FE simulations reveals that there is a critical phase configuration that maximizes damage. Voids are more likely to initiate in channels of percolated ferrite aligned perpendicular to the main tensile direction and constrained by the surrounding martensite. The present understanding of the role of residual ferrite in MSS should enable the design of microstructure with enhanced mechanical properties.

Keywords: automotive, hot stamping, martensitic stainless steel, ductile damage, martensite, ferrite, strength contrast, FE model

*Speaker

Combining interfacial and bulk plasticity for ductile failure with the thick level set approach (TLS)

Nicolas Moës * [1]

[1] Ecole Centrale de Nantes – Ecole Centrale de Nantes, CNRS : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France

The presentation addresses an issue with ductile failure that is not often looked at : the insertion of displacement discontinuity within the bulk softening zone to ensure the progressive and eventually full failure of the part. The capability to introduce displacement discontinuity is important to avoid infinite strain and accompanying element distortion. The Thick Level Set approach has been successful in combining an evolving displacement discontinuity within a diffuse damaging zone, for quasi-brittle failure. The presentation will discuss this capability for ductile failure. The key ideas will be presented in a 1D setting. We will demonstrate the capability of the model to shift smoothly within the following sequence of regimes : elastic, softening plasticity in the bulk (with a length regularization provided by the TLS), activation of a cohesive zone within the bulk plasticity acting concurrently with the bulk plasticity, contact and friction of the interface as a fully formed crack appears.

Keywords: plasticity, cohesive zone, thick level set, failure

*Speaker

Void Coalescence Mechanism for Combined Tension and Large Amplitude Cyclic Shearing

Kim Lau Nielsen * [1], Rasmus Andersen [1], Viggo Tvergaard [1]

[1] Technical University of Denmark, Department of Mechanical Engineering (DTU Mechanical Engineering) – Nils Koppels Allé, Bld. 404, Denmark

Void coalescence at severe shear deformation has been studied intensively under monotonic loading conditions, and the sequence of micro-mechanisms that governs failure has been demonstrated to involve collapse, rotation, and elongation of existing voids. Under intense shearing, the voids are flattened, such that the void volume diminishes, whereafter the flattened crack-like voids rotate and elongate until interaction with neighboring micro-voids dominates the material response and coalescence sets in. Eventually, this leads to a complete loss of load carrying capacity. The severe shear loading, imposed at the far boundary, is in an early state of the deformation associated with significant stretching of parts of the void surface, while other parts remain practically un-deformed. A largely uneven distribution of the strain hardening, therefore, evolves along the void circumference and, thus, one cannot expect the void to return to its original shape in the case where the far-field loading is reversed. The present numerical work aims to investigate the evolution of micro-voids subject to constant tension and large amplitude cyclic shearing. The far-field loading, the void shape, and the void growth are monitored, and the calculations are pushed to coalescence and complete loss of load carrying capacity. The initially circular cylindrical voids are predicted to develop protrusions in the shearing plane with normal in the direction of the applied tensile load. These protrusions evolve during repeated cyclic shearing and spread towards neighboring voids - eventually being responsible for void coalescence.

Keywords: Damage, Ductile failure, Low cycle fatigue, Constant mean stress

*Speaker

Ductile fracture modeling of aluminum thin CT and KAHN specimens with bimodal void distribution and Coulomb fracture model.

Gilles Rousselier * [1], Thilo Morgeneyer [1]

[1] Centre des Matériaux (MAT) – CNRS : UMR7633, MINES ParisTech - École nationale supérieure des mines de Paris – Centre des matériaux P. M. Fourt RN 447 - BP 87 91003 EVRY CEDEX, France

In aluminum thin sheets, complex ductile fracture mechanisms can be observed: damage with micrometer and sub micrometer voids, transgranular fracture without prior void damage. The self-consistent polycrystalline model is a powerful tool for the easy integration of various deformation and fracture mechanisms. The framework of physically based polycrystalline metal plasticity has also intrinsic advantages in describing the anisotropy and distortion of the yield surface, as well as non-proportional loadings (when damage and/or fracture are modeled, local loading paths are highly non-linear, even if the structure is in proportional loading). For reasonable computation times, the finite element calculations require the use of a "reduced texture" with a small number of crystallographic orientations (12 "grains" in the present applications). The plasticity model parameters *and* the reduced texture parameters (Euler angles and volume fractions) are determined from *mechanical* experiments through inverse optimization. For the large voids, a macroscopic porous plasticity model is reformulated in the polycrystalline framework. The small voids observed in shear bands (void sheets) are modeled with similar equations at the slip system scale. The Coulomb fracture model at the slip system scale is used for transgranular fracture. The parameters of the damage models are determined with the experimental data: load-displacement curves, SEM and 3D laminography observations. Through trial and error, the two Coulomb parameters are calibrated with the two specimen geometries CT and KAHN. The experimental and numerical results are in good agreement with regard to fracture strains and locations, macroscopic and microscopic features. The effects of the second population of voids are discussed.

Keywords: ductile fracture, porous plasticity, transgranular fracture, aluminum, finite elements

*Speaker

Numerical implementation and validation of a homogenized model for nanoporous metallic materials

Jean-Michel Scherer * [1], Jérémy Hure [2]

[1] CEA Saclay (CEA) – Commissariat à l'énergie atomique et aux énergies alternatives – 91191 Gif-sur-Yvette cedex, France
[2] CEA Saclay (CEA) – Commissariat à l'énergie atomique et aux énergies alternatives – 91191 Gif-sur-Yvette cedex, France

Nanoporous metallic materials are observed in industrial applications such as structural alloys used in nuclear power plants under irradiation, where nanovoids have been shown to contribute to the ductile fracture through classical void growth to coalescence mechanisms. Assessing the structural integrity of these components requires using homogenized models relevant for nanoporous materials. Homogenized models for porous materials have been widely developed and used for the last decades. However, as voids size decreases to the nanoscale, size effects are expected in the fracture of ductile solids. In particular, accounting for the presence of an interface associated with an interfacial energy may be mandatory for nanovoids. Homogenized growth and coalescence yield criteria and their associated flow rules taking into account interfacial stresses and void shape effects have been proposed recently in the literature. These criteria introduce a dimensionless parameter comparing void radius to a typical microstructural length, and exhibit size effects. The aim of this work is first to implement them numerically and second to assess their predictions by performing finite element calculations on porous unit cells. For the sake of compatibility with various finite element codes, numerical implementation of the constitutive equations has been performed with the open source code generator MFront with a Newton-Raphson algorithm. In addition to the yield criteria, hardening is considered following the heuristic evolution proposed originally by Gurson and based on local/global energy dissipation balance. Assumption of matrix plastic incompressibility and geometry lead to governing evolution laws of porosity and void size, shape parameters. Assessment of the homogenized model hypotheses is performed by comparing the predictions to finite element simulations. Porous cubic unit-cell are considered, assuming periodic boundary conditions and constant stress triaxiality. Interfacial stresses are accounted for by adding 2D-elements following a von Mises type flow rule at the matrix/void interface. Unit-cell simulations show that the evolution of void shape is strongly dependent of the size of the void, as stronger interfacial stresses for small voids tend to reduce void shape evolution. A new evolution law is proposed that depends on the dimensionless parameter introduced in the homogenized model, and a good agreement is finally observed between homogenized model predictions and unit-cell results.

Keywords: Ductile fracture, Coalescence, Size effects

*Speaker

Study of crack propagation on double notched steel specimen – numerical and experimental results comparisons

Jérémy Serveaux * [1,2], Carl Labergere [1], Khemais Saanouni [1], Frédéric Bumbieler [2]

[1] University of Technology of Troyes – ICD-LASMIS UMR CNRS 6281 – 10300 Troyes, France
[2] Andra – Direction de la R&D – 92290 Châtenay-Malabry, France

Predicting ductile fracture under complex loading path remains challenging, in particular for heterogeneous materials for which failure mechanisms depend on microstructural properties. In this paper, a study of crack propagation in the case of ductile damage is presented. A comparison between numerical simulations and experiments is necessary to check the efficiency of the numerical model used.
This work is a part of a study concerning the behavior of a welded steel overpack containing high level radioactive wastes which are planned to be disposed of in deep geological repository. During its lifetime, the overpack will be subject simultaneously to mechanical loading and corrosion. The main objective is to know if the numerical model is able to reproduce the behavior of this overpack under different representative loading paths. In order to validate the model, many investigations are conducted, belong them, the ductile fracture of double notched specimen constituted from homogeneous material is studied. So, the initiation and evolution of cracks must be accurately predicted using appropriate models and the results have to be compared to the experimental results.

The ductile behavior of the steel under concern has been studied in previous experiments. An elastoplastic behavior model with mixed nonlinear hardening (isotropic and kinematic) strongly coupled with ductile isotropic damage is adopted to model this material. It is formulated based on the classical thermodynamics of irreversible processes with state variables at the macroscopic scale, developed in Lemaitre $[L09]$, Saanouni $[S12]$. Materials parameters have been identified on standard tensile tests in previous works and allows the numerical model to predict good results in comparison with experiments.

In order to study the cracks propagation, tensile tests on double notched specimen have been carried out on specimen inspired by Takeda $[T16]$ who found interesting results. Different configurations of the notches have been tested and their impact on the direction of propagation of failure are compared.

The main objective of this paper is to compare the numerical and experimental results for the crack initiation and propagation during the tensile test of the double notched specimen. The influence of the shape radius and the initial positon of the notches on the crack propagation is analyzed.

Digital Image Correlation is used to measure the 2D spatial displacements vector on the external surface of the specimen. Displacement field given by the model is compared to theses experimental DIC measurements. In addition, the macroscopic cracks localization, the force – stroke curves are also compared in order to show the efficiency of the model in different cases.

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Keywords: ductile damage, double notched specimen, FEM, DIC

In-situ analysis of microstructural damage in advanced ultra-high strength automotive steel

David Wilkinson *† [1], Javad Samei‡ [1], Linnfeng Zhou [1], Diyar Salehiyan [1], Jidong Kang [2]

[1] McMaster University – Canada
[2] CanmetMATERIALS – Canada

There has been considerable progress in the development of ultrahigh-strength (UTS $>$ 1 GPa) low alloy steels for application in stamped automotive components. Greater utilization of such materials will depend on obtaining not only high strength but also good formability and crashworthiness. Due to combination of high strength and good formability, dual phase (DP) and quench and partitioning (Q&P) steels are amongst the ultra-high strength steels with great potential for application in future vehicles. In the current research, two fine-grained (FG) and ultrafine-grain (UFG) DP1300 steels and one commercial QP980 steel were tested in uniaxial tension coupled with in-situ scanning electron microscopy (SEM) and X-ray computed tomography (XCT). The UFG DP1300 was produced by adding 0.14 wt% of vanadium to the FG DP1300 steel which reduced ferrite grain size from 4.9 to 1.6 μm in the rolling direction and from 2.9 to 0.8 μm in the transverse direction. Grain refinement led to significant improvement of ductility in this DP1300 steel. The micromechanisms of damage evolution were similar in the DP1300 and QP980 steels. SEM observation during tensile testing indicated that only a small amount of microstructural damage occurred before the onset of necking; however, nucleation of voids and formation of micro-cracks developed progressively after necking. Martensite cracking and localized deformation at the ferrite/martensite interface are found to be the major and secondary micromechanisms of damage in both steels. XCT analysis also showed that notable void nucleation and growth began after necking; and hence, most of voids are located just below the fracture surface. Quantitative XCT determined that void volume fractions are 0.73, 0.42 and 0.44 vol% in the fractured FG and UFG DP1300 and QP980 steels, respectively. The lower damage level in the UFG compared to the FG DP1300 can be attributed to martensite refinement in the vanadium-added steel, which led to significant decrease of martensite cracking. Furthermore, nanoindentation tests have indicated that the mechanical compatibility between ferrite and martensite was improved in the UFG DP1300 steel which reduced ferrite/martensite decohesion and therefore suppressed nucleation and growth of interfacial voids.

Keywords: ductile fracture, damage, steel, xray tomography, in situ

*Speaker
†Corresponding author: wilkinso@mcmaster.ca
‡Corresponding author: samaeij@mcmaster.ca

Fracture investigation on Al/NiTip composite manufactured by friction stir processing

Lv Zhao * [1], Aude Simar [1], Sergio Turteltaub [2]

[1] Université Catholique de Louvain – Belgium
[2] Delft University of Technology – Netherlands

Fracture investigation on Al/NiTip composite manufactured by friction stir processing
Lv Zhao, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

Aude Simar, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

Sergio Turteltaub, Delft University of Technology, Delft, The Netherlands

Fracture strength involves one of the key parameters in the design of metal-based structures in automobile and aerospace applications. Over the past few years, increased attention has been paid on metal matrix composites (MMCs) because of the flexibility of tailoring their mechanical properties. However, controlling damage remains a challenging issue in these composites due to the prevailing failure at the interface between matrix and reinforcement agents [1, 2]. Shape memory alloys (SMAs) are considered good candidates to overcome this problem since they permit to introduce local compressive residual stresses that may delay fracture initiation. This concept, which has been studied numerically [3], requires further experimental validation.

The present work investigates the fracture behavior in friction stir processed Al1050/NiTip composite. In order to trigger the shape memory effect (SME) of the integrated NiTi particles, cold rolling and heat treatment were consecutively performed following the composite manufacturing. *In-situ* tensile tests were performed in a scanning electron microscope to monitor the crack paths in both Al/NiTip and pure Al (also friction stir processed and cold rolled) samples. Fracture initiation and propagation were separately investigated in crack-free and pre-cracked samples. It is found that the Al/NiTip composite involves higher yield stress and ultimate tensile strength than the pure Al. The real time monitoring on the pre-cracked samples shows that the NiTi particles lead to fracture path deviation in the composite, while the crack growth is quite straight in the pure Al. Moreover, when looking at the fracture surface, a flat to slant transition is observed in Al/NiTip, in contrast to the fracture of pure Al in which only the so called "flip-flap" feature is involved. The strength improvement is found to be dependent of the volume fraction of NiTi particles. The largest increase of the fracture strength achieved in the present work is nearly 35%, which is much higher than that reported in previous works on Al/NiTip composites [4, 5]. The strengthening effect is proposed to stem from not only the shape memory effect of NiTi particles, but also some local stresses induced by the cold rolling in the heterogeneous Al/NiTip composite, according to finite element simulations.

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Keywords: Metal matrix composite, shape memory alloys, fracture resistance, in, situ tensile tests

Quantitative assessment of the impact of second phase particle arrangement on damage and fracture anisotropy

Florent Hannard [1], Aude Simar [*†] [1], Thomas Pardoen [1], Eric Maire [2]

[1] Institute of Mechanics, Materials and Civil Engineering, IMMC, Université catholique de Louvain – B-1348, Louvain-la-Neuve, Belgium
[2] Matériaux, ingénierie et sciences [Villeurbanne] (MATEIS) – Institut National des Sciences Appliquées de Lyon, Centre National de la Recherche Scientifique : UMR5510, Université Claude Bernard Lyon 1 – Bâtiment Blaise Pascal 7, avenue Jean Capelle 69621 VILLEURBANNE CEDEX, France

The fracture anisotropy of the three aluminium alloys Al 6056, Al 6061 and Al 6005A has been characterized in tension. In the three alloys, the onset of yielding and strain hardening behaviour do not depend much on the direction of loading. However, while the fracture strain is close to isotropic in the alloys Al 6061 and Al 6005A, the alloy Al 6056 exhibits significant anisotropy. In situ tensile tests in X-ray tomography reveal that there exist two coalescence stages that include intra- and inter-cluster coalescence. A quantitative approach is proposed to relate this propensity to fracture anisotropy to a simple microscopic parameter characterizing the degree of anisotropy in the spatial distribution of second phase particles. The new indicator which quantifies the degree of connectivity or percolation between clusters is successfully assessed for the three Al alloys.

Keywords: X, ray tomography, Ductile damage, Anisotropy, Aluminium alloys

*Speaker
†Corresponding author: aude.simar@uclouvain.be

S7: Fatigue, reliability and lifetime predictions

Fatigue behaviour of an industrial synthetic rubber

Thomas Balutch * [1,2], Bertrand Huneau† [1], Yann Marco [3], Pierre Charrier [2], Clément Champy [2]

[1] Institut GeM – École Centrale de Nantes, Ecole Centrale de Nantes – France
[2] CAE Durability Prediction – Vibracoustic – France
[3] IRDL – ENSTA Bretagne – France

Anti-vibration solutions in automotive are crucial to ensure comfort, safety and durability in vehicle systems. Most of the parts that are designed to provide these functions are made of rubber, and particularly of natural rubber, known for its good fatigue resistance that is often attributed to the faculty to crystallize under tension [1]. Because of the significant heat experienced by some parts near car's hot spot, natural rubber can no longer be used (long period with $T > 90 \circ C$). As a consequence, synthetic rubbers such as EPDM are preferred because of better heat aging resistance. However, this matrix presents little or no strain-induced crystallization which leads to a lower resistance to fatigue crack growth when compared to natural rubber [1], and this lower resistance also has to be considered. Moreover, fatigue prediction for this material is difficult due to an important scattering of the lifetime results that could be related to the influence of geometrical flaws as the parting line. Finally, it has to be noted that only few scientific papers are dealing with the fatigue behaviour of such material [2, 3, 4].
Tools and methods that were developed during a previous study [5] to investigate the fatigue resistance and associated damage mechanisms of natural rubber are adapted here for synthetic rubbers. In the present work, fatigue tests in relaxing conditions and displacement control are performed using an experimental device with five diabolo-shaped samples tested at once. Four strain levels and five samples per levels are chosen for the construction of a fatigue lifetime curve, with an adapted frequency at each level to limit the self-heating. In addition, twenty five samples are tested at one given level in order to estimate more accurately the related scattering of the results. All the fracture surfaces of the tested specimens are then analyzed using binocular microscopy and SEM (Scanning Electron Microscopy) to identify the root causes of failure. Initiation mechanisms around inclusions and geometrical flaws, as well as propagation mechanisms, are investigated thanks to interrupted fatigue tests with regular observations of the samples surface.

The established fatigue lifetime curve confirms the important scattering of fatigue results as expected for such polymer (more than two decades of scattering in figure 1). Furthermore, all the fracture surfaces exhibit a single initiation site having various origin, such as rubber's inclusions or geometrical flaws. It appears that even if there is a competition between these two different root causes, there is no clear influence on the fatigue results. For the sample's failure, the following damage scenario can be considered thanks to the interrupted fatigue tests:
- Multi crack initiations on both parting lines and inclusions, but without cracks coalescence. The number of cracks is very low compare to what is observed in NR;
- Slow propagation of some cracks;
- Fast macroscopic propagation of one of them.

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*Speaker
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Keywords: Fatigue, EPDM, Rubber, Crack initiation, Fracture surfaces analysis

Heat Sources Effects on the Stress Intensity Factor for a Long Fatigue Crack

Zaid Boussattine * [1,2], Nicolas Ranc [1], Thierry Palin-Luc [2]

[1] Procédés et Ingénierie en Mécanique et Matériaux [Paris] (PIMM) – Centre National de la Recherche Scientifique : UMR8006, Arts et Métiers ParisTech – 151 boulevard de l'hôpital, 75013 Paris, France
[2] Institut de mécanique et d'Ingénierie [Talence] (I2M) – Centre National de la Recherche Scientifique : UMR5295, Arts et Métiers ParisTech – Esplanade des Arts et Métiers, 33405 TALENCE Cedex, France

By subjecting a cracked specimen to a cyclic loading, thermal effects take place and create a strongly heterogeneous temperature field around the crack tip. Those thermal effects are associated with dissipative and coupling heat sources, namely: (i) The heat source due to dissipative plastic deformation located at the reverse cyclic plastic zone near the crack tip; (ii) the intrinsic dissipation related to self-heating phenomena originating from plasticity at the scale of microstructure; (iii) the heat source due to elastic deformation leading to a thermo-elastic coupling. The aim of this work is to separately study the effects of each heat source on the mode I stress intensity factor in a center cracked specimen in C40-steel under cyclic loading.
The first dissipative heat source due to plasticity at the crack tip is evaluated by an experimental procedure based on infrared measurements technique [1]. Indeed, the temperature is initially measured near the crack tip by an infrared camera. Then, it is averaged ahead of the crack tip over a zone with less temperature gradient to minimize the measurements errors. Secondly, the heat diffusion equation is solved by finite element analysis for a unit heat source, the temperature is then computed in the same zone ahead of the crack tip. Finally, by using the linearity of the heat diffusion equation, the heat source due to plasticity at the reverse cyclic plastic zone is estimated.

The second dissipative heat source has an intrinsic property making it dependent on the material. Under cyclic loading, microplasticity occurs in all the material and dissipates into heat. It mainly depends on the loading frequency, the loading ratio and the applied stress amplitude. The estimation of this heat source is carried out by classical self-heating tests on non-cracked specimen [2].

The third coupling heat source is a periodically varying heat source. It describes the thermo-elastic coupling power deriving from the elastic deformation of the material [3]. It is directly proportional to the stress amplitude in the material and the loading frequency. It has been computed by a home-made Matlab thermo-mechanical framework.

For each heat source and by using finite element analysis, the temperature field in the whole cracked specimen is calculated. This temperature field is heterogeneous at the crack tip, and due to thermal expansion phenomena, it induces a heterogeneous stress field which can be computed by using an isotropic thermo-elastic constitutive equation to model the material behavior outside the reverse cyclic plastic zone. Thus, the mode I stress intensity factor due to each heat source is calculated by using the Green's function method [4].

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Keywords: Fatigue, Plastic dissipation, Reverse cyclic plastic zone, Infrared measurements, Thermoelasticity, SelfHeating, Stress intensity factor

Microstructure Sensitive Crack Nucleation in PM Ni Alloys

Bo Chen * [1], Jun Jiang [1], Fionn Dunne [1]

[1] Imperial College London – United Kingdom

Fatigue crack nucleation in a powder metallurgy produced nickel alloy containing a non-metallic inclusion has been investigated through integrated small-scale bend testing, quantitative characterisation (HR-DIC and HR-EBSD) and computational crystal plasticity which replicated the polycrystal morphology, texture and loading. Multiple crack nucleations occurred at the nickel matrix/inclusion interface and both nucleation and growth were found to be crystallographic with highest slip system activation driving crack direction. Local slip accumulation was found to be a necessary condition for crack nucleation, and that in addition, local stress and density of geometrically necessary dislocations are involved. However, the local stored energy density alone (of a Griffith-Stroh kind) unambiguously identified all the crack nucleation sites as those giving the highest magnitudes of stored energy.

Keywords: PM Nickel alloys, crystal plasticity, fatigue

*Speaker

Thermal cycling of Phase Change Material: a coupled method for the identification of thermal properties

Tanguy Davin * [1], Alain Guillet [2], Benoît Lefez [1]

[1] Groupe de physique des matériaux (GPM) – Centre National de la Recherche Scientifique : UMR6634, Université de Rouen Normandie – Avenue de l'Université, BP 08, 76801 Saint-Etienne-du-Rouvray Cedex, France
[2] Groupe de physique des matériaux (GPM) – Institut National des Sciences Appliquées – Technopôle du Madrillet UFR Scie Avenue de lÚniversité - BP 12 76801 ST ETIENNE ROUVRAY CEDEX, France

Phase Change Materials are commonly used for thermal storage or cooling purpose. In particular, transport industries like aeronautics or automotive applications. These compounds are submitted to severe thermal aging conditions. It is important to verify the thermal stability of such materials. In order to do so, an experimental bench was specially designed and an associated model was programmed.
The lumped system analysis (also known as nodal method), which is a relatively easy and adaptable formulation, was adopted. Also, the enthalpy-based modelling was chosen to avoid the heavy computation of the interface tracking. Hence, the variations of the PCM effective heat capacitance Cp(T) permits to render the change in enthalpy as a function of temperature. For the representation of real materials, the model takes into account of the subcooling, one of the main drawbacks of PCMs. The model aims at rendering the dynamic phenomena by considering microscopic crystallization parameters, such as the solidification speed. The conservation of enthalpy is checked during the numerical representation of this particularly delicate phenomenon. An inverse solving algorithm was implemented to identify these parameters and the thermo-physical properties. Thereby, the stability of the PCM can be controlled.

This experimental-modelling method was applied on the aging of erythritol, an organic compound often considered in the literature for cooling and thermal storage applications. The sample was placed in the designed setup to undergo aging conditions. Temperatures were recorded during the cycles comprising thermal loads. The experimental bench can thereby be described as a macro-DSC apparatus. The number of thermal cycles are analyzed to see its influence on the thermo-physical and crystallization parameters.
In this study, the experimental apparatus and the associated model are presented. Also, the identification procedure and the identified parameters of interest are described. Thanks to this coupled method, it is then possible to characterize the stability of the tested material during its use.

Keywords: experimental/numerical approach, thermal cycling, Phase Change Material (PCM), organic compound, identification model, subcooling

*Speaker

The Effect of the Environment on High Temperature Fatigue Behaviour of Carbon/Polyimide Textile Composites for Aircraft Applications

Federico Foti * [1], Yannick Pannier [2], David Mellier [1], Marco Gigliotti [1]

[1] Institut Pprime (PPRIME) – CNRS : UPR3346, Université de Poitiers, ENSMA – 1, avenue Clément Ader, BP 40109 F86961 FUTUROSCOPE CHASSENEUIL, France
[2] Institut Pprime (PPRIME) – CNRS : UPR3346, Université de Poitiers, ENSMA – ISAE-ENSMA - Teleport 2 1 Avenue Clement Ader - BP 40109 F86961 FUTUROSCOPE CHASSENEUIL Cedex, France

The employment of organic matrix/carbon fiber composites (OMC) is foreseen for the realization of "warm" aircraft structures: these parts may be subjected, in service, to mechanical fatigue (e.g. fan/compressor blades turbo-engines), thermal cycling and thermo-mechanical fatigue (e.g. aircraft structural parts). Though there is a consistent literature concerning the fatigue behaviour of woven composites (see, for instance, [1]), while the interaction between fatigue and environmental degradation at high temperature has been poorly explored. This work aims at characterizing and modelling - for carbon fiber/organic matrix (polyimide) textile composites – the thermomechanical behaviour, the onset and the development of damage related to cyclic mechanical mechanisms (fatigue) under controlled (temperature and gas) environment. It is known that thermoset polymers at high temperature may suffer from thermo-oxidation phenomena leading to embrittlement and damage in OMC ([2]). An experimental setup is specifically developed in order to perform fatigue tests under controlled environment (Tmax: 350∘C, pmax: 5 bar, environment: air, O2, N2). Sample properties evolution during fatigue tests at 250∘C are monitored using in-situ Digital Image Correlation (DIC) and damage assessment is provided by ex-situ X-ray microtomography (μCT). μCT scans are carried out to evaluate the type and the extent of damage during fatigue. The long-term aim of the study is to provide experimental and numerical tools to strengthen the understanding and the modelling of mechanics/damage/environment coupling for durability prediction.

Keywords: environment, fatigue, organic composite material, carbon/polyimide, textile composites

*Speaker

A crystal-plasticity based model for the early stages of fatigue damage

Charles Mareau * [1]

[1] Laboratoire Angevin de Mécanique, Procédés and innovAtion (LAMPA) – Arts et Métiers ParisTech – Arts et Métiers ParisTech - Centre d'Angers 2, Boulevard du Ronceray BP 93525 49035 Angers Cedex 01, France

In metallic materials, the process driving to fatigue failure is often complex, mostly because of the significant influence of microstructural heterogeneities during the initiation and propagation stages. Polycrystalline plasticity models, because they explicitly consider such heterogeneities, provide a way of understanding and quantifying the role of microstructure on the fatigue behavior of metallic materials. For fatigue applications, such models often rely on the a posteriori computation of some indicators (e.g. stress-based, strain-based and/or energy-based) to determine whether the conditions for crack nucleation are met or not [e.g. McDowell and Dunne 2010, Przybyla et al. 2010, Robert et al. 2012, Guerchais et al. 2014]. However, while these approaches are useful for investigating initiation, the transition to the following propagation stage cannot be described as the local degradation of mechanical properties is not accounted for.

This work aims at proposing a non-local constitutive model for describing the nucleation and propagation of short fatigue cracks (stage I) in polycrystalline metallic materials. The constitutive relations are written within the context of crystal plasticity, which allows considering the kinematics of crystallographic slip. Also, to include the progressive degradation of local stiffness properties, the general framework of continuum damage mechanics is used [Lemaitre 1996, Desmorat et al. 2007]. More specifically, the anisotropic nature of fatigue damage is included by adopting the strategy initially proposed by Saanouni and Abdul-Latif [1996], which consists of associating a damage variable to each slip system. An internal length scale is introduced by extending the set of internal variables to include the spatial gradient of damage variables. The driving forces associated with the different internal variables (i.e. plastic shear strains, damage variables, damage gradient variables and hardening variables) are then derived from a thermodynamic potential. Finally, a rate-dependent formalism is used to connect the time derivatives of the different internal variables to the corresponding driving forces.

The above constitutive model is implemented within a spectral (i.e. FFT-based) solver which allows solving the equations associated with equilibrium and compatibility conditions [Moulinec and Suquet, 1998]. For an illustration purpose, the model is then used to investigate the fatigue behavior of a copper polycrystal. More specifically, the model is used (i) to evaluate the influence of loading conditions on damage development (ii) to discuss the connection between plasticity and damage.

Keywords: Crystal plasticity, Damage, FFT, Non, local model

*Speaker

On the crystallographic, stage I-like, character of fine granular area formation in internal fish-eye fatigue cracks

Thilo Morgeneyer * [1], Hayat Abdesselam [1], Jérôme Crépin [1], André Pineau [1], Anne-Laure Rouffie [2], Pierre Gaborit [3], Léa Menut-Tournadre [3]

[1] Centre des Matériaux (MAT) – CNRS : UMR7633, MINES ParisTech - École nationale supérieure des mines de Paris, Ecole des Mines de Paris – Centre des matériaux P. M. Fourt RN 447 - BP 87 91003 EVRY CEDEX, France
[2] Safran Tech, Pôle M&P – SAFRAN (FRANCE) – Rue des Jeunes Bois, Châteaufort, 78772 Magny les Hameaux,, France
[3] Safran Aircraft Engines – SAFRAN (FRANCE) – Villaroche, Rond-Point René Ravaud-Réau, 77550 Moissy-Cramayel, France

The aerospace industry is constantly looking for new technologies that will meet the objectives of performance, safety and reduction of fuel consumption. High strength steels have become well suited for weight reduction and guaranteeing the reliability of structures for long term service. Large variability in fatigue life is often found for ultra-high strength steels [1]. This fact requires using high coefficients of security for structural design. S-N curves of these steels have a distinct knee point within the high cycle and the very high cycle fatigue regimes with a plateau between them. Experimental data can be divided into two characteristic failure types on non-metallic inclusions: surface fracture mode at higher stress level leading to fewer loading cycles and interior fracture mode at lower stress levels leading to very long fatigue lifetime and sometimes to a formation of a fine granular area (FGA) around the particle [2] [3] [4] [5]. Thus, there is a stress level for which the crack initiation changes from the surface to the internal structure of the material, which is associated with substantially longer fatigue lives.
In the present work [6], the crystallographic character of FGA formation from internal particles in martensitic high strength steel has been revealed by an assessment of the plastic zone size at the FGA border. This plastic zone size corresponded to about 3 times the martensite lath width. Tests at different temperatures (20∘C, 200∘C and 400∘C) revealed a decreasing FGA size with increasing temperature at constant applied stress amplitude. As a consequence, the critical stress intensity factor varied as the FGA decreased with temperature. In contrast, the critical plastic zone size remained constant and equal to the sizes of microstructural features. This represents a strong similarity between crystallographic, stage I-like, crack propagation and FGA formation in a vacuum.

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Keywords: Fine Granular Area (FGA), Plastic zone, Stage I, like, VHCF, Optically dark area, ODA, GBF, Martensitic High Strength Steel

Fatigue behavior of notched short glass fiber reinforced thermoplastics

Ilan Raphael *† [1,2], Nicolas Saintier [1], Lucien Laiarinandrasana [2], Gilles Robert [3]

[1] Institut de Mécanique et d'Ingénierie de Bordeaux (I2M) – Arts et Métiers ParisTech – I2M - Site : Arts et Métiers ParisTech, Esplanade des arts et métiers 33405 TALENCE Cedex, France
[2] Centre des Matériaux (MAT) – CNRS : UMR7633, MINES ParisTech - École nationale supérieure des mines de Paris – Centre des matériaux P. M. Fourt RN 447 - BP 87 91003 EVRY CEDEX, France
[3] Solvay (France) – Solvay (France) – France

Short glass fiber reinforced thermoplastics allow for a weight reduction of structures, especially in the car industry. They exhibit good specific mechanical properties, are easy to manufacture and prove to be cost effective.
Having a good understanding of the fatigue behavior of such materials is key for an optimized durability of the industrial parts. As those parts exhibit complex geometries, one of the current challenges is to provide proper experimental data and models needed to get a better understanding of the notch effect.
An experimental campaign was performed on RH50 reinforced PA66 loaded in tension-tension (R=0.1) with a frequency of 0.5Hz. The usual fiber orientations (0○, 45○, 90○) as well as two different notch geometries were tested. Digital Image Correlation was used to evaluate the cyclic behavior in the notch root during fatigue tests. Both the local cyclic strain and mean strain field were evaluated in order to identify the numerical constitute model. Based on micro-tomography and and fractography observations a fatigue damage mechanism a fatigue model are proposed for these materials.

Keywords: Fatigue, Composite, Thermoplatics, Notch

*Speaker
†Corresponding author: ilan.raphael@ensam.eu

Cyclic loading and delayed hydride cracking in Zr-alloys

Luca Reali *† [1], Daniel Balint [2], Mark Wenman [3], Adrian Sutton [1]

[1] Department of Physics [Imperial College London] – Department of Physics, South Kensington Campus, Imperial College London, SW7 2AZ London UK, United Kingdom
[2] Imperial College London (ICL) – Imperial College London, South Kensington Campus, London SW7 2AZ, United Kingdom
[3] Imperial College London (ICL) – Imperial College London, South Kensington Campus, London SW7 2AZ, United Kingdom

The Zr-alloy cladding, which is a critical component in fission reactors, has to safely withstand both fatigue and delayed hydride cracking (DHC) due to thermo-mechanical loads in a corrosive environment. During DHC a crack opens by sequential precipitation and fracture of hydrides, and this has been a major industrial concern for over 60 years. Currently, the industrial regulations consider them separately, and indeed no theoretical framework that couples them exists in the literature. The proposed analysis aims at filling this gap with a physically based model rooted in stress-assisted diffusion. It takes as an input the TEM characterisation of the microstructure and then combines an analytical description of dislocations and a numerical integration of the two-dimensional diffusion equation. We focus first on how the microstructural effects of cyclic plastic strain can influence hydrides precipitation, resulting in a fatigue-enhanced DHC. Second, also the influence of the loading frequency on DHC is investigated.
When cyclic plastic strain localises in slip bands, low-energy edge dislocation patterns emerge. Importantly, they form vacancy dipoles which act as traps for hydrogen. The hypothesis is that hydrogen accumulated in Cottrell atmospheres sets the path for the DHC propagation. A multiscale approach bridges the microscopic scale of dislocation clusters and hydrides, and the hydrogen accumulation around dislocations and subsequent diffusion.

In the literature, the crystallographic dislocations generated during fatigue have been described by equivalent edge dipoles. Here, the similar concept of equivalent vacancies is applied to the vacancy dipoles. In order to test the model, the dislocation patterns typical of fcc metals were employed due to the abundance of data, but the distribution of the vacancies is completely flexible. A crack is then placed close to the vacancies and propagated by nucleation of hydrides at its tip. The process at place is similar to conventional DHC, although, by including the features of the defects introduced with fatigue, this model establishes a link between these two phenomena.

Preliminary calculations were performed under the assumption, rooted in experimental literature, that the dislocation patterns in zirconium and in fcc metals are comparable. By comparing the DHC velocity with and without vacancies, the fatigued microstructure gives a crack propagation enhancement by 91 % at 500 K under a constant mode-I stress intensity factor of 10 MPa(m)1/2. This may have a big impact as the safety of these components is of the utmost importance. The proposed coupling may be confirmed if supplemented by an experimental TEM characterisation.
Since the process reaches a steady state, the resulting DHC velocity could be readily used to estimate the lifetime of the cladding, given the initial thickness and the minimum ligament length. Finally, when including the effect of a sinusoidal loading, two different regimes emerge. At the lower frequencies, DHC does not depend on the frequency, whereas for frequencies higher than 1 Hz (at 500 K and load ratio 0.1) DHC is inhibited. Both the regimes can be explained by comparing the typical diffusion time and the period of the oscillations.

*Speaker
†Corresponding author: luca.reali16@imperial.ac.uk

Keywords: Crack propagation, Fatigue, Delayed Hydride Cracking, Zirconium alloys

Micromechanistic and microstructural design of titanium alloys for resisting cold dwell fatigue

Zhen Zhang * [1], Fionn Dunne [1]

[1] Department of Materials, Imperial College London – United Kingdom

A micromechanical study has been conducted on low temperature dwell fatigue resistance in multiphase titanium alloys. The origin of the observed peak in strain rate sensitivity (SRS) over temperature (Zhang et al., 2015) has been explained by the transition from high-stress/low-temperature to low-stress/high-temperature thermally activated dislocation escape. The SRS peak is found also to depend on texture and phase morphology in multiphase titanium alloys, which is different from binary alloys.
Basal slip in titanium alloys has been found to be more rate dependent than that for prismatic and pyramidal systems at low temperature. This leads to stronger load shedding during cold creep in a hard and soft grain combination and greater slip transfer when the neighbourhood grains are soft. A computational investigation of crystallographic texture shows that a stronger rate sensitivity results from polycrystals with higher fractions of grains well-orientated for basal slip activation. This has also been demonstrated in independent experimental studies (Amouzou et al., 2016).

Basket weave structures with multiple a variants have been shown to give the lowest SRSs (Zhang and Dunne, 2017), for which the mechanistic explanation is that the β lath structures provide multiple, small-scale α variants which inhibit creep and hence stress relaxation, thus producing more uniform, diffuse stress distributions across the microstructure through *intragranular kinematic confinement.* The critical consequence of this is that alloy Ti-6246, typically having multi-variant basket weave structure, remains free of dwell fatigue debit whereas Ti-6242, associated with globular colony structures, suffers significant dwell debit. The micromechanistic basis for this is: (1) microscale kinematic confinement imposed by multi (α)-to-single (β) BOR relations (i.e. multiple α variants sharing the same parent β grain); (2) macro-textural confinement; (3) the intrinsic anisotropic strain rate sensitivities of β and α phase slip systems; (4) multiple intragranular α variants. This understanding is important in microstructural design of titanium alloys for resisting cold dwell fatigue.

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Keywords: low temperature fatigue, microstructures, texture, morphology, multiphase alloys

*Speaker

Multiscale modelling study of low cycle fatigue behaviour of an austenitic stainless steel processed by Surface Mechanical Attrition Treatment

Jianqiang Zhou *† [1], Zhidan Sun [1], Pascale Kanouté [2], Delphine Retraint [1]

[1] ICD, P2MN, LASMIS, University of Technology of Troyes, UMR 6281, CNRS, Troyes – University of Technology of Troyes – France

[2] ONERA, The French Aerospace Lab, 29 avenue de la Division Leclerc, 92322 Chatillon Cedex, France – ONERA – France

It is important to understand the materials characteristics responsible for their performance in service, in particular their cyclic deformation response. Residual stress, as a main feature of metallic materials, can be generated during their manufacture or treatment, and it is often coupled with work hardening/softening activities. Both residual stress and work hardening can significantly influence the properties of metallic materials. Thus being able to thoroughly understand and precisely characterize these two parameters is of great importance for material processing design and optimization. Surface mechanical attrition treatment (SMAT), based on mechanical impacts of materials by metallic balls at high strain rate, can generate high compressive residual stress and work hardening fields in the near surface region, along with a thin nanostructured layer on the treated surface, which enables better improvement of the in-service performance of materials. This work consists in studying the effect of SMAT on low cycle fatigue (LCF) of a stainless steel with multiscale modelling method. SMAT is performed on cylindrical specimens in austenitic stainless steel 316L. The generated gradient microstructure is characterized by a thin grain-refined layer on the treated surface, and an in-depth variation of residual stress as well as work hardening in the near surface region, according to the measurement/analysis using Electron BackScatter Diffraction (EBSD), micro-indentation, and X-ray diffraction (XRD). The effect of residual stress and work hardening on the cyclic behaviour of material constitutes the main task of this study through homogenizing the response of all the considered grains using a self-consistent method. Several representative volume elements (RVE) for numerical simulation are constructed so as to represent the typical in-depth features of SMATed material. A phenomenological micro-macro constitutive law based on the plastic slip is used for each grain and slip system, and the material dependent parameters are identified from the cyclic behaviour of the studied material through correlating with the evolution of back stresses and effective stresses obtained with LCF tests. Typical residual stress state evaluated by XRD in the given depth can be considered as the local macroscopic residual stress, and thus directly applied on the RVEs. Whereas, the work hardening is strongly dependent on the deformation history, and accordingly an analysis of plastic flow history during SMAT is performed in the microscopic scale to generate a microscopic residual stress field and plastic slips in each grain corresponding to the initial condition of the SMATed material. The strain controlled cyclic loading is simulated using the constructed homogenization models, to analyse the evolution of microscopic residual stress and plastic slips as well as their effects on the mechanical behaviour of RVEs during cyclic loading. In addition, a comparison between the results of simulation and the ones of experimental investigation for the material state obtained after LCF tests is performed.

Keywords: Residual stress, Work hardening, SMAT, Low cyclic fatigue, Multiscale modelling, Homogenization.

*Speaker

†Corresponding author: jianqiang.zhou@utt.fr

Fatigue behavior and life prediction of Flax fibre thermoplastic composites

Haggui Mondher * [1], El Mahi Abderrahim [1], Jendli Zouhaier * [2], Akrout Ali [3], Haddar Mohamed [3]

[1] Laboratoire d'Acoustique de l'Université du Maine (LAUM) – Laboratoire d'Acoustique de l'Université du Maine – Avenue Olivier Messiaen, 72085 Le Mans, France
[2] ESTACA'Lab (PôleMécanique des Matériaux Composites et Environnement) – ESTACA, ESTACA – PôleMécanique des Matériaux Composites et Environnement, Parc universitaire Laval-Changé Rue Georges Charpak -BP 76121 53061 Laval Cedex 9, France
[3] Laboratoire de Mécanique, Modélisation et Productique (LA2MP) – Ecole Nationale d'Ingénieurs de Sfax Sfax 3038, Tunisia

The aim of the present study is to highlight the fatigue properties of flax fibre composites as a potential alternative to synthetic fibres. The considered materials were manufactured by liquid infusion process and consist of thermoplastic Elium resin reinforced by flax fibre. Mechanical characterizations coupled with control techniques were conducted and the behaviors of the composites were discussed. First, static tests performed to determine the failure parameters and characteristics used in fatigue tests. Then, two configurations of materials, unidirectional and cross-ply laminates, were subjected to a cyclic tensile fatigue tests. In order to more understanding the response of complex phenomena exhibited by natural fibre structures subjected to fatigue loads, acoustic emission technique and microscopic analysis were used to identify and characterize the damage mechanisms. During cyclic tests, the stiffness degradation is evaluated and presented as effective mean that describe the state of the material. Moreover, some parameters, such as dissipated energy and loss factor, were evaluated to quantify the damage. The lifetime prediction of composite is represented by the mean of Wohler curve which show that the flax / Elium composite could be a promising solution for many industrial applications as well as synthetic fibres composites.

Keywords: Flax fibre, fatigue, acousticemission, damage.

*Speaker

S8: Failure of quasi-brittle materials

Discrete element simulation of concrete fracture under different loading velocities using polygonal elements

Birgit Beckmann *† [1], Manfred Curbach [1]

[1] Institute of Concrete Structures, TU Dresden (IMB, TU Dresden) – August-Bebel-Straße 30/30A, 01219 Dresden, Germany

Simulation of concrete fracture phenomena is presented in this work. Special focus is laid on the investigation of crack propagation under different loading velocities. As a matter of principle, the consideration of different loading velocities is an important, basic step in the context of impact modeling. A two-dimensional numerical simulation based on the discrete element method (DEM) is used for the analysis of concrete behaviour under compression load. Thereby, crack patterns, crack initiation and damage evolution are analysed. In the simulation, the cracks are discrete just as in real laboratory experiments. Cracks are the absence of concrete material. The cracks arise due to the interaction of the concrete particle elements and without the predefinition of any crack zones or crack elements. Regarding the particle shape, polygonal particles are chosen. One of the reasons for this choice is the generation of a dense particle ensemble. Another reason is the shape stability and, therefore, the optionality of cohesion modeling. This means, that cohesion and tensile forces between the particles can optionally be modeled, but need not necessarily to be modeled. Due to the polygonal particle shape, the simulation is limited to only two dimensions up to now, although the simulation is principally designed with three dimensions, of course. With regard to the calculation of the interaction forces of contacting particles, a convex shape of the particles is necessary. In order to consider both convex and concave specimen geometries, particles on a concave corner are divided into subparticles during particle generation. This is to preserve the convex shape of the particles themselves even in the case of concave geometries of the whole test specimen. The simulation results are compared to the ones of laboratory experiments. Damage accumulation is investigated. In the simulation, the same virtual concrete specimens are loaded with lower and with higher velocities. The crack patterns and the break loads of both loading cases are compared. As a result of the simulation it is shown that the ultimate load is higher and the concrete behaviour is more brittle for higher loading velocities than for lower loading velocities. It is the complex processes of failure mechanisms, crack propagation and damage evolution which are specifically investigated rather than to investigate the concrete behaviour within a range of safe working loads. The simulation results show that particle simulations and DEM simulations are a suitable and reasonable approach for the numerical investigation of concrete behaviour and crack propagation.

Keywords: concrete, discrete element simulation, crack evolution, fracture, damage accumulation, loading velocity

*Speaker
†Corresponding author:

A flexible 'two-surface' gradient-extended damage model for quasi-brittle and ductile materials

Tim Brepols* [1], Stephan Wulfinghoff [1], Stefanie Reese † [2]

[1] Institute of Applied Mechanics, RWTH Aachen University (IFAM) – Mies-van-der-Rohe-Strasse 1, D-52074 Aachen, Germany, Germany
[2] Institute of Applied Mechanics, RWTH Aachen University (IFAM) – Mies-van-der-Rohe-Strasse 1, D-52074 Aachen, Germany, Germany

Damage and fracture models are of utmost importance in computational mechanics since they allow for a convenient and adequate way of modeling failure processes taking place in materials and structures. In this regard, Continuum Damage Mechanics (CDM) has proven to be a suitable theoretical framework in which one or several damage variables are introduced in the mathematical formulation that account for damage effects in an averaged sense. Furthermore, it is nowadays commonly acknowledged to work with, e.g. 'nonlocal' or gradient-extended models which can counteract the well-known mesh dependence problem which otherwise occurs in finite element simulations involving conventional (i.e. 'local') CDM models. Even though a lot of progress has been made in the past decades with regard to the theoretical understanding of these models, there is still a pressing need for further research in this area, especially with regard to today's computing power that enables engineers to study their behavior under ever more realistic simulation conditions.

In this study, a generic 'two-surface' gradient-extended model is presented which is able to describe coupled damage-plasticity material behavior (Brepols et al. [2017]). The terminology 'two-surface' comes from the fact that the latter phenomena are treated as distinct dissipative mechanisms by taking into account independent damage and yield criteria as well as corresponding sets of loading/unloading conditions. This makes the model especially flexible and adaptable to various situations: the considered material's behavior can either be (quasi-)brittle-like, ductile-like or possibly anything in between. The model is thermodynamically motivated and fits into the general micromorphic framework as proposed by Forest [2009], the latter being an approach for unifying concepts among the various existing types of gradient extensions in the literature. Theoretical and numerical aspects of the model are discussed, as e.g. the constitutive characteristics or the algorithmic treatment of the model which requires special considerations due to the applied 'two-surface' methodology. Finally, the model's behavior and mesh regularization properties are assessed numerically in several structural benchmark simulations.

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Keywords: gradient extended damage, two surface model, micromorphic approach

*Corresponding author: tim.brepols@rwth-aachen.de
†Speaker

Damage modeling of concrete affected by the alkali-silica reaction in varying environmental conditions.

Martina Colombo [1], Claudia Comi *† [1]

[1] Department of Civil and Environmental Engineering, Politecnico di Milano – Piazza Leonardo da Vinci, 32 20133 Milano, Italy

The slow development of the alkali-silica reaction (ASR) in concrete structures built several decades ago can modify the stress state, can induce an increase in the displacements and a pattern of diffuse micro-cracks. These phenomena can compromise the structural safety and functioning, therefore their correct modelling is of paramount importance for strategic structures such as large dams.

The kinetics of the ASR strongly depends on the temperature and on the humidity evolutions, as described in [1-2]. In the present work, we discuss a phenomenological two-phase isotropic damage model for ASR induced degradation, accounting for the simultaneous effect of the temperature and humidity, [3]. In the frame of the Biot's theory of porous media, the material subject to alkali-silica reaction is described as a continuous medium consisting of two phases: the solid skeleton of concrete and the expansive products of the reaction.

The model is used for the analysis of an existing arch dam affected by ASR. A weakly coupled approach is followed: starting from real monitoring data, a preliminary heat diffusion analysis and moisture diffusion analysis allow computing the varying fields of temperature and humidity, which are the input of the subsequent chemo-damage analysis.

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Keywords: Concrete, damage, ASR, poromechanics

*Speaker
†Corresponding author: claudia.comi@polimi.it

Rapid crack propagation in pharmaceutical tablets

Benjamin Croquelois *† [1], Jean-Benoit Kopp [2], Jérémie Girardot [1], Pierre Tchoreloff [3], Vincent Mazel [1]

[1] Institut de Mécanique et d'Ingénierie de Bordeaux (I2M) – Institut polytechnique de Bordeaux, Arts et Métiers ParisTech, CNRS : UMR5295, Université de Bordeaux, Université de Bordeaux – Site ENSCBP Bât A 16 avenue Pey-Berland 33607 Pessac Cedex, France

[2] Institut de Mécanique et d'Ingénierie de Bordeaux (I2M) – Université de Bordeaux, Arts et Métiers ParisTech, Institut polytechnique de Bordeaux, Centre National de la Recherche Scientifique : UMR5295, Arts et Métiers Paris Tech – Site ENSCBP Bât A 16 avenue Pey-Berland 33607 Pessac Cedex, France

[3] Institut de Mécanique et d'Ingéniérie (I2M) – Université de Bordeaux (Bordeaux, France), CNRS : UMR5295, Bordeaux-INP, Arts et Métiers Paris Tech – UFR des Sciences Pharmaceutiques, 146 rue Léo Saignat, 33076 Bordeaux cedex, France

The tablet is the most common pharmaceutical form. As any pharmaceutical product, it must fulfill a number of requirements. Among them, the mechanical strength plays an important role. This property guaranties the integrity of the tablet from the ejection from the tablet press to the dispensation to the patient. Moreover, the mechanical strength is also linked with classical issues that arise during the manufacturing of tablets like capping, lamination or chipping. A good quantification of the mechanical behavior of a tablet is thus of great importance from an industrial perspective. The classical approach in the pharmaceutical field for the characterization of the mechanical strength of tablets is the use of fracture tests. The common practice is to use the diametral compression test (also known as Brazilian test) to calculate the tensile strength. This classical test, which is relatively easy to perform, presents nevertheless some defects with this kind of material. The introduction of flat ends on the compacts, for example, limits contact "problems" between the tablet and the platens and therefore ensures a crack initiation at the center of the specimen. As a pharmaceutical tablet is obtained from powder compression, the final material is a porous solid which intrinsically contains structural defects. These defects, which influence the fracture behavior, are also difficult to characterize. In order to evaluate their influence, defects larger in size than the defects intrinsically present in the material are introduced. These changes in the experimental test make it possible to limit as much as possible the influence of the structure in the material response. Rapid crack propagation was captured with the help of a high speed camera. Cracks initiate and propagate dynamically from the center to the pole of the specimen. First results seem to indicate a crack speed between 400 and 800 m.s-1 for one of the tested products. This makes it necessary to take into account inertial effects, which could affect the crack propagation, in the estimate of a material parameter. The fracture stress of the specimen is easily calculated from the results of the Brazilian Test. It is proposed here to estimate numerically the dynamic energy release rate which takes into account inertial effects. These effects vary especially as a function of the crack speed and the specimen geometry. Finally, as it is not possible to perfectly dissociate material from structure response with the diametral compression test, a more classical fracture test is proposed: the Disk-shaped Compact Tension Test (DCT). The Linear Elastic Fracture Mechanics formalism will be used to access a material parameter as the energy release rate or the stress intensity factor.

Keywords: dynamic fracture, Pharmaceutical tablet, Brazilian test, energy release rate

*Speaker

†Corresponding author: benjamin.croquelois@u-bordeaux.fr

Two-dimensional intergranular crack propagation in a mesh independent framework with explicit damage update

Zoltan Csati * [1], Thierry J. Massart [2], Nicolas Moës [3]

[1] École Centrale de Nantes (ECN) – Ministère de l'Enseignement Supérieur et de la Recherche Scientifique – 1 rue de la Noë - BP 92101 - 44321 Nantes cedex 3, France
[2] Université libre de Bruxelles (ULB) – Belgium
[3] GeM, École Centrale de Nantes – Ecole Centrale de Nantes – France

Modelling distributed microcracking in heterogeneous materials, like rocks is important in engineering applications. In crystalline rocks such as granite, experiments show that mechanical loading mainly induces the initiation and propagation of cracks along grain boundaries. Based on this assumption, a model able to incorporate all a-priori known potential crack path is aimed at. We use this assumption, i.e. all possible crack paths are supposed to be known from the beginning.

The generation of a conforming mesh for many configurations involving many grains (which can be concave, elongated and of different sizes) is challenging particularly in 3D. Therefore, the fictitious node method [1] is applied, an element technology enabling the straightforward representation of strong discontinuities within an element (and similar to the extended finite element method [2]). Overlapping meshes are used together with Lagrange multipliers that enforce the continuity of the displacement field until the material separates. The naive use of the Lagrange multiplier method on non-matching grids often leads to unstable formulations that fail to satisfy the LBB condition. The creation of a stable Lagrange multiplier space was performed for linear [3] and quadratic [4] triangular elements crossed by a single interface. This work provides a systematic approach for many interfaces possibly intersecting, using bilinear quadrangular elements. A robust and general method is created to handle the situation in which an interface is close to a node.

In quasi-brittle materials under scrutiny, the fracture process zone cannot be neglected, and an extrinsic cohesive zone method is therefore used. To avoid the use of a penalty stiffness before the cohesive zone opening initiates, we rely on a two-field formalism proposed in [5]. A modified Lagrangian formulation is introduced that modifies the cohesive law with a change of variable and the traction-separation law is recast by introducing an internal damage variable [6]. The dual of this variable represents the energy release rate, from which the evolution laws can be written. A cost-efficient explicit algorithm suggested in [6] is applied to update the damage field. This allows decoupling the solution of the mechanical problem from the damage update, resulting in a computationally efficient procedure. On the one hand, the value of the dual variable is directly determined from the modified Lagrange multipliers obtained from the solution procedure. On the other hand, the damage update only alters a small block matrix in the system, and therefore most matrices need to be assembled and factorized only once.

The robustness of using the mesh independent discretization along with the explicit damage algorithm is evaluated on different assembly of grains and various loading situations.

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Keywords: cohesive zone, Lagrange multiplier, crack, damage, quasibrittle, XFEM

Homogenizing the thermoelastic behavior of a microcracked polycrystal: correlated cracks and crystallographic orientations

Jean-Baptiste Gasnier [1], François Willot [1], Dominique Jeulin [1], Hervé Trumel *† [2], Maxime Biessy [2], Jacques Besson [3]

[1] MINES ParisTech, PSL – Research University, CMM – Centre for Mathematical Morphology – Ecole Nationale Supérieure des Mines de Paris – 35, rue St Honoré, F-77300 Fontainebleau, France
[2] Le Ripault – CEA, DAM – F-37260 Monts, France
[3] Mines ParisTech, PSL - Research University, Centre for Materials – Ecole Nationale Supérieure des Mines de Paris – 63-65 Rue Henri Auguste Desbruères, F-91100 Corbeil-Essonnes, France

This work deals with the homogenization of the thermoelastic properties of quasi-brittle materials, and more precisely those of polycrystals in the presence of microcrack populations. To the authors' knowledge, this problem has yet received no satisfying solution with self-consistent-like methods, and three-dimensional finite element full-field homogenization becomes hardly tractable in the case of thousands of microcracks.
Therefore, an attempt is made here to solve the problem with a Fourier-based full-field homogenization method, for arbitrary crystal symmetry and arbitrary (though reasonable) microcrack densities. This is done in the simplified context of macroscopic isotropy of the sound polycrystal and of the distribution of microcrack orientations. Such populations are presumed to be representative of the isotropic state of damage induced, for instance, by low temperature cooling. The method relies on a Voronoí or Johnson-Mehl-based description of the polycrystal, supplemented by populations of either inter- or transgranular microcracks, each one being described by a thin layer of void voxels. Therefore, only open microcracks are accounted for in the present work.

The ability of the Fourier methods to deal with microcracks is first assessed. The 2D plane strain case of a periodic array of parallel cracks embedded in a homogeneous matrix submitted to mode I loading is considered. The fields near the crack tip provided by the Fourier simulation compare well to the Williams asymptotic expression. On the one hand, local fields are slightly less accurate than those predicted by finite element computations of comparable resolution. This is attributed to the necessarily finite thickness of the crack in Fourier simulations. The latter are, on the other hand, much less demanding in terms of memory allocation.

The technique is then applied to a quasi-brittle energetic material, whose single crystals are triamino- trinitrobenzene (TATB), a strongly anisotropic organic triclinic crystal, As expected, the effective bulk and shear moduli decrease monotonically with increasing microcrack density, and a percolation threshold microcrack density is found in the intergranular case. For the case of planar transgranular microcracks, if no correlation between microcrack and crystallographic orientations is considered, then the effective thermal expansion coefficient varies only very slightly. Conversely, it is shown to vary strongly when microcrack orientations are aligned with crystallographic axes of the crystals, This is shown to be linked to the crystal elastic anisotropy, and the sign of the variations of the thermal expansion coefficient depends on the orientation of the crystallographic plane in which each microcrack is embedded.
Finally, the interest of performing full-field simulations involving several thousands of microcracks is highlighted by the study of local fields, which reveal so-called van Hove singularities in the probability distribution function

*Speaker
†Corresponding author: herve.trumel@cea.fr

of local strain components, induced by microcracks interaction. Those singularities are shown to be linked to the existence of weakly-loaded "dead" zones.

Keywords: polycrystal, microcracking, Fourier computational method, 3D full, field homogenization, thermoelasticity

Calibration for material mechanical parameters in PFC2D and the ability of PFC2D to model crack initiation and propagation for quasi-brittle material

Guixian Liu * [1], Georg Koval [1], Cyrille Chazallon [1]

[1] Laboratoire des sciences de língénieur, de línformatique et de límagerie (ICube) – Ecole Nationale du Génie de l'Eau et de l'Environnement de Strasbourg, université de Strasbourg, Institut National des Sciences Appliquées – 300 bd Sébastien Brant - BP 10413 - F-67412 Illkirch Cedex, France

Abstract: Wedge-splitting tests (WST) of asphalt concrete samples presenting a longitudinal interface are analyzed by discrete element modeling. Curves of opening force versus displacement provide information about the fracture energy during interfacial crack propagation. A parametric study is performed aiming at relating the influence of the properties of the different materials, interface adhesion, and interface thickness on WST results. A random packing structure of multi-dispersed disks is adopted to model the asphalt concrete and the interface material composed by an asphaltic emulsion. The elastic properties of both materials (i.e. Young's moduli and Poisson's ratios) are related to the contact (normal and tangential) stiffness by a calibration procedure based on simulations of tension tests. A cohesive contact model is adopted to describe the strength and the fracture energy at a local level. The contact forces are elastic inside a defined limit of displacement, which also defines contact strength. Once this limit is overpassed a softening behavior, described by an affine decrease of the force for increasing displacements is adopted, which defines a contact rupture energy. Despite the simplicity of the local contact model, a complex sample behavior is observed, which is consistent with experimental results. Thin interfaces with lower elasticity and lower strength, seems to dominate the sample global behavior where the asphalt concrete contributes only as a rigid substrate. In those cases, the sample elasticity is directly related to the stiffness of the interface. For a given local strength, the global fracture energy also seems to be linearly dependent on the contact rupture energy; although sample strength improvement presents a more complex dependence on fracture energy. A theoretical model is then proposed to explain completely the effect of thin soft interfaces on sample force-displacements response. For thicker soft interfaces, the crack propagation is also strongly dependent on the interface properties. Nevertheless the dependence on the thickness becomes negligible and the samples behave as a sample without any pre-existing interface. Stiffer interfaces tend to behave as zones composed by asphalt concrete, and similarly, the effect of the interface fades away. Hence, the general response of the analyzed wedge-splitting samples is located between two limit cases: thin-soft interface behavior and the absence of interface.

Keywords: Wedge, splitting test, asphalt concrete, interface, fracture, discrete element modeling, cohesive contact law

*Speaker

Combining bulk damage and cohesive zone models with the Thick Level Set approach to quasi-brittle fracture

Benoît Lé * [2,1], Nicolas Moës [1,2], Grégory Legrain [2,1]

[2] Research Institute of Civil Engineering and Mechanics (GeM) – Research Institute of Civil Engineering and Mechanics – 1 Rue de La Noe, 44321 Nantes, France
[1] Ecole Centrale de Nantes (ECN) – École Centrale de Nantes, Ecole Centrale de Nantes – 1 Rue de La Noe, 44321 Nantes, France

Damage and fracture mechanics are both widely used to study quasi-brittle failure, each one having its own strength and weakness. Some approaches allowing to couple the advantages of these two categories of models exist, most of them consisting in introducing a traction free or cohesive crack when the damage variable reaches a certain critical value. The main difficulty of these approaches is the proper way to introduce this crack (orientation, form of the cohesive traction/separation model, etc). In this presentation, the Thick Level Set (TLS) approach to fracture is used as a natural way to combine damage and cohesive zone models. The first version of the TLS (TLS V1) was originally introduced in [1,2] as a way to regularize damage models. Based on the use of a level set function, it allows to introduce a traction-free discontinuity when the material is fully damaged. In the TLS V2 framework, which is the object of this presentation, a cohesive crack is introduced prior to the full damage state of the material. Compared to the already existing approaches, it is made easier by the use of a unique level set function, which is used both to determine the crack location, and to drive the bulk and cohesive damage evolutions.

The TLS V2 makes up for most of the drawbacks of both damage and cohesive zone models. From the cohesive zone models point of view, diffuse damage brings the ability to initiate, branch and coalesce, as well as a natural propagation criterion. It also allows to take into account stress triaxiality, which is necessary to model splitting tests for instance. From the damage mechanic point of view, the use of level set functions makes easy the insertion of displacement discontinuities, and therefore to extract macro-cracks opening. Introducing a cohesive crack prior to the material being fully damaged (instead of a traction-free displacement jump) avoids infinite strains, and allows mesh coarsening for reduced computational costs. It can also be used to model complex interfacial behaviors like frictional contact, something which is not trivial with diffuse damage modeling.

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Keywords: Damage mechanics, Fracture Mechanics, Cohesive zone, Thick Level Set, X, FEM, Level Set

*Speaker

A new rate dependent damage model to simulate dynamic crack propagation in quasi-brittle materials

Prithvi Mandapalli *† [1], Lambertus Sluys *

[2], Jaap Weerheijm *

[3,4]

[1] Fluidyn-Consultancy&Software – India
[2] Delft University of Technology (TU Delft) – PO Box 5048,2600 GA Delft, The Netherlands, Netherlands
[3] TNO, Rijswijk – Netherlands
[4] Delft University of Technology – Netherlands

Concrete is a commonly used construction material and concrete structures have a high risk of being subjected to extraordinary events like explosions, earthquakes and high velocity impacts. Under these high loading rate situations concrete develops complex fracture and fragmentation patterns and therefore it becomes very important to develop numerical tools to faithfully predict the failure behavior and determine the residual load bearing capacity of concrete structures.
It is well known from experiments that concrete is a highly rate dependent material. Existence of many rate dependent concrete models suggests that the dynamic behavior of concrete is not completely understood, though the possible physical mechanisms responsible for rate dependency as indicated by experiments and numerical simulations can be attributed firstly to resistance of moisture in the capillary pores at low or moderate loading rates, secondly due to the effects of inertia at micro-level and diffusion of damage over a wider zone, at higher loading rates. Damage evolution is dependent on the processes taking place at various material length scales i.e. micro, meso and macro scales. Numerical simulation of concrete considering all the individual constituents would implicitly take into account the inertia at micro level, which is responsible for the micro crack growth retardation at high loading rates, ultimately leading to a strength increase observed at macro-level [1]. Therefore when concrete is modelled explicitly considering all its constituents, a rate independent material model can be used, but often modelling concrete at micro-meso level is computationally expensive. Alternatively a homogeneous macroscopic model can be developed with rate effects included in the constitutive material law to capture all the processes taking place at different length scales. Therefore the constitutive material law including the rate dependency is dependent on the length scale of the problem of interest. Macro-scopic inertia effects are implicitly accounted for by the equation of motion.

In the present work a new rate dependent damage model coupled with a non-local model is developed in order to study dynamic crack propagation and branching. The nonlocal strain is modified to take the micro-meso level structural inertia effects into account. To achieve this, nonlocal strain evolution is delayed by coupling it with a Duhamel type integral, thus introducing the dynamic delay concept commonly referred to as micro-inertia effects. The formulation is based on a similar concept presented in [2]. The model is tested for dynamic crack propagation and validated against experimental results. It is found that the model realistically describes the crack propagation and branching.

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*Speaker
†Corresponding author: prithvir.bv@gmail.com

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Keywords: Nonlocal model, Damage, Rate dependent, Dynamic crack propagation

Multi-cracking of brittle thin films on compliant elasto-plastic substrates

Guillaume Parry * [1], Ilhem Ben Cheikh [1], Rafael Estevez [1], Davy Dalmas [2]

[1] Science et Ingénierie des Matériaux et Procédés (SIMaP) – Université Grenoble Alpes – 1130 rue de la Piscine, BP 75 38402 Saint Martin DHères, France
[2] Laboratoire de Tribologie et Dynamique des Systèmes (LTDS) – Ecole Centrale de Lyon, Ecole Nationale des Travaux Publics de l'Etat, Ecole Nationale d'Ingénieurs de Saint Etienne, Centre National de la Recherche Scientifique : UMR5513 – 36 Avenue Guy de Collongue, 69134 Ecully Cedex, France

Thin films coatings are used in many high technology applications particularly in microelectronics devices. Using flexible polymers as a substrate on which thin films (metal, oxides or organic) are bonded can give rise to new industrial applications such as OLED, flexible electronics or flexible photovoltaics devices. The mechanical stability and failure behavior of multilayer structures deposited on flexible substrate has been extensively studied both experimentally and theoretically [1-3]. Several relaxation mechanisms in thin films have been identified such as channel cracks, debonding or buckle delamination.
The objective of this study is to understand the multi-cracking of zinc oxide layers of various thicknesses coated on elastoplastic substrates (ETFE). In the process of cracking many parameters have to be taken into account, such as the elastic modulus mismatch between the film and the substrate, the plasticity of the substrate and the ductile or brittle nature of the film.

In the literature several experimental and analytical studies can be found. In [4], after experimental investigations, the existence of three different fracture stages was confirmed, the third one being a saturation stage of the cracks density at high strain with large opening of the existing cracks. Considering a purely elastic substrate, as in Xia & Hutchinson model [3], does not lead to the correct saturation pattern. The "Shear lag" formalism [1,2] focuses its analysis on slip at the film/substrate interface to explain saturation, and does not allow to capture large cracks opening.

In order to further investigate the mechanisms leading to those experimental observations, we present a model that uses a cohesive zone strategy in order to simulate both the interface debonding and the cracking inside the film. This model also takes into account the plastic behavior of the substrate. The different stages of cracking observed experimentally, including the nucleation stage were simulated by finite element calculations. A relationship between the film toughness, the saturation stress level in the film and the saturation distance between the cracks under deformation is evidenced. We show that the mechanism responsible for saturation is actually involving plasticity in the substrate well below the interface.

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*Speaker

Keywords: modeling, thin films mechanics, finite elements method, cohesive zone models

Developing an interface model to investigate the damage and Fracture in Hard Nano-coating Layers

Shahed Rezaei *† [1], Stephan Wulfinghoff [1], Stefanie Reese [1]

[1] Institute of Applied Mechanics [Aachen] – Mies-van-der-Rohe-Str. 1D-52074 Aachen, Germany

Coating layers are usually applied on different manufacturing tools in, e.g., plastic extruder in order to increase their lifetime and to improve the surface properties of the final parts. New coating deposition techniques such as high-power impulse magnetron sputtering (HPPMS) can provide more parameters to control the coating mechanical properties, therefore they result in producing coating layers with better performance and perhaps higher damage resistance. In order to be able to compare the effect of different parameters on damage behaviour of the coatings, a cohesive zone (CZ) element model has been applied. The fracture modes are divided into an intergranular fracture inside the coating and delamination between the coating layer and the substrate. The developed numerical model allows predicting the damage initiation and propagation within various types of coating systems in different setups such as nanoindentation. Numerical studies of nanoindentation tests show that the intergranular cohesive tractions, residual stresses, elastic and plastic properties and the grain morphology of the coating layers are the most effective parameters in order to produce stronger coatings.

Keywords: interface model, damage, fracture, grain boundary sliding

*Speaker
†Corresponding author: shahed.rezaei@rwth-aachen.de

Estimating the stiffness and strength increase of a ceramic biomaterial due to bone regeneration by means of a micromechanical approach

Stefan Scheiner *† [1], Vladimir Komlev [2], Alexej Gurin [3], Christian Hellmich [1]

[1] Vienna University of Technology (TU Wien) – Austria
[2] Russian Academy of Sciences – Russia
[3] Central Scientific Research Institute of Dentistry and Maxillofacial Surgery – Russia

Bone replacement materials must fulfill various requirements, such as biocompatibility and appropriate mechanical properties. In particular, the latter include suitable stiffness and sufficient strength. Finding biomaterials with adequate mechanical properties based on experimental trial-and-error approaches is cumbersome and ineffective, thus mathematical modeling is considered a promising complement. Here, a hydroxyapatite-based, granular biomaterial, developed as bone replacement material with the human mandible as targeted application region, is studied. This material exhibits a distinctive hierarchical organization, with different types of pore spaces of characteristic lengths ranging from nanometers to millimeters. Additionally, once exposed to the targeted physiological environment (i.e. the immediate vicinity of mandibular bone tissue), new bone tissue forms around the biomaterials granules, whereas the hydroxyapatite crystals undergo resorption. The presented work aims at estimation of both stiffness and strength of this material, taking into account the compositional changes due to bone ingrowth and hydroxyapatite resorption. For this purpose, micromechanical homogenization techniques are employed, yielding a three-step stiffness homogenization scheme, giving access to the macroscopic stiffness tensor of the scaffold material. On the other hand, the micromechanical model also takes into account quasi-brittle failure of the hydroxyapatite needles, based on which the loading type-specific macroscopic strength of the scaffold material can be deduced. The above-sketched micromechanical model gives access to stiffness and strength estimates for the scaffold material, as functions of various material and design parameters of the material, including the macro-porosity, the granule size, the density of cracks, as well as the rates of bone formation and scaffold resorption. The presented modelling approach provides insights beneficial both for the scaffold material design process and for a clinician actually applying such material. Namely, the aforementioned material and design parameters could be tuned based on model predictions, to optimize the mechanical properties of the scaffold material. Complementing this way the experimental trial-and-error strategy that, in this respect, still is the gold standard, would lead to a significant improvement of the design process.

Keywords: Micromechanics, Biomaterials, Homogenization, Predictive design

*Speaker
†Corresponding author: stefan.scheiner@tuwien.ac.at

Cohesive stress heterogeneities and the transition from intrinsic ductility to brittleness

Döme Tanguy * [1]

[1] Institut Lumière Matière (iLM) – Université Claude Bernard - Lyon I – Bâtiment Léon Brillouin - étage 2- 6 rue Ada Byron 69622 Villeurbanne cedex France, France

Nanoscale cavities may be involved in the cracking of metals, in a wide range of conditions, such as: fatigue, hydrogen embrittlement and irradiation damage. We present a study, based on atomistic simulations, of their impact on the fracture of grain boundaries. The crack crystallography is chosen such that dislocation emission is easy. Increasing the grain boundary coverage leads to a transition from a ductile behavior of the tip to a brittle one, in good agreement with recent experiments from the literature. Even at the highest coverage, the character of the crack is highly sensitive to the initial position of the tip with respect to the smallest cavities. The transition is not sharp. This complexity cannot be accounted for by the usual criterion based on the drop of the work of separation with the amount of damage in the structure (Rice and Thomson criterion). Instead, it is shown that a cohesive zone model, with parameters extracted from the simulations and enriched with a criterion for plasticity, can describe the transition. It emphasizes the role of cohesive stress heterogeneities along the interface and rationalizes the complexity found in the simulations. A parametric study determined the characteristics of the heterogeneity which constitutes an obstacle to brittle crack propagation. These could be guidelines to designing interfaces more resistant to solute embrittlement, in general.

Keywords: Fracture, Embrittlement, Grain boundaries, Atomistic simulations

*Speaker

Stress-based gradient-enhanced damage models with vanishing length scale

Bram Vandoren *† [1], Angelo Simone [2,3]

[1] Hasselt University, Faculty of Engineering Technology (UHasselt) – Martelarenlaan 42, 3500 Hasselt, Belgium
[2] Delft University of Technology, Faculty of Civil Engineering and Geosciences (TU Delft) – PO Box 5048, 2600 GA Delft, Netherlands
[3] University of Padova, Department of Industrial Engineering – Via Venezia, 1, 35131 Padova PD, Italy

While gradient-enhanced damage models show excellent regularization properties for avoiding mesh-dependency in strain localization, it is known that these models suffer from spurious spreading of damage and unphysical damage initiation [1,2]. To overcome these issues, we propose a class of anisotropic stress-based gradient-enhanced damage models in which the gradient activity vanishes when damage increases.
The first model is based on principal stresses and is directly inspired by the stress-based integral nonlocal model by Giry, Dufour and Mazars [3]. It will be shown that this model does not perform well in case of shear-dominated failure problems, leading to tortuous force-displacement curves caused by a mismatch between the evolving level of gradient activity and damage: nonlocal interactions are cancelled too soon with respect to damage. The second model solves this problem by employing a nonlocal equivalent stress-based gradient parameter, which is linked to the measure of the equivalent strain that drives damage evolution. Nonlocal averaging is thus more at pace with the evolving level of damage, similar to the recently proposed model by Poh and Sun [4] in which a damage-based parameter is used inspired by micromorphics.

It will be shown that both models lead to a correct location of damage initiation and significantly reduce the spreading issue. However, the models suffer from unphysical strain oscillations caused by a gradient parameter that becomes too small with respect to the mesh size, reintroducing some degree of mesh-dependency. It will be demonstrated that these oscillations can be cancelled by using an element-specific lower bound value of the gradient parameter. The performance of the proposed models is evaluated by means of shear and bending tests.

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Keywords: gradient enhanced damage, anisotropic damage, evolving length scale

*Speaker
†Corresponding author: bram.vandoren@uhasselt.be

Limitations of the delay damage model and the need for spatial regularization

Jihed Zghal *† [1,2], Nicolas Moës‡ [1,2]

[1] École Centrale de Nantes – École Centrale de Nantes – 1 rue de la Noë, 44321 Nantes cedex 3 - France, France
[2] GeM Institute, UMR CNRS 6183 – GeM Institute, UMR CNRS 6183 – 1 rue de la Noë 44321 Nantes cedex 3 - France, France

One of the major problems of damage simulation is the mesh dependency and the artificial localization. In statics to avoid these problems, non local models or a second-gradient theories are used. However, these are not suited for dynamic problems because they require a significant modification in standard software leading to a high computational cost [Suffis et al., 2007]. As a solution to simulate damage in dynamics problems, a delayed damage model was introduced by [Ladeveze, 1992]. The main idea of this model is to complement a traditional damage model with an equation which controls the damage rate.
Through this work, we want to investigate the limitation of delay damage model in dynamics. For this purpose, we simulate the failure of a bar submitted to pulses. Damage and dissipated energy evolution are analysed for different pulse intensity. The mesh dependency is also pointed-out. We simulate also the failure of of a guitar string initially at rest. We consider a 1D bar submitted to a quasi-static load on which we introduce a small damage perturbation, discharging wave appears and system goes into dynamics. Damage, dissipated energy and mesh dependency are also investigated.
The results show the limitations of the delay damage model and point-out mesh dependency. One of the proposed solution is the use of a spatial regularization in order to avoid these problems. Additional simulation using Thick Level Set approch (TLS) and coupling betwwen TLS and delay damage model are performed. A Comparaison between the different approach is made.

Keywords: Delay damage model, Thick Level Set approch (TLS), Dynamics

*Speaker
†Corresponding author: jihed.zghal@ec-nantes.fr
‡Corresponding author: nicolas.moes@ec-nantes.fr

S9: Functional and architectured materials

Finite deformation of fibre-reinforced magneto-elastic rods

Jacopo Ciambella * [1], Antonino Favata [1], Giuseppe Tomassetti [2]

[1] Department of Structural and Geotechnical Engineering - SAPIENZA University of Rome – Via Eudossiana 18, 00184 Rome, Italy, Italy
[2] Engineering Department - Rome Tre University – Rome, Italy, Italy

Magneto-Rheological Elastomers (MREs) are a class of functional materials whose mechanical properties can be controlled upon the application of an external magnetic field by dispersing into a non-magnetic soft matrix, magnetic hard particles. The use of magnetic field to achieve actuation is advantageous over other type of actuation as it offers remote and contactless control and it does not produce any polarization of the media nor chemical alteration. Several type of magnetic particles are nowadays commercially available including ferromagnetic, paramagnetic or diamagnetic fillers. Owing to such a large availability of filler types and shapes, MREs provide a much larger design space compared to other type of soft actuators but yet require models able to account for all these features. Upon final cure, the rigid particles are locked in place into the elastomeric matrix, and the composite possess a high degree of flexibility combined with tunable stiffness that makes it capable of bearing large deformations. Moreover, if a magnetic field is applied during the elastomer cross-linking process, the induced magnetization of the spherical particles make them orient along the field lines in a chain-like structure which in turn makes the cured composite transversally isotropic. Therefore, proper models need to be formulated in the framework of large strain transversally isotropic elasticity coupled with magneto-statics.
In this contribution, we present a derivation from the consistent theoretical framework of 3D magneto-elasticity of the governing equations for the finite motion of a magneto-elastic rod reinforced with spherical or ellipsoidal inclusions. The particles are assumed weakly and uniformly magnetised and therefore the potential energy of the system is additively decomposed into a purely mechanical term plus a part accounting for the interaction between the deformation and the applied field. The particles are further assumed rigid and firmly embedded into the elastomeric matrix, this in turn makes the demagnetization tensor dependent only on the current orientation of the particles and not on their stretch. These simplifying assumptions made possible to derive a closed form expression in terms of the external magnetic field of the (body) forces and distributed couples that act on the rod. Finally, we show that the motion of a planar rod is governed by the classical elastica equation with forcing terms controlled by the applied mangetic field, which we call the *magneto-elastica* equation.

Keywords: magnetic rods, elastica, instability, soft, actuators

*Speaker

Mechanical Behavior of Ni-Ti Shape Memory Alloy Honeycombs Obtained by Investment Casting

Carlos Jose De Araujo * [1], Jackson Simões [2], Paulo Sales Da Silva [1], Denis Favier [3]

[1] Universidade Federal de Campina Grande (UFCG) – Brazil
[2] Universidade Federal Rural Semi-Árido (UFERSA) – Brazil
[3] Techniques de l'Ingénierie Médicale et de la Complexité - Informatique, Mathématiques et Applications, Grenoble (TIMC-IMAG) – CNRS : UMR5525, Université Joseph Fourier - Grenoble I – Domaine de la Merci - 38706 La Tronche, France

In this work, two types of honeycombs were fabricated from a Ni-Ti shape memory alloy (SMA) using centrifugal casting and models printed in ABS plastic. After obtaining honeycombs with hexagonal and circular cells, these architectured smart structures were analyzed by differential scanning calorimetry (DSC), confirming the presence of the characteristic martensitic phase transformation of SMA. These structures were mechanically tested at room temperature (about 25 ∘C) by cyclic compression tests up to 6% maximum deformation, in steps of 1% deformation. For these levels of deformation, the forces imposed varied between 400 N and 1400 N, with honeycombs of circular cell those that require greater force for deformation. The experimental analysis of the superelastic mechanical behavior of the Ni-Ti SMA honeycombs was complemented by a numerical analysis using the finite element method with ANSYS 16.0 software, which showed a good agreement with the experimental results.

Keywords: Shape memory alloys, Ni, Ti alloys, Architectured materials, Honeycombs, Mechanical behavior

*Speaker

Elastic Wave Propagation in Finitely Deformed Laminates

Pavel Galich * [1], Stephan Rudykh [1]

[1] Faculty of Aerospace Engineering, Technion – Israel Institute of Technology – Israel

Finite deformations can significantly transform elastic wave characteristics even in the relatively simple initially isotropic materials. Therefore, elastic wave propagation in soft laminates can be manipulated by deformation. Note that layered structures are observed in soft biological tissues, which frequently experience large deformations due to various physiological processes, e.g., growth or recovery. Hence, investigation of elastic wave propagation in finitely deformed laminates can be beneficial for biomedical applications such as ultrasound testing.
In this work, we focus on propagation of small amplitude shear and pressure waves in finitely deformed laminates with isotropic elastic phases. By employing a micromechanics based approach and Bloch-Floquet approach, we investigate influence of deformation induced changes in geometry and physical properties of the layers on the elastic wave propagation and band gaps, in particular. Thus, in laminates with relatively simple compressible neo-Hookean phases shear wave band gaps (SBGs) are independent of deformation, because deformation induced changes in geometry and physical properties of the phases completely compensate each other. However, SBGs are tunable by deformation in laminates with highly nonlinear phases, e. g., Gent and Arruda-Boyce. This is because deformation induced changes in geometry do not fully compensate corresponding changes in the physical properties of the phases anymore. Remarkably, pressure wave band gaps (PBGs) significantly depend on deformation even in the laminates with neo-Hookean phases. Hence, complete BGs – frequency ranges where neither shear nor pressure waves can propagate – are tunable by deformation regardless of the laminate composition.

Keywords: elastic waves, laminates, finite deformations, band gaps

*Speaker

Magnetomechanical macroscopic instabilities in magnetorheological elastomer composites with periodic microstructures

Artemii Goshkoderia * [1], Stephan Rudykh [2]

[1] Aerospace Engineering, Israel Institute of Technology (Technion) – Haifa, Technion city,3200003, Israel
[2] Technion – Israel

We study magnetomechanical macroscopic instabilities in magnetorheological elastomer (MRE) composites undergoing finite strains in the presence of a magnetic field [1, 2]. In particular, we consider MRE composites with circular and elliptical inclusions embedded in a soft matrix. We analyze the influence of the applied magnetic field and finite strains, as well as the microstructure geometrical parameters and material properties, on the stability of the MRE composites. We implement the stability analysis (see, for example, [3] for mathematically analogous dielectric elastomer composites) into a numerical finite element based tool, and through the numerical evaluation of the tensors of magnetoelastic moduli, the unstable domains were identified.
We present numerical algorithm of identification of critical condition of macroscopic magnetomechanical instabilities in periodic incompressible composites [4]. In order to determine the onset of magnetomechanical instabilities, we utilize the general macroscopic stability condition [3, 5]. We show that MRE stability can be tailored (increased or even decreased) by applying proper magnetic field or by changing geometrical parameters of the inclusions while keeping the volume fractions.

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Keywords: Magnetorheological elastomers, Stability, Composites, Finite Deformation, Microstructure

*Speaker

An analytical and a micro-sphere based electroelastic model of dielectric elastomers resulting from molecular chain statistics

Mikhail Itskov * [1], Vu Ngoc Khiêm [1], Sugeng Waluyo [1]

[1] Department of Continuum Mechanics, RWTH Aachen University (KM RWTH) – Kackertstr.9 52072 Aachen, Germany

Mechanical response of dielectric elastomers can be influenced or even controlled by an imposed electric filed. It can, for example, cause mechanical stress or strain without any applied load. The latter phenomenon is referred to as electrostriction. There are many phenomenological hyperelastic models describing this electro-active response of dielectric elastomers. There, coupled electro-elastic terms are of special importance. So far, these terms have not got any physical reasoning. In the simplest case, the electric potential is represented by a quadratic function of an electric variable such as electric field, displacement or polarization. Some polyconvex electroelastic strain energies have also been proposed. In this contribution, we propose an electro-mechanical constitutive model based on molecular chain statistics. The model considers polarization of single polymer chain segments and takes into account their directional distribution. The latter one results from the non-Gaussian chain statistics taking finite extensibility of polymer chains into account. The so resulting (one-dimensional) electric potential of a single polymer chain is further generalized to the (three-dimensional) network potential. To this end, we apply directional averaging on the basis of the numerical integration over the unit sphere. A numerical algorithm with 45 points on a half-sphere has been utilized. In a comparative study it was shown that this cubature provides the best compromise between the amount of anisotropy artificially induced by the integration and computational efforts. In a special case of the eight-chain (Arruda-Boyce) model the directional averaging is obtained analytically. It results in an analytical invariant-based electroelastic constitutive model of dielectric elastomers. The proposed model is able to predict not only the above mentioned electro-active response and electrostriction but also electroelastic instability (so called pull-in instability) observed in experiments on thin dielectric films. The model includes a few number of physically interpretable material constants and demonstrates good agreement with experimental data.

Keywords: electroelasticity, dielectric elastomers, electrostriction, full network model, eight, chain model, pull, in instability

*Speaker

Multiscale homogenization of strain-induced nonlinear magneto-electric coupling

Matthias Labusch * [1], Jörg Schröder * † [1]

[1] University Duisburg-Essen – Germany

Multiferroic materials combine two or more ferroic characteristics and can exhibit an interaction between electric and magnetic fields. This magneto-electric (ME) coupling can find applications in sensor technology or in magneto-electric data storage devices [1]. Since most ME single-phase materials show such a coupling far below room temperature the manufacturing of two-phase composites, consisting of a ferroelectric matrix with magnetostrictive inclusions, becomes important. Due to the interaction of both constituents the composites generate a strain-induced ME coupling at room temperature, where we distinguish between the direct and converse ME effect. The direct effect characterizes magnetically induced polarization, where an applied magnetic field yields a deformation of the magnetostrictive phase, which is transferred to the ferroelectric phase. Due to the electro-mechanical properties of the matrix material the composite exhibit a change in polarization. On the other hand, the inverse ME effect characterizes electrically induced magnetization. The ME coupling significantly depends on the microscopic morphology and the ferroic properties of the individual constituents. In order to take both aspects into account, a finite element (FE^2) homogenization approach is performed, which combines via a scale bridging the macro- and microscopic level [2]. Thereby, the microscopic morphology is characterized be representative volume elements and the ferroic properties of the phases are described by suitable material models. The typical ferroelectric hysteresis curves are modeled by considering the switching behavior of the spontaneous polarizations of barium titanate unit cells [3], whereas the magnetic hysteresis loops are described by a Preisach operator [4].

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Keywords: homogenization, magneto, electric, composites, nonlinear, coupling

*Speaker

†Corresponding author: j.schroeder@uni-due.de

Multiferroic nanocomposites: Comparison of experimental data and FEM simulation

Veronica Lemke * [1], Matthias Labusch [1], Jörg Schröder [1], Heiko Wende [1]

[1] University Duisburg-Essen – Germany

By combining ferroelectric and ferromagnetic materials into multiferroic composites, the possibilities regarding technical sensors and data storage devices are enlarged [1]. This is due to the property of these magneto-electric (ME) materials to convert a physical ferroic quantity into another i.e. an applied magnetic field changes the electric polarization of the ferroelectric part of the composite. Magneto-electric single-phase materials also exist in nature, but since their synergy between polarization and magnetization is only active at very low temperature, these materials are not convenient in most of the technical applications.
Therefore, ME composites are a good alternative considering that they yield a strain-induced magneto-electric product property at room temperature [2]. Two different effects can be distinguished in ME composites, the direct and the converse ME effect.
For the first one, the magnetically induced polarization, a magnetic field is applied which than generates a deformation in the ferromagnetic phase. The deformation is transferred to the second phase and evokes a polarization in this ferroelectric material.
The second observed effect, which characterized the reaction vice versa, describes an electrically caused magnetization.
In this contribution, our focus is on a (1-3) composite which is based on the experiments described in [3] and [4]. The experiments investigate cobalt ferrite nanopillars which where embedded in a barium titanate matrix. For the numerical FEM-simulation, we take the material coefficients from [5] and [6], and we compute the changes of the strain-induced in-plane polarizations of the ferroelectric matrix around one cobalt ferrite nanopillar. Then, we compare these results with the experimental measurement outcomes. Furthermore, we take a closer look on the magneto-electric coupling coefficient.

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Keywords: Nanocomposites, Multiferroic

Role of mineral bridges in staggered bio-inspired composites

Aman Mahar *† [1], Siladitya Pal * ‡ [2]

[1] Aman Mahar – Multi-scale Mechanics and Multi-physics lab, Mechanical and Industrial Engineering Department, IIT Roorkee, India
[2] Siladitya Pal – Multi-scale Mechanics and Multi-physics lab, Mechanical and Industrial Engineering Department, IIT Roorkee, India

Natural exoskeleton, such as Nacre (mother of pearl), bone, and teeth boast a prominent amalgamation of mechanical facets such as stiffness, strength and toughness. Merger of these properties in engineering materials is still a challenge. Nacre, which is an inner shell layer of many sea-shells, primarily made of 95% of brittle mineral (calcium carbonate), however; it exhibits superior mechanical properties as compared to their major constituents. Micro-structure of nacreous layer reveals the staggered 'brick-bridge-mortar' architecture in which polygonally shaped mineral tablets are stacked. Presence of organic layer and mineral bridges act as a glue and interconnection between platelets, respectively. Imitations of the architecture of these high-performing biological hybrid materials have captured the attention of research community. Bio-inspired high-performance composites require in-depth knowledge of the structure-properties-function relationship. Therefore the goal of the present study is to provide a detailed understanding of the role of mineral bridges along with various geometric parameters towards the origin of extraordinary properties. In this work, we will investigate the mechanical behaviour of staggered architecture using finite element framework under quasi-static loading condition. The fracture of the staggered composite will be simulated using a combination of continuum and discrete cohesive zone models accounting the failure of interlayers and mineral bridges, respectively. In this study, we will provide a parametric understanding of geometrical features such as overlap ratio, aspect ratio, bridge density and bridge distribution on emergent stiffness, strength and toughness. Finally, detail design map will be constructed that will assist to develop novel architectured composites with desired mechanical properties.

Keywords: cohesive zone modeling, architectured composite, mineral bridges

*Speaker
†Corresponding author: amanmahar135@gmail.com
‡Corresponding author: spal.fme@iitr.ac.in

Mechanical behavior of steel scaffolds made by selective laser melting

Jean-Marc Olive *† [1,2], Andrzej Zielenski [3], Jean-Pierre Lariviere [1], Tomek Semarak [3], Michel Mesnard [4], Fabienne Jordana [5]

[1] Institut de Mécanique et d'Ingénierie de Bordeaux (I2M) – CNRS : UMR5295 – I2M - Site : Université Bordeaux 1 Bât A4 RDC 351 cours de la Libération 33405 TALENCE Cedex, France
[2] Centre National de la Recherche Scientifique - CNRS – Centre National de la Recherche Scientifique - CNRS – France
[3] Gdansk University of Technology – Poland
[4] Université de Bordeaux – Bordeuax – CNRS UMR 5295, France, France
[5] University of Nantes – Université de Nantes, CHU de Nantes, INSERM U1229, Université de Nantes – UFR d'Odontologie, 1 Place Alexis Ricordeau, BP 84215, 44042 Nantes cedex 1, France

A mechanical analysis of different architectures of scaffolds processed by selective laser melting (SLM) of 316L stainless steel powder is proposed. Experimental compression tests of scaffolds obtained with different SLM parameters are compared with FEM computations. Identification of the mechanical behavior law parameters of the constitutive material of the scaffolds is made. It is shown that for non post heat treated scaffolds, the identified parameters on a specific architecture are not transferable to predict the compression behavior of an other architecture.

Keywords: Scaffolds, stainless steel, selective laser melting, mechanical behavior

*Speaker
†Corresponding author: jean-marc.olive@u-bordeaux.fr

Instabilities in the deformation of magnetoelastic membranes

Narravula Harshavardhan Reddy [1], Prashant Saxena [*†1]

[1] Department of Mechanical and Aerospace Engineering, Indian Institute of Technology Hyderabad – India

We study the inflation of magnetoelastic membranes in the presence of an externally applied magnetic field. Two geometries – cylindrical and toroidal – are studied using a variational formulation based on magnetization [1] and under the assumption of a weakly magnetized material [2]. We observe that the traditional elastic limit point in the inflation of membrane can be altered by the magnetic field. For a given pressure and magnetic field, multiple stable equilibrium configurations can be achieved. Magnetic limit point, a phenomenon first introduced by Barham et al. [2], refers to the state corresponding to a loss of equilibrium solution. This observation is reconfirmed both for a toroidal and cylindrical membrane in our study [3,4]. Furthermore, we also make some predictions about the onset of wrinkling instability and its dependence on the externally applied magnetic field by using the concept of a relaxed energy density.

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Keywords: magnetoelasticity, membrane, limit point, instability analysis

*Speaker
†Corresponding author: prashant_saxena@iith.ac.in

Onset of Macroscopic Instability in Dielectric Elastomer Composites with particulate microstructures

Stephan Rudykh * [1], Artemii Goshkoderia [2]

[1] Aerospace Engineering, Technion - Israel Institute of Technology (Technion) – Israel
[2] Aerospace Engineering, Israel Institute of Technology (Technion) – Haifa, Technion city,3200003, Israel

Dielectric elastomers (DE) are a class of electroactive soft material that can develop large deformations in response to electric excitations. Potential applications of DEs include actuators and sensors, energy harvesting devices, and soft robotics. These materials, however, require high electric field to be actuated, thus, limiting the development of the DE based technologies. Recently, the usage of microstructured composite materials has been explored to enhance the electromechanical performance of soft DE composites. Moreover, the microstructured DE composites have the potential for tunable phonic crystals and elastic wave manipulation by electric field [1]. Here, we examine the electromechanically coupled behavior of microstructured dialectic elastomers (DE) subjected to finite strains and external electrostatic stimuli. In particular, DE composites with circular and elliptical inclusions embedded in soft matrix are studied. We analyze the role of the material properties, and geometrical parameters, and applied electromechanical loadings on the effective properties of the DE composites. We specifically focus on the instability phenomenon in the DE composites with periodically distributed circular and elliptical particles embedded in soft matrix. The corresponding unit cells are constructed and analyzed by means of a finite element code [2]. The applied electromechanical loadings are imposed in terms of periodic boundary conditions. To determine the onset of electromechanical instabilities, a general stability condition is utilized. We identify the unstable domains in terms of material and microstructure parameters and electromechanical loading [2].

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Keywords: dielectric elastomers, DE, instabilities, microstrutures, electroactive materials

*Speaker

Modeling of Auxetic Metamaterials Based on Micro-Dilatation Theory of Elasticity

Yury Solyaev *† [1], Sergey Lurie [1], Anastasia Ustenko [1]

[1] Institute of Applied Mechanics of Russian Academy of Science (IAM RAS) – Leningradsky ave., 7, Moscow, Russia

Metamaterials with re-entrant type lattice structure with cubic symmetry are studied. We show that the continuum micro-dilatation theory (theory of elastic materials with voids) [1, 2] generalized to the case of media with cubic symmetry can adequately describe the effective properties of a wide class of considered lattice structures as continuum media. Identification of the micro-dilatational elastic constants for the cellular metamaterials with negative Poisson's ratio is carried out. Methods for identifying the parameters of the micro-dilatation theory of media through the structural and rigidity parameters of lattice structures are developed.It is shown that material constants of the micro-dilatation theory can be directly linked with the geometrical and elastic parameters of the unit cell of the metamaterial. In particular, "void stiffness" modulus and voids diffusion parameter depend linearly on the stiffness of re-entrant structures in the unit cells and coupling modulus depends significantly only on the geometry of the unit cell. This result is obtained using micro-dilatational analytical solution of the homogeneous elasticity problem and FE modeling of the uniaxial tension, hydrostatic compression and simple shear of the beam lattice metamaterial models [3]. The problem of non-homogeneous uniaxial deformation of the rod and the problem of the pure bending of the beam were used to determine the voids diffusion parameter. It is shown, in particular, that the coupled and scale effects are equivalent for the studied continuum and lattice models of the metamaterials in the considered range of parameters. Developed approach is also extended for the refined prediction of the metamaterial strength in the frame of continuum modeling using found relation between the micro-dilatation function in continuum model and the stress state of the metamaterial unit cells.

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Keywords: microdilatation theory of elasticity, cellular metamaterial, auxetics, lattice structure, continuum modeling, strength

*Speaker

†Corresponding author: yos@iam.ras.ru

Molecular dynamics simulations of surface welding and shape memory behaviors of Diels-Alder networks

Hua Yang * [1]

[1] China University of Mining and Technology, Beijing (CUMTB) – Xueyuan Road Ding No. 11, Haidian District, Beijing, China

As a notable example of the recently emerged covalent adaptable network (CAN) polymers, Diels-Alder (DA) networks could depolymerize at high temperature through the reversible DA reactions, which bestows interesting behaviors of thermosetting polymers, such as malleability, surface welding behavior, and recyclability. Recently, there are increasing research interests in combining CANs with shape memory polymers (SMPs) to enable the next generation reprogrammable and recyclable actuation materials. However, our macromolecular-level understanding of DA networks that are intended for SMP applications is still limited. In this work, we established a molecular dynamics method to investigate the surface welding and shape memory behaviors of DA networks. The mechanical properties of fresh and fully welded networks are examined by uniaxial tension measurements. The results indicate that with sufficient welding time, the welded networks can fully recover the mechanical properties as those of fresh network. The glass transition temperature of welded network with varying weight fractions of epoxy monomers are studied, and the simulation results agree well with experiment results. In addition, the shape fixity and recovery simulations reveal ideal shape memory property of the DA networks. Parametric studies revealed that with a decreased end-to-end distance of polymer chains, the DA networks exhibit higher flexibility, which significantly influences their mechanical and shape memory properties.

Keywords: Diels Alder reaction, shape memory effect, surface welding, covalent adaptable network polymers, molecular dynamics simulation

*Speaker

Kirigami based mechanical metamaterials

Jie Yin *† [1]

[1] Temple University – Department of Mechanical Engineering, Philadelphia, PA 19122, United States

Mechanical metamaterials are artificial materials, which are becoming the emerging frontier in scientific research and engineering innovation due to their unprecedented physical properties, such as negative acoustic indices, negative Poisson's ratio, and vanishing shear modulus, arising from the innovative geometrical design of their unit cells. When in response to stimuli, metamaterials can be reconfigured beyond their original design by reversibly changing the size, shape, and symmetry. Reconfigurable metamaterial offers an enhanced flexibility in performance due to its coupled dynamically changing structural configuration with tunable properties. It synergistically integrates mechanics, geometry, design, properties and functionality, which is of tremendous interest in design of flexible electronics, actuators, sensors, and photonic devices.

In this talk, we will discuss our recent studies in kirigami-based mechanical metamaterials with a focus on their mechanics, geometry, and potential applications. *Kirigami* ("*kiri*" means cut) is a close cousin of Japanese paper art *origami* combining both folds and cuts. *kirigami*-based metamaterial is generated by applying cuts or folds to a rigid 2-D thin sheet and stretchable/shearable thin sheet considering real material properties. Cuts divide the original continuous thin sheet into a discretely connected units-based structure through hinges, *i.e.* the uncut marginal parts. Depending on the types of cuts, the deformation of the structure is achieved either through rotation of units, without deforming the unit itself and thus units are acting as being rigid, or through the out-of-plane buckling to largely mitigate the stress to the cut hinges to realize high stretchability.

We will discuss two examples of kirigami metamaterials. One is the simplest kirigami metamaterials constructed by introducing one-dimensional (1-D) parallel line cuts to a thin sheet to generate an extremely stretchable and dynamically tunable structure. We shows that the tilting orientation of the 1D kirigami structure can be manipulated in a controlled fashion from homogeneous to heterogeneous and patterned distribution of the tilting orientations in each cut unit in both contact-based mechanical way and remote thermal actuation. The mechanics on the buckling of the 1-D kirigami structures is revealed and its potential application for kirigami-based building envelope for energy saving will be discussed. The second example is the hierarchical kirigami metamaterials constructed by introducing hierarchical two-dimensional (2-D) orthogonal cuts to a thin sheet. We demonstrate that the hierarchical cut concept can be used to design of ultra-soft materials with tailorable and nonlinear mechanical properties. The uniaxial stress–strain behavior of hierarchical metamaterials exhibits highly nonlinear and strain hardening material characteristics, as well as tunable auxetic mechanical response, which we show is the result from the deformation transition from bending-dominated to stretching-dominated deformation. However, severe stress concentration is found in the local region of the hinges, especially at the level 1, contributing to the ultimate structural failure. Through rational design of the local cut shape and global hierarchical hinge structures, we show enhanced extreme expandability and high tensile strength in both hyperelastic and brittle materials.

Keywords: mechanical metamaterial, kirigami, buckling, functional kirigami

*Speaker
†Corresponding author: jieyin@temple.edu

A Simple Higher Order Shear Deformation Theory to Study a Dynamic Behavior of Functionally Graded Plates

Zaoui Fatima Zohra * [1], Tounsi Abdelouahed [2], Ouinas Djamel [1]

[1] Laboratoire de Modélisation Numérique et Expérimentale des Phénomènes Mécaniques (LMNEPM) – université Abdelhamid Ibn Badis, Mostaganem, 27000, Algeria
[2] Laboratoire des Matériaux et Hydrologie, université de SIDI BEL ABBES – Laboratoire des Matériaux et Hydrologie, université de SIDI BEL ABBES. BP 89 cite Ben M'hidi 22000 SIDI BEL ABBES, Algérie, Algeria

In This study, an analytical solution to the free vibration analysis of functionally graded plates is presented by using a simple refined trigonometric shear deformation theory in which the stretching effect is included. The material properties of plates are assumed to be varied according a power law distribution in terms of the volume fractions of the constituents. Equations of motion are derived from Hamilton's principle and Navier-type solutions for simply-supported plates are compared with the available solutions to verify the validity of the proposed theory. Numerical results are obtained to investigate the effects of the power-law index and side-to-thickness ratio on the natural frequencies.

Keywords: free vibration, functionally graded material, natural frequencies, plate, stretching effect

*Speaker

Elastic instabilities and wave propagation in buckled compressible layered composite

Jian Li * [1], Stephan Rudykh† [1]

[1] Department of Aerospace Engineering, Technion – Israel Institute of Technology – Israel

We study the influence of compressibility on the instability and wave propagation in buckled layered composites. We employ the Bloch-Floquet analysis to detect the onset of instability for LCs with different compositions. We show that the change in compressibility has a significant influence on the critical stretch ratio and wavenumber at high compressibility range, and this effect is more significant for the change in the stiff layer compressibility. We show that the instability induced wavy pattern expands the width of shear wave band gap and shifts it to higher frequency range, and this effect increases with a decrease in compressibility, whereas its effect on pressure wave band gap varies with the change in compressibility. A comparison between the band gaps of the stressed unit cell (in which both local material property change and geometry pattern change are considered) and stress-free unit cell (in which only the geometry pattern change is considered), reveals that the geometry pattern shifts shear and pressure wave band gaps to lower frequency ranges under contraction deformation, and the geometry pattern change plays a dominant role in affecting the location of pressure wave band gaps.

Keywords: Layered composite, compressibility, instability, band gap, postbuckling, wave propagation

*Speaker
†Corresponding author: rudykh@technion.ac.il

S10: Coupled problems in material mechanics

Effective transient behaviour of heterogeneous media in diffusion problems

Laurence Brassart *† [1], Laurent Stainier [2]

[1] Department of Materials Science and Engineering, Monash University – Australia
[2] Institut de Recherche en Génie Civil et Mécanique (GeM) – Université de Nantes, Ecole Centrale de Nantes, Centre National de la Recherche Scientifique : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France

The general context of this work is the identification of macroscopic continuum theories to describe diffusive transport coupled to mechanics in materials. This can be addressed within a homogenization framework, which requires a micromechanical analysis on a Representative Volume Element (RVE) of the microstructure in order to identify effective parameters to be used at the macroscopic scale. For diffusion problems, it is usually assumed that the microscopic fields instantaneously reach a steady-state in the RVE, while transient diffusion is handled at the level of the macroscopic boundary-value problem. The assumption of microscale steady-state becomes however questionable when there is a high contrast between the diffusivities of the constituents. In this case, transport through the slow phase may induce a memory effect at the macroscopic scale, which needs to be included in a macroscopic continuum description.
Here we investigate the memory effect induced by microscale diffusion in model systems consisting of a slow inclusion phase dispersed in a fast percolating matrix. A first-order homogenization framework is adopted, and expressions for the effective concentration rates and fluxes (conjugated respectively to the macroscopic chemical potential and its gradient) are derived invoking a Hill-Mandel macro-homogeneity condition. Simple mean-field models are also proposed based on the transient solution for a single inclusion [1]. The obtained effective constitutive relations include a local dissipative term involving a non-equilibrium chemical potential associated with the memory effect. The model is similar to our previously proposed phenomenological models [2]-[3]. The consequences of the theory are illustrated in several chemo-mechanical boundary value problems at the macroscale.

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Keywords: Homogenisation, Diffusion, Memory effect

*Speaker
†Corresponding author: laurence.brassart@monash.edu

Integrated modeling and experiments of viscoelastic polymeric gels

Shawn Chester * [1]

[1] New Jersey Institute of Technology – United States

Polymeric gels are polymeric materials swollen with a solvent. The volume and apparent mechanical properties of gels are typically significantly different compared to those of the same dry polymer. One of the factors that determines the properties of the gel is the concentration of the solvent, or fluid content. In this talk we report on a recent experimental program designed to determine the coupled behavior of gels, while concurrently obtaining data for use towards validating constitutive models. Specifically, we consider a gel system comprised of an acrylic elastomer, VHB 4910, swollen with multiple solvents. We have performed free swelling experiments to equilibrium, as well as uniaxial tension at various states. The influence of the fluid content is clearly observable from our measurements, and initial data shows many existing constitutive models are inadequate to describe the observed behavior.

Keywords: elasticity, viscoelasticity, polymeric materials, coupled problems, multifield modeling

*Speaker

Recent advances in magnetorheological elastomers and harnessing instabilities in film/substrate systems

Kostas Danas * [1]

[1] LMS, CNRS, Ecole Polytechnique (CNRS, Ecole Polytechnique) – CNRS : UMR7649, Centre National de la Recherche Scientifique - CNRS, Ecole Polytechnique - X – LMS, Ecole Polytechnique, Route de Saclay, 91128 Palaiseau Cedex, France, France

Magnetorheological elastomers (MREs) are ferromagnetic particle impregnated rubbers whose mechanical properties are altered by the application of external magnetic fields. In addition, these composite materials can deform at very large strains due to the presence of the soft polymeric matrix without fracturing. From an unconventional point of view, a remarkable property of these materials is that while they can become unstable by combined magneto-mechanical loading, their response is well controlled in the post-instability regime. This, in turn, allows us to try to operate these materials in this critically stable region. In this work, we study experimentally and numerically the response of such an assembly subjected to transverse magnetic fields and in-plane stresses. The film is made up of an isotropic MRE material and non-magnetic silicon substrate. We find that the critical magnetic field can be substantially reduced in the presence of compressive prestress of the assembly, thus opening the possibility of controlling haptic interfaces with low magnetic fields.

Keywords: magnetoelasticity, film, smart materials, finite elasticity, experiments, finite elements

*Speaker

Concurrrent two-scale analysis of composites embedding phase change particles

Kossi-Mensah Kodjo *† [1,2,3], Julien Yvonnet‡ [1], Karam Sab [2], Mustapha Karkri [3]

[1] Laboratoire de Modélisation et Simulation Multi Echelle (MSME) – Université Paris-Est Marne-la-Vallée, Université Paris-Est Créteil Val-de-Marne - Paris 12, Centre National de la Recherche Scientifique : UMR8208 – Université Paris-Est, 5 Bd Descartes, 77454 Marne-la-Vallée, Cedex 2, France

[2] Laboratoire Navier (NAVIER UMR 8205) – Institut français des sciences et technologies des transports, de l'aménagement et des réseaux, Ecole des Ponts ParisTech, Centre National de la Recherche Scientifique : UMR8205 – Ecole des Ponts ParisTech 6 / 8 avenue Blaise Pascal 77455 CHAMPS SUR MARNE, France

[3] Centre dÉtudes et Recherches en Thermique, Environnement et Systèmes [Créteil] (CERTES EA3481) – Université Paris-Est Créteil Val-de-Marne - Paris 12 – 61, avenue du Général de Gaulle 94010 Créteil Cedex, France

To improve thermal inertia of buildings and reducing energy consumption, several works have demonstrated the effectiveness of concrete embedding Phase Change Materials (PCMs). The structures are made of cementitious materials including micro-capsules of PCM (paraffin wax with melting point at 27 ∘C in a shell). During thermal phase changes, PCMs can store or release a significant amount of thermal energy thanks to latent heat. Preliminary analyses show that for high contrast of mechanical properties between the PCM and the matrix, a linear homogenization assumption can be safely used for the mechanical behavior. In the present work, we propose a FE^2 method to predict the effective thermo-mechanical behavior of heterogeneous materials embedding thermal-phase change inclusions within an elastic matrix. In this framework, the temperature and the temperature gradient are transfered between micro and macro scales to evaluate the equilibrium at both scales. On the fine scale, an apparent heat capacity method is used to model the thermal phase change of the PCM. At the coarse scale, transient heat equation is solved with physical properties obtained from the micro-scale. An iterative process between the macro-scale model and micro-scale problems is repeated until convergence. Time-dependent results show that the offset between the applied temperature and the temperature in the structure increases with the radius of the PCM's capsules.

Keywords: Multiscale, thermomechanics, phase transformations, computational homogenization

*Speaker

†Corresponding author: jeromekodjo@hotmail.fr

‡Corresponding author: julien.yvonnet@univ-paris-est.fr

Homogenization of elastic dielectric composites containing space charges

Oscar Lopez-Pamies * [1]

[1] University of Illinois Urbana-Champaign (UIUC) – United States

In this talk, I will present the derivation of the homogenized equations for the macroscopic response of elastic dielectric composites containing space charges (i.e., electric source terms) that oscillate rapidly at the length scale of the microstructure. The derivation will be carried out in the setting of small deformations and moderate electric fields by means of a two-scale asymptotic analysis. Two types of rapidly oscillating space charges will be considered: passive and active. The latter type corresponds to space charges that appear within the composite in response to externally applied electrical stimuli, while the former corresponds to space charges that are present within the composite from the outset. The obtained homogenized equations will reveal that the presence of (passive or active) space charges within elastic dielectric composites can have a significant and even dominant effect on their macroscopic response, possibly leading to extreme behaviors ranging from unusually large permittivities and electrostriction coefficients to metamaterial-type properties featuring negative permittivities. These results suggest a promising strategy to design deformable dielectric composites — such as electrets and dielectric elastomer composites — with exceptional electromechanical properties.

Keywords: Electrets, Dielectric elastomer composites, Metamaterials, Multiscale asymptotic expansions

*Speaker

Computational homogenisation of thermoplastic composites

Andreas Menzel *† [1], Rolf Berthelsen [1]

[1] TU Dortmund (TU Do) – Institute of Mechanics Leonhard-Euler-Str. 5 44227 Dortmund, Germany

Many tailored materials are designed by composition of different constituents with different physical properties in order to achieve particularly designed effective material behaviour. Examples for such tailored materials of technological interest are electroactive polymers, thin laminated structures, metal-matrix-composites or hard materials. In order to predict the effective material behaviour during the development stage of products, numerical analysis can help to reduce costs of manufacturing and testing prototypes. The coupling of mechanical and thermal loads is often of particular interest. In order to capture and simulate the influence of the micro-scale within the finite element method, a thermomechanically coupled two-scale finite element framework is discussed for thermoplastic response. Several representative boundary value problems show the applicability of the developed thermomechanically coupled FE2 formulation.

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Keywords: Multiscale modelling, Finite element method, Thermomechanics, Homogenisation

*Speaker

†Corresponding author: andreas.menzel@udo.edu

Mechanics and fracture of tough hydrogels below water-freezing temperature

Xavier Morelle *† [1], Widusah Illeperuma [1], Kevin Tian [1], Ruobing Bai [1], Zhigang Suo [1], Joost Vlassak [1]

[1] Kavli Institute for Bionano Science and Technology, John A. Paulson School of Engineering and Applied Science, Harvard University (Harvard SEAS) – 29, Oxford Street, Cambridge, MA - 02138, United States

Hydrogels are cross-linked networks of a hydrophilic polymer chains dispersed in water. Current hydrogels are typically soft stretchable solids with useful water-like transport properties. The combination of rubber-like toughness and stretchability along with biocompatibility, ionic conductivity and optical transparency have considerably enlarged the range of applications of recent hydrogels, going from tissue engineering and drug delivery to ionic skin and soft robot actuators, as well as stretchable electroluminescent devices. However, if the temperature is decreased below 0∘C, the water in the hydrogel freezes and the hydrogel becomes rigid, brittle and non-conductive, thereby losing their desirable properties. Here we demonstrate a class of hydrogels that have much lower freezing points or that freeze over a range of temperatures, therefore retaining some of their critical attributes of stretchability and conductivity at much lower temperatures. These hydrogels are synthesized by soaking in a suitable amount of salt into the hydrogel. The actual freezing point depression is determined by the nature of the salt and its concentration inside the gel. The present study focuses on a polyacrylamide-alginate hydrogel equilibrated with aqueous solutions of 10wt% and 30wt% calcium chloride. The resulting hydrogels are capable of retaining high stretchability and fracture toughness even at temperatures far below 0∘C. In particular, we show that the mechanical properties of these salts-containing hydrogels can be further improved by going through a "slurry" state, coexistence of a mixed phase of ice crystals and salt solution inside the gel network, before fully freezing. We give a comprehensive explanation of the reasons of this optimum through a micro-mechanical understanding of the observed modified failure scenario. We foresee that this new class of hydrogels will prove useful in the development of applications operating over a broad range of atmospheric conditions.

Keywords: non freezing hydrogels, high toughness, slurry state, water freezing temperature, microdamage and crack deflection

*Speaker
†Corresponding author: morelle.xavier@gmail.com

Isogeometric analysis for modeling chemical transformations front kinetics

Aleksandr Morozov * [1,2], Alexander Freidin [3,4], Sergei Khakalo [5], Viacheslav Balobanov [5], Jarkko Niiranen [5], Müller Wolfgang [1]

[1] Institute of Mechanics, Faculty of Mechanical Engineering, Berlin University of Technology (TU Berlin) – Straße des 17. Juni 135, 10623 Berlin, Germany, Germany
[2] Institute of Mechanical Engineering Problems [St. Petersburg] (IPME) – V.O., Bolshoj pr., 61 199178 St. Petersburg Russia, Russia
[3] Institute for Problems in Mechanical Engineering of Russian Academy of Sciences (IPME RAS) – 61 Bolshoy Pr. V.O., St. Petersburg 199178, Russia, Russia
[4] Peter the Great St. Petersburg Polytechnic University (POLYTEC) – Polytechnicheskaya Str. 29, St. Petersburg 195251, Russia, Russia
[5] Department of Civil and Structural Engineering, School of Engineering, Aalto University (Aalto University) – 00076 AALTO Rakentajanaukio 4 A, Espoo, Finland, Finland

Abstract

Various experimental and theoretical observations of chemically reacting and transforming materials (e.g., [1,2]) show the influence of mechanical stresses on chemical reaction rate. The chemical reaction front also affects the mechanical stress-strain behavior via chemical transformation strains. As a result, one faces a complex coupled problem of mechanochemistry with a moving chemical reaction front. Recently it was shown that the configurational force driving the reaction front is the normal component of the chemical affinity tensor and that the reaction rate depends on the orientation of the surface element at which the reaction takes place (see, e.g., [3] and references therein). A kinetic equation was formulated in terms of the reaction front velocity depending on the normal component of the affinity tensor. In this approach the stresses affect the front velocity through the chemical affinity tensor.

In a numerical simulation, the front propagation is realized as a front movement in the normal direction proportionally to the front velocity by utilizing the chemical affinity tensor concept. The simulation is based on isogeometric analysis [4] together with ABAQUS user defined subroutines and elements [5]. By solving various boundary value problems numerically we demonstrate a variety of front behaviors depending on material parameters, boundary conditions, and the initial configuration. We show that the reaction front can be retarded and even blocked by mechanical stresses. Special attention is paid to the front behavior in the vicinity of chemical equilibrium that corresponds to front blocking. Straightforward analogies between the stability behavior of equilibrium interfaces in phase and chemical transformations are emphasized.

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*Speaker

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Keywords: mechanochemistry, isogeometric analysis, chemical affinity tensor, chemical reaction front kinetics, phase transitions, reaction blocking, reaction front stability, numerical simulations

Stress-affected chemical reactions in non-linear viscoelastic solids: Two-phase lithiation of Si particles

Mikhail Poluektov *† [1], Alexander Freidin [2,3], Lukasz Figiel [1]

[1] University of Warwick – University of Warwick, Coventry CV4 7AL, UK, United Kingdom
[2] Institute for Problems in Mechanical Engineering of Russian Academy of Sciences – 61 Bolshoy Pr. V.O., St. Petersburg 199178, Russia, Russia
[3] Peter the Great St. Petersburg Polytechnic University – 29 Polytechnicheskaya Str., St. Petersburg 195251, Russia, Russia

Silicon particles offer promising means for capacity enhancement of Li-ion batteries [1]. However, extreme volumetric expansion of Si during lithiation leads to the emergence of mechanical stress, which can cause failure of the anode and thereby the capacity fade of the battery. Moreover, as observed experimentally, mechanical stress can influence the kinetics of the chemical reaction between Si and Li even up to the reaction arrest [2]. There is a variety of models that were designed to describe the influence of mechanical stresses on the kinetics of chemical reactions. In some approaches, stress dependencies of the reaction rate parameter and the diffusivity are postulated, e.g. [7,8]. Other models are based on stress-dependent scalar chemical potentials, e.g. [5,6].
In this talk, the stress-affected two-phase silicon lithiation process is modelled by adopting the chemomechanical framework, in which the chemical affinity tensor (see [3,4] and reference therein) is used in combination with the finite-strain non-linear viscoelastic constitutive model. The reaction is localised at the reaction front. The reaction rate and, thus, the reaction front velocity are determined by the normal component of the chemical affinity tensor, which depends on the stresses and strains at the reaction front. Since the reaction front is the moving boundary for the mechanical and the diffusion boundary value problems, there is stress-diffusion-reaction coupling, even if the diffusion flux does not depend on the stresses and the stresses are not generated by the diffusion. In present talk, this coupling mechanism is explored and the factors influencing the nature of the coupling are highlighted. For example, in few cases (e.g. spherical symmetry and elastic materials) the stress and the diffusion equations can be decoupled; however, for viscoelastic materials, the coupling is present even in the case of spherical symmetry, as opposed to the elastic case.

The coupled problem is solved using the finite element approach to predict propagation of the reaction front during the two-phase lithiation of a spherical Si particle. The stress distribution within the particle and the evolution of stresses during the reaction front propagation are studied in detail in connection with the reaction front kinetics. The retardation and the blocking of the reaction are shown, which corresponds to experimental observations.

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*Speaker
†Corresponding author: m.poluektov@outlook.com

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Keywords: chemical affinity tensor, mechanochemistry, lithiation of silicon, chemical reaction front kinetics, finite, strain, elasto, viscoplasticity

A mechanoluminescent glass matrix particulate composite

Tanguy Rouxel * [1,2], Marion Dubernet [2], Yann Gueguen [2], Patrick Houizot [2], Emilie Bruyer [2], Xavier Rocquefelte [2]

[1] University of Rennes 1, IPR, UMR UR1-CNRS 6251, Department of Glass Mechanics (UR1) – CNRS : UMR6251 – University of Rennes 1, Rennes 35042, France
[2] University of Rennes 1 – Université de Rennes I – France

A material is considered as mechanoluminescent when it emits light under mechanical loading. We have developed of a transparent glass-matrix particulate composite exhibiting this remarkable property. A green light is produced during loading in the elastic regime, which depends much on the loading cycle and loading type (shear versus isostatic). Experiments show the linear dependence of the mechanoluminescence intensity with the mechanical power. A rheological model is proposed, based on the physics of delayed processes (in analogy to viscoelasticity), and on the electron trapping and de-trapping process that is at the source of this phenomenon. An in-depth DFT analysis was conducted to get insight into the physics of mechanoluminescence in this peculiar composite material and to understand the mechano-optical coupling.

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Keywords: Mechanoluminescence, glass, mechano, optical coupling, experimental, theoretical, Density Function Theory

*Speaker

Thermodynamics and multi-physical model in metal subject to corrosive environment

Kanssoune Saliya *† [1], Benoit Panicaud [1], Carl Labergere [1]

[1] Department of Engineering Mechanics and Mechanics of Materials. University of Technology of Troyes (ICD/LASMIS, CNRS UMR 6281) – Université de Technologie de Troyes – CS 42060, 10004 Troyes Cedex, France, France

Abstract: In various industrial sectors, some metal parts of more or less complex shape have to be carefully dimensioned to resist with time to thermo-mechanical stresses, but also to a more or less aggressive environment. When a metal structure must withstand thermo-mechanical stresses over very long periods, the problem arises to take also into account the degradation of these mechanical properties by the presence of gas such as hydrogen, which can diffuse into the material and weaken it. The presence of oxygen could also be considered, which generally oxidizes its surface. The degradation of materials subjected to such aggressive environments put significant challenges for engineering. To achieve such a goal, it is necessary to predict at least with accuracy the diffusion of hydrogen and/or oxygen, which generates indirectly a degradation of mechanical properties, in order to improve the reliability and predictivity of such models.
For hydrogen, its effects on mechanical response are now qualitatively well known. Metals and alloys are degraded in the presence of hydrogen [1]. One of this phenomena is known as hydrogen embrittlement. Embrittlement by hydrogen is explained by a great number of theories, but two of them are the most developed: hydrogen enhanced decohesion (HEDE) and hydrogen locally enhanced plasticity (HELP).

Several authors have proposed models for the study of hydrogen embrittlement near a crack tip [1-2]. All these models consider two kinds of sites for hydrogen diffusion: normal interstitial lattice sites and microstructural trapping sites such as dislocation cores, grain boundaries, and interfaces between the matrix and various second-phase particles. Most of these models use the postulate of Oriani [3].

The existing models, although they allow studying the effects of hydrogen diffusion on the mechanics and reciprocally, are not fully based on the thermodynamics of irreversible processes. The only model which is based on the thermodynamics of irreversible processes is the one of Di Leo et al. [2].

In our work, we base our developments on the thermodynamics of irreversible processes and develop a constitutive model taking into account the couplings between volume diffusion, chemical reactions at surface, and thermo-mechanical behavior including ductile damage. This model includes both kinematic and isotropic hardening in the material. At our knowledge, this is the first time that a coupled theory for species diffusion and thermo-elasto-visco-plastic model takes into account simultaneously ductile damage and both kinematic and isotropic hardenings with chemical effects. The model supposes the presence of several chemical species such as hydrogen from the environment. In this case, the flux of the considered specie *n* may depend on the gradient of the chemical potentials of the others species *m*.

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*Speaker
†Corresponding author: kanssoune.saliya@utt.fr

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Keywords: Modeling, Diffusion, Mechanochemistry, Thermo, Visco, Plasticity, Damage

A discrete twin-boundary approach for simulating the magneto-mechanical response of Ni-Mn-Ga

Doron Shilo * [1], Eilon Faran [2], Leonardo Riccardi [3]

[1] Faculty of Mechanical Engineering, Technion – Israel
[2] Technion – Israel
[3] Leonardo Riccardi – ETO MAGNETIC GmbH, 78333 Stockach, Germany, Germany

The design and optimization of ferromagnetic shape memory alloys (FSMA)-based devices require quantitative understanding of the dynamics of twin boundaries within these materials. Here, we present a discrete twin boundary modeling approach for simulating the behavior of an FSMA Ni-Mn-Ga crystal under combined magneto-mechanical loading conditions. The model is based on experimentally measured kinetic relations that describe the motion of individual twin boundaries over a wide range of velocities.
The calculated results show good agreement with experimental measurements performed on a specially designed Ni-Mn-Ga linear spring – mass actuator. The effects of the actuator's mass and the twin boundary density on the resonance response and the actuator performance are explored numerically and reveal several new effects that have not been considered before.
The model simulations show that the use of a linear kinetic law that is commonly applied in phase field models is inadequate and results in incorrect predictions. The strength of the new modeling approach is that it enables exploring the relations between basic (atomistic-scale) twin boundary properties and actuator performances. Our results show that the magnitude of the lattice barrier that resists twin boundary motion is the important property that determines the level of actuation strain at relevant frequencies, while the contribution of twinning stress property is minor.

Keywords: FSMA, magneto, mechanical problem, Ni, Mn, Ga, Twin boundary, interface motion, SMA

*Speaker

Multi-physics modeling of fracture in polycrystalline cathode in Lithium-ion battery

Avtar Singh * [1], Siladitya Pal * † [1]

[1] Department of Mechanical and Industrial Engineering [Roorkee] (IIT Roorkee) – IIT Roorkee Roorkee, Uttarakhand India, India

Electrochemical energy storage (EES) devices are the prominent technologies for portable electronic devices, transformation of hybrid electric vehicles to all electric vehicles and large-scale grid integration for electric power supply when electric energy is harvested from various renewable energy sources such as wind mills and solar accumulators. EES devices based on lithium-ion battery are attractive candidates for many applications for its high specific energy and power density. In the drive towards the development of high capacity electrochemical energy storage devices for Li-ion battery, polycrystalline cathode material such as LiCoPO4, LiFePO4, LiMnPO4, LiNi1/3Mn1/3Co1/3O2and LiCoO2 etc. are the next generation electrode materials for Li-ion batteries due to the faster ion and electron transport, higher surface reactivity and relief of stresses and improved mechanical stability. During the lithium diffusion, volumetric change occurs leading differential strain that causes mechanical stress in the electrode. However, attendant mechanical stress develops inter- or trans-granular cracks upon electrochemical cycles that can hinder the transport of Li-ions as well as electrons resulting capacity fading. Therefore, there is strong need for multi-physics description for understanding the fracture behavior of polycrystalline cathode at the micro-structural level for various grain sizes and charge rates during the electrochemical cycle. In the present study, we will develop a numerical framework to understand the fracture behavior of polycrystalline cathodes. Of particular interests are the role of different crystallographic orientations and anisotropic diffusion parameters at the microstructure level. Mass transport of Li-ion along with mechanical equilibrium conditions will be considered. A cohesive zone model will be incorporated to simulate the debonding of grain boundaries. A finite element framework will be adopted and Newton-Raphson scheme will be used to perform linearization of coupled equations. To discretize the equation in the time domain, an implicit time stepping scheme will be employed. Polycrystalline cathodes with desired micro-structural features will be realized using custom made grain generation code. A finite element discretization of grains will be performed and cohesive zone finite elements will be inserted at the grain boundaries. A representative volume element with large number of grain structure will be simulated using in house code in parallel computing architecture. A systematic parametric study will be performed to construct a failure map for various micro-structures, materials and electrochemical cycle parameters.

Keywords: Polycrystalline, Cathode, Fracture, Li, ion battery, Cohesive Zone Model

*Speaker
†Corresponding author: siladitya.pal@gmail.com

Modelling of heat generation in vehicle components made of rubber using FEM

Veronika Szüle *† [1,2]

[1] szule.veronika@sze.hu (szule.veronika) – 9026 Győr Egyetem tér 1, Hungary
[2] University of Széchenyi István, Department of Applied Mechanics – Győr, Hungary

Vehicle components made of rubber usually exhibit large deformations. Cyclic finite deformations may induce increasing temperature in hyperelastic materials. This case where changes in deformation and in temperature occur simultaneously is called coupled thermomechanical problem. Both the mechanical and thermal processes have their own governing equations, that is why special techniques are needed for the computation. A widely used numerical method for solving such problems is the Finite Element Method (FEM).

Rubber can be classified as a so-called hyperelastic polymer which has a typical geometrical and material nonlinear behaviour. The geometrical nonlinearity is easy to handle mathematically, however the material nonlinearity is only described approximately [1, 2]. Furthermore, a number of material laws for rubber can be found in literature [3], for example the Neo-Hooke-, the Mooney-Rivlin, the Yeoh- and the Arruda-Boyce material models. Cyclic finite deformations may induce increasing temperature in hyperelastic materials [4].

The goals of this paper are the following:

It is necessary to summarize the applied equations and the basic physical laws which are responsible for the theoretical background. It is necessary to extend these relationships like equilibrium of the linear and angular momentum and the first and second laws of thermodynamics to the high deformation of rubber and rubberlike polymers. For the solution of the thermomechanical exercise the Neo-Hooke material law is applied [3]. Finally, the numerical solution and the computation of the coupled thermomechanical problem will be presented and an example will be solved. The present numerical algorithm is the basis of the further fatigue and lifetime-calculations.

NUMERICAL SOLUTION

The position vector is determined from the weak form of the mechanical problem, the temperature field is determined from the weak form of the thermodynamical problem. Let us consider the mechanical model of a silent block, where A, B and C are axisymmetric bodies. The A and C bodies are rigid bodies, while B is a deformable one. The external body (A) is fixed and the internal one is imposed by a given rotation.

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*Speaker
†Corresponding author: szule.veronika@sze.hu

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Keywords: hyperelastic materials, high deformations, thermodynamics, Neo, Hooke material law, coupled problem

Studying Energy Dissipation Mechanisms in Pseudoelastic Thin Film Shape Memory Alloys for Vibration Damping

Frank Wendler * [1], Shahabeddin Ahmadi [2], Kiran Jacob [2], Manfred Kohl [3]

[1] Chair of Materials Simulation, Department of Materials Science, Friedrich-Alexander University of Erlangen-Nürnberg (WW8, FAU) – Dr.-Mack-Strasse 77, 90762 Fürth, Germany, Germany
[2] Institute of Microstructure Technology, Karlsruhe Institute of Technology (IMT KIT) – Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany, Germany
[3] Institute of Microstructure Technology, Karlsruhe Institute of Technology (IMT KIT) – Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany, Germany

Due to the high work density shape memory alloys (SMAs) represent optimal materials for damping of vibration and shock impacts, until now only exploited in large-scale applications like the protection of buildings against seismic activity. Here, we present recent work on thin-film NiTi-based miniature devices in form of predominantly tensile loaded bridge structures, which are potential vibration dampers for portable electronics. Pseudoelasticity and one-way shape memory effect are possible mechanisms to dissipate vibrations, which allow for passive, semi-active and active damping strategies.
Models for SMA materials have to tackle the complex thermomechanical coupling with mutual conversion of elastic into chemical (phase state) and thermal energy, which leads to stress-strain hysteresis and a high temperature sensitivity of the mechanical response. Previously, we presented an FEM based mesoscale model which implements transition state kinetics for the phase change martensite-austenite (M-A) and contributions for the M-A interface energy from a phase-field approach [1]. Experimentally observed martensitic strain bands and thermal patterns in tensile loading are resolved in the simulations. The strain band density increasing with strain rate is a consequence of the limiting thermal transport, leading to an increase of the transformation stress. The model is extended to dynamics conditions and more general loading states, where the external spring-mass system is represented by an ODE and coupled to the FEM domain as a boundary condition. For parameterization, macroscopic as well as local material properties are evaluated by a set of tensile testing, DIC (digital image correlation), thermal IR and DSC experiments. Additionally, we develop a test protocol to identify dynamic model parameters, applying both forced vibrations and transient excitation of a test mass.

In the simulations, both pseudoelastic and quasiplastic SMA materials are investigated, for the latter using temperature pulses by Joule heating for resetting. In both cases we find a strong dependency of the damping loss of the thin film device on the SMA prestrain, martensitic fraction and temperature. With an optimal control of the operation point, the vibration energy of a shock load can be fully reduced in few oscillation cycles.

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Keywords: shape memory alloy, transition state theory, phase, field model, damping, vibration control

*Speaker

S11: Mechanics of biological materials & biomechanics

Investigating the Uncertainty in Constitutive Model Calibration for the Hyperelastic Behavior of Brain Tissue

Patrick Brewick * [1], Kirubel Teferra [1]

[1] US Naval Research Laboratory (NRL) – United States

This work is focused on developing a Bayesian calibration technique to probabilistically characterize model parameters for constitutive laws that describe the mechanical behavior of brain tissue. The mechanical behavior of brain tissue is challenging to characterize because of the need to extrapolate ex-vivo measurements to in-vivo conditions as well as the complexity, viscoelasticity, and high compliance of soft biomaterials. As a result, there is an extremely large degree of uncertainty and disagreement in the experimentally-determined stress-strain curves that have been published over the years. The predictive ability of computational models to quantify the mechanical response within the brain under loading scenarios causing traumatic brain injury relies, among many factors, on the accurate characterization of the mechanical properties of biological tissue. Therefore, uncertainty quantification of the constitutive models characterizing the mechanical behavior of brain tissue is an important prerequisite towards improving the reliability of mechanical response predictions of computational models. The Bayesian calibration framework enables the variability in the measurement data, modeling assumptions, and other epistemic uncertainties to be factored into the model calibration process. By modeling the constitutive model parameters as a random vector, Bayes' law is employed to formulate its joint posterior distribution, which is calculated through a novel enrichment of state-of-the-art simulation techniques. The results of a study comparing model calibration techniques for constitutive models that describe the hyperelastic behavior of brain tissue are presented. One and two-term Ogden models are fit to two different sets of stress-strain experimental data for brain tissue using both least squares optimization and Bayesian estimators. The joint posterior distribution of the constitutive parameters is calculated by employing Hamiltonian Monte Carlo (HMC) sampling, which is a type of Markov Chain Monte Carlo method. The HMC method is enriched in this work to intrinsically evaluate Drucker stability by formulating a nonlinear parameter constraint function that ensures the constitutive model produces physically meaningful results. Through application of the nested sampling technique, the 95% confidence bounds on the constitutive model parameters are identified. These bounds are then propagated through the constitutive model to produce the resultant bounds on the stress-strain response. Despite some similarity between the two data sets, the resulting distributions are noticeably different, even for models with the same number of terms. The results from this study demonstrate that increasing the model complexity (i.e., adding an additional term in the Ogden model) improves the accuracy of the best-fit set of parameters while also increases the uncertainty via the widening of the confidence bounds of the calibrated parameters. This study also examines the limitations of Gaussian assumptions on the posterior distributions, assumptions that are mitigated through the application of nested sampling.

Keywords: Bayesian model calibration, Ogden hyperelastic constitutive model, Brain tissue, Hamiltonian Monte Carlo sampling, Drucker stability

*Speaker

On the application of a new methodology to identify the initiation of damage in modelling human aneurysms

Karunakaran C *† [1], K. Kannan [1]

[1] Indian Institute of Technology Madras (IITM) – Chennai-600036, Tamilnadu, India

Most approaches to damage assume the body to be homogeneous and introduce a damage parameter that depends on the stress or strain for which one has to know a reference configuration in which the body was stress or strain free to start measuring from. Exploiting the fact that damage is a consequence of the inhomogeneity of the body, Alagappan et al. [1] has developed a new methodology that studies damage considering the body to be inhomogeneous. The material parameters were defined in terms of reference density and the determinant of the deformation gradient. As the material properties of the body depend invariably on the density among the other variables in the current configuration, density in the current configuration was used as a means to identify the onset of damage in a class of materials. The damage criterion suggested by the study is the derivative of the norm of the Cauchy stress with respect to the current density. It bears out to be appropriate as this criterion comes purely from the current configuration and no other extra damage parameters are needed.
The work is based on applying this new methodology for identifying the initiation of damage in human aneurysms. An aneurysm is a localized dilatation developed in the artery whose rupture will lead to hemorrhage and finally may lead to death. The objective is to model and simulate the human aneurysms to discover the causes of its initiation and rupture using this new damage approach. The artery wall is modeled with spots of inhomogeneity based on the density. Boundary value problem is formulated with hyperelastic models representing the artery tissue. Applying internal pressure, the governing equations are solved numerically to locate the spot of development of bulge (dilatation) from the artery wall and the simulations are continued till the initiation of damage occurs at some local point in the developed bulge. This provides a basic justification about the initiation phase. The growth and remodeling mechanisms will be incorporated later.

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Keywords: damage, inhomogeneity, aneurysm, hyperelastic

*Speaker
†Corresponding author: karunakaranvictory@gmail.com

Influence of angle on failure of growth rods in H3S2 construct

Maïté Croonenborghs * [1], Karim Ismail† [1], Maryline Mousny [2], Thomas Pardoen‡ [1]

[1] iMMC-UCLouvain – Belgium
[2] Department of Orthopedics, Cliniques Universitaires Saint-Luc – Belgium

Scoliosis is an abnormal three-dimensional deformation of the vertebral column with an angle larger than 10◦ in the frontal plane. This deformation can appear at any time during life, but it is particularly problematic during childhood growth period. Depending on the amplitude of the deformation, different treatments are applied. Arthrodesis consists in merging vertebrae together; however, for children this can have a negative impact on the development of other organs. Children can be immobilized using braces. However, if the brace does not provide a significant result and if the child still has an important growth potential, surgery is unavoidable.
Surgery consists in inserting one or two growth rods along the column to straighten it. The so-called H3S2 setup "3 hooks 2 screws", which uses one long cylindrical beam, has been studied in this work. Since children keep growing and the column tries to return to its initial deformed configuration, varying stresses are constantly induced in the rods. In 36 percent of treatments, the rod fails inside the body weeks or months after surgery [Yang2011]. The failure mechanism is usually due to a fatigue cracking process. During the surgery, the surgeon bends the rod to fit the natural shape of the patient spine. This bending process as well as the marking of the material due to contact during bending are believed to affect the fatigue resistance of the rod.

The aim of this research is to characterize and model the failure mechanisms in the rods by means of mechanical tests and numerical simulations. The decrease of rods lifetime due to the bending process is investigated by carrying static and fatigue tests as well as finite element simulations on pre-bent or as-received specimens. Rods made of pure titanium, titanium alloy TiAl6V4 and cobalt-chromium alloy, which are typically used in surgery, were selected. Particular attention is put on the development of internal stress, on the fatigue life, on failure mechanisms, on Bauschinger effect and on the strain hardening capacity in order to generate a quantitative understanding of the problem. These results provide guidelines towards selecting more adapted procedures and materials.

Keywords: Growth rods — H3S2 — Rod contour — Rod failure — Fatigue life — Internal stresses — Strain hardening

*Speaker
†Corresponding author: karim.ismail@uclouvain.be
‡Corresponding author: thomas.pardoen@uclouvain.be

Homeostatic ensemble for cells

Vikram Deshpande * [1]

[1] Department of Engineering [Cambridge] – Cambridge University, Department of Engineering, Trumpington Street, Cambridge CB2 1PZ, United Kingdom, United Kingdom

Complex bio-chemical processes attempt to maintain constant time-averaged concentrations of a range of proteins within cells in a process commonly referred to as cellular homeostasis. These chemical processes cause fluctuations of the state of cells that depends on the extra-cellular environment. A statistical mechanics view to model these fluctuations will be presented which will enable a unifying treatment of range of disparate cellular phenomena. First the probability of observing a cell in a so-called spread micro-state is estimated in terms of the free-energy of that state using the basic idea of Gibbs entropy. Next a model is presented to estimate this free-energy. The model includes stress-fiber reorganisation and the associated contractility by considering the energetics of the actin/myosin functional units that constitute the stress-fibers. This model then used to elucidate the range of states over which the cell can fluctuate in a particular environment and the probability of observing each of those states. Finally some predictions are presented for a range of experimentally observed phenomena using this approach. This includes: (i) the spreading and shape of cells as a function of the stiffness of the substrate; (ii) durotaxis whereby cells tend to migrate guided by rigidity and chemical gradients on substrates and (iii) differentiation of stem cells guided by the stiffness of substrates and as well as cell shape as controlled by the chemical environment.

Keywords: mechano, biology, cytoskeleton, myosin contractility

*Speaker

Coupled problems in biomechanics of growth

Alexander Freidin * [1,2,3], Yanina Izmaylova [2], Valeriia Khashba [2]

[1] Institute for Problems in Mechanical Engineering of Russian Academy of Sciences (IPME RAS) – 61 Bolshoy Pr. V.O., St. Petersburg 199178, Russia, Russia
[2] Peter the Great St. Petersburg Polytechnic University (POLYTEC) – Polytechnicheskaya Str. 29, St. Petersburg 195251, Russia, Russia
[3] St. Petersburg University (SPBU) – Russia

The concept of the chemical affinity tensor, which was developed and applied for modeling of chemical reaction fronts propagation in the case of stress-assisted chemical reactions (see e.g. [1,2] and reference therein), is applied for modeling biological growth. Various experimental and theoretical observations show the influence of mechanical stresses on growth rate (see e.g. [3,4] and reference therein). In the present paper it is derived from fundamental laws and entropy inequality that the growth rate is controlled by the configurational force equal to the normal component of the driving tensor similar to the affinity tensor that in turn depends on stresses/strains and the concentration of the supplied matter. Then the stresses affect the growth via this tensor. On the other hand, stresses depend on the current configuration of the growing body. The kinetic equation is formulated in the form of the dependence of the growth rate on the configurational force. Note that driving force approach was also presented in other papers (see e.g. [5] and reference therein).
The model developed is examined in two processes: bone remodeling and axon growth. Special attention was paid to the choice of the stress dependent supplying function which controls the amount of the matter incoming into bone tissue. This function provides additional coupling between stresses, growth rate and the matter supply. Bone growth and resorption was studied at various stress states. In the case of the longitudinal axon growth the combination of volume and surface growth is studied. The solution of the advection-diffusion equation for the supply of the substance in the case of axonal growth is presented and the influence of the transport parameter value on the growth kinetics is examined. The influence of mechanical stress on the kinetics of axonal growth is analyzed.

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*Speaker

Keywords: coupled problems, biomechanics, growth, chemical affinity tensor, bone remodeling, axon growth

Exploring the influence of damage accumulation on collagen fibre remodelling in arteries under supra-physiological loads

Milad Ghasemi *† [1,2], David Nolan [1,2], Robert Johnston [1,2], Caitríona Lally [1,2]

[1] Department of Mechanical and Manufacturing Engineering, Trinity College Dublin, Ireland – Mechanical & Manufacturing Engineering Parsons Building Trinity College Dublin Dublin 2 Ireland, Ireland
[2] Trinity Centre for Bioengineering, Trinity College Dublin, Ireland – Trinity Biomedical Sciences Institute Trinity College Dublin 152-160 Pearse Street Dublin 2 Ireland, Ireland

Carotid atherosclerotic plaque rupture is one of the leading causes of stroke [1]. Angioplasty, stenting and endarterectomy are among the most common endovascular treatments to re-open atherosclerotic and narrowed arteries. These treatments can apply supra-physiological loads on the vessel wall, from the deployment of the intravascular device itself or through external tissue clamping during surgery.
The mechanical behaviour of arteries is commonly modelled using a structural hyperelastic anisotropic material model, where two families of collagen fibres are embedded in a soft matrix [2]. Collagen fibres are the most significant load bearing constituents of the arterial wall [2, 3]. Fibre orientation has been the primary focus of investigations into collagen fibre remodelling within soft tissues [3, 4], however, the inherent quality of collagen fibres may be of equal importance [5]. The main aim of this research is to explore the role of damage accumulation on fibre reorientation and remodelling. To achieve this, a constitutive model has been developed which can capture collagen fibre reorientation and collagen fibre quality in arterial tissues. This constitutive model is applied to real vessel geometries of stenosed carotid arteries. This computational framework may provide objective support for clinical decisions on the need for medical intervention, even in asymptomatic patients, by assessing both distribution of fibres and damage accumulation in the arterial wall and consequently the risk of plaque rupture.

Within this study, realistic vessel geometries are constructed based on medical images obtained from atherosclerotic human carotid arteries, following an approach previously described in [6]. Collagen fibre directions evolve to maximize the load bearing capacity of the tissue [3, 4]. In this research, reorientation of collagen fibres follows a periodic distribution function where both fibre direction and dispersion are subjected to remodelling rules according to the two largest principal strains, similar to [4]. A continuum damage mechanics approach is used to investigate the response of arteries to supra-physiological loading conditions. Four primary mechanical phenomena can be captured in the arteries using this approach: softening (known as Mullins effect), permanent set, hysteresis (continuous damage) and fibre rupture.

The results of this research demonstrate the influence that progressive damage accumulation has on fibre remodelling in real carotid geometries. Preliminary results suggest that damage in fibres can occur even at physiological blood pressure in the presence of atherosclerotic plaques. A highly aligned distribution of fibres has also been predicted at plaque shoulders. The difference between the optimum fibre distribution and the orientation of fibres in diseased arteries could be used as a metric for distinguishing the areas at greatest risk of rupture. The future goal of this project is to fully validate this constitutive model using experimental and clinical data.

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*Speaker
†Corresponding author: ghasemim@tcd.ie

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Keywords: Atherosclerosis, Plaque rupture, Collagen fibres, Damage, Reorientation, Remodelling

Biomechanics of human cornea modeled via a generalized statistical approach

Alessio Gizzi * [1], Marcello Vasta [2], Anna Pandolfi [3]

[1] University Campus Bio-Medico of Rome, Department of Engineering – Via A. del Portillo 21, 00128 Rome (IT), Italy
[2] Università di Chieti-Pescara – Viale Pindaro 42, Pescara, Italy
[3] Politecnico di Milano – Piazza Leonardo da Vinci 32, 20133 - Milano, Italy

The human cornea is a biological tissue characterized by a high microstructural complexity and a wide variability between different components [1]. The cornea belongs to the class of fiber-reinforced composite materials characterized by multiple sets of collagen fibers, modeled often by assuming the mechanical superposition of distinct contributions of the material constituents [2].

In the view of applications to the human cornea, we develop a generalized statistical approach for the description of fully three-dimensional fiber-reinforced materials [3], resulting from the coupling of two indepen- dent probability distribution functions [4, 5]. The investigation is motivated by recently published experimental evidences of the existence of complex spatial architectures of reinforcing collagen fiber distributions [6, 7]. We discuss the consequences of the proposed formulation on the constitutive behavior of fibrous materials. Upon suitable assumptions, the generalized formulation recovers previous alternative models, constructed through averaged structure tensors [8, 9]. We demonstrate that the generalized formulation embeds standard models such as planar isotropy and transverse isotropy, while any intermediate behavior is easily obtained through the suitable choice of two material parameters.

We apply the model to the numerical analysis of the in-plane organization of the stromal collagen in the human cornea, variously modelled to include one or more features of the newly evidenced collagen architectures. In particular, we investigate numerically the implication of the local organization of collagen in the stroma on the response of the human cornea to mechanical tests.

Keywords: Human cornea, Distributed fibers, Statistical modeling, Biomechanics, Finite Elements.

*Speaker

Mechanical properties of flax fibers: from the stem to the cell walls

Camille Goudenhooft * [1], Alain Bourmaud [1], Samuel Réquilé [1], Christophe Baley [1]

[1] Institut de Recherche Dupuy de Lôme (IRDL) – PRES Université Européenne de Bretagne [UEB], CNRS : FRE3744 – Centre de Recherche C. HUYGENS Rue de Saint-Maudé - BP 92116 56321 LORIENT Cedex, France

The development of composites reinforced by flax fibers, used for more environmentally friendly materials, requires a better knowledge and understanding of inherent fiber properties. In this perspective of optimization of flax-based composites, the present study focuses on to the understanding of structural parameters of a stem, comparable to a composite material. In fact, the flax plant itself can be assimilated to a composite structure. It is composed of several biological tissues, each of them having a particular function. For instance, the strengthening of flax stems is ensured by flax fibers that, long before their use as reinforcement for industrial applications, constitute the supporting tissues of the plant.
The study is realized following a multi-scale approach, to provide a general understanding of the mechanics of this natural composite.

At the stem scale, the mechanical properties the different biological tissues are evaluated by a three-point flexural test, combined with a microstructural analysis of stems to determine the fiber distribution. Analyzed as a tube formed by a first layer of supporting fibers, a second layer of internal xylem and a central lacuna, the flax stem is considered as a model composite; the contribution of each part of the stem to the bending stability is evaluated by testing the samples before and after manual removal of the fibers. The mechanical characterization shows flax fibers contribute to 70 % to the flexural stiffness of a stem. This contribution is significant, especially when compared to other fiber plants such as hemp (for which the fiber contribution to the flexural stiffness reaches about 50%). In addition, this result could be linked to the impressive slenderness of flax among other plant species, fibers having a key role in its slenderness.

At the fiber scale, tensile tests on elementary flax fibers are performed in order to evaluate their apparent mechanical performances. These results are compared with the fiber properties estimated at the stem scale and are well-correlated.
The fiber cell wall scale is finally relevant to get better insights in the origin of the high mechanical performances of the fibers. In this way, an investigation the characteristics of cell wall properties of flax fibers during plant development is performed using Atomic Force Miscroscopy (AFM) using Peak-Force Quantitative Nano-Mechanical property mapping (PF-QNM). This technique shows that changes in the morphology and mechanics of the secondary cell-walls take place over cell maturation. Mature thickened fibers have a homogeneous morphology, leading to greater indentation modulus. Moreover, the highlighted changes of indentation modulus enable to have better insights of the evolutions of plant stability and risks of lodging over plant growth. These later parameters are of great importance, both for the development of flax cultivation and for the production of fibres having high performances.

Keywords: Flax fiber, Stem, Cell wall, Mechanical properties, Composite

*Speaker

Modeling the load-carrying properties of collage-fiber reinforced soft biological tissues

Amir Hamedzadeh [1], T. Christian Gasser * [2], Salvatore Federico [1]

[1] The University of Calgary, Calgary, Alberta, Canada – Canada
[2] KTH Solid Mechanics, Stockholm, Sweden – Sweden

Collagen is the most abundant protein in mammals and equips soft biological tissues with stiffness, strength and fracture toughness. Alteration and degradation of collagen, are involved in a large number of Extra Cellular Matrix (ECM) disorders. Consequently, modeling the load-carrying mechanisms of collagen may not only contribute to our understanding of soft biological tissues biomechanics, but could also help to better understand collagen-related tissue disorders.
This work proposes a finite-strain constitutive model that considers recruitment and rupture of collagen fibrils being the key factors in determining the characteristics of the tissue biomechanics at higher load levels. Similarly to other published models, our model employs Probability Distribution Functions (PDFs) to express the progressive recruitment and subsequent rupture of collagen fibrils. The kinematics follow the multiplicative decomposition of the deformation gradient, and the constitutive description revises (corrects) and generalizes a model proposed earlier [1]. Although derived very differently, we demonstrate that such generalization defines a model that is equivalent to the recruitment and damage model proposed elsewhere [2]. Finally, in order to account for collagen fibers that are dispersed aligned in the tissue, we apply the general theory of fibrous connective tissue [3, 4]. The integration over the unit sphere is carried out by *t*-designs [5], and the model has been implemented into the Finite Element (FE) package FEAP (University of California at Berkley).

Stress-stretch properties predicted for a single collagen fiber (Mathematica, Wolfram Research Inc.) are used to explore parameter sensitivity, to verify the FE implementation and to test the plausibility of the physical assumptions made in our model. Finally, tearing apart a segment of the Achilles tendon demonstrated organ-level application of the proposed constitutive model, and yielded good quantitative [6] and qualitative [7] agreement with data from in-vitro experimental testing.

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Keywords: Non, linear tissue model, Anisotropy, Collagen, Damage, Finite strain

Interfibrillar damage accumulation causes fatigue of soft fibrous tissues: multi-scale mechanics and constitutive modeling

Markus Hillgärtner * [1], Kevin Linka [1], Mikhail Itskov [1]

[1] RWTH Aachen University, Department of Continuum Mechanics – Germany

In a recent experimental study of tendon pathology, cyclic loading with different strain amplitudes on rat tail tendon fascicles have been conducted, while the fibril strain was quantified by using a confocal microscope. Accordingly, tendon pathologies are correlated with an irreversible change of the tendon interfibrillar microstructure, which alters the microscopical tissue stress-response. In this contribution, a multi-scale constitutive model ranging from the tropocollagen (TC) molecule level up to bundles of collagen fibers is proposed and utilized to predict the elastic and inelastic long-term tissue response. The collagen fibrils are considered as a cross-linked assembly of TC molecules. The TCs inside a fibril can be in an entropic or energetic state, depending solely on their current configuration. Material failure of collagen fibrils is elucidated by a detachment of non-covalent bonds of the interfibrillar matrix. This kinetics is considered within a probabilistic framework of adhesive detachments of molecular linkages providing collagen fiber integrity. The final constitutive equations are validated against recent experimental data available in literature and show good agreement. All material parameters of the proposed model have a clear physical interpretation.

Keywords: Damage, Collgen, Fatigue

*Speaker

Optimization of Magnetic Resonance Imaging (MRI) based Patient Specific Models with mechanical property estimation from inverse finite element analysis

Robert Johnston * [1,2], David Nolan [1,2], Dorian Botella-Barillot [3], Milad Ghasemi [1,2], Christian Kerskens [4], Caitriona Lally† [1,2]

[1] Trinity Centre for Bioengineering, Trinity College Dublin, Ireland – Trinity Biomedical Sciences Institute Trinity College Dublin 152-160 Pearse Street Dublin 2 Ireland, Ireland
[2] Department of Mechanical and Manufacturing Engineering, Trinity College Dublin, Ireland – Mechanical & Manufacturing Engineering Parsons Building Trinity College Dublin Dublin 2 Ireland, Ireland
[3] Mechanical Engineering & Interactive Design Department, Polytech Montpellier, University of Montpellier, France – Polytech Montpellier, University of Montpellier – University of Montpellier Place Eugène Battalion - CC 419 34095 MONTPELLIER CEDEX 5, France
[4] Trinity College Institute of Neuroscience, Trinity College Dublin, Ireland – Trinity College Institute of Neuroscience Lloyd Building Trinity College Dublin Dublin 2 Ireland, Ireland

Vulnerable atherosclerotic plaque rupture is one of the main contributors to major cerebrovascular and cardiovascular events [1]. The distribution of stress in the arterial wall alters during atherosclerotic plaque progression [2]. Quantifying these stress distributions could offer a means to distinguish symptomatic and asymptomatic patients at risk of vulnerable plaque rupture. The objective of this study is to highlight the key factors that affect the finite element (FE) model reconstruction and the stress distributions within atherosclerotic carotid arteries. Patient specific finite element models can locate regions of high stress in an atherosclerotic vessel, which can in turn be used to quantify the risk of plaque rupture [3]. Real vessel geometries can be constructed from anatomical T2 weighted black blood MRI scans by delineating the vessel wall and interpolating between slices. By shifting the field of view (FOV), an increase in the axial data can be obtained improving the interpolation. High quality, hexahedral meshed finite element models can then be created from these registered segmented images.

An inverse finite element approach is used to compliment these patient specific models to estimate the mechanical properties of the healthy and diseased vessel walls *in vivo*. Adapting the process discussed in [5]: the first step in the inverse approach requires reconstruction of the artery geometry in systole and diastole. The artery is then given high stiffness linear elastic material behaviour and the so-called apparent stress at systolic and diastolic pressures is computed using the respective geometries. This can be done by implementing cardiac triggering of the pulse sequences to obtain the vessel wall and plaque in the desired phase. The second step involves building an objective function, where non-linear anisotropic material parameters are optimized to match the stress fields and mapped deformation gradients fields of the systolic and diastolic configurations computed in step 1. Using this technique, personalised geometries and mechanical properties can be calculated for healthy and diseased models.

This study determines the importance of MRI scanning parameters, such as the FOV and slice thickness in the reconstruction of patient specific models for stress analyses in carotid arteries. The accuracy of the stress field throughout these constructed models depends on both the in-plane resolution and the number of axial slices obtained. Qualitative and quantitative comparisons between the stress distributions for both healthy and diseased

*Speaker
†Corresponding author: lallyca@tcd.ie

models are made for a range of imaging parameters. All vessels are assigned optimized material properties based on estimations of the apparent stress field in the systolic and diastolic phases of the cardiac cycle.

Optimization of the scanning parameters in MRI is critical to accurately capture the geometry and material properties of healthy and diseased arteries *in vivo*. These optimized models could enable non-invasive identification of carotid plaques at risk of rupture.

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Keywords: Carotid Bifurcation, Finite Element Analysis, Magnetic Resonance Imaging, Constitutive Parameter Estimation

Characterization of irreversible physio-mechanical processes in stretched fetal membranes

Yulia Marom *† [1], Shlomit Goldman [2], Eliezer Shalev [2,3], Doron Shilo [1]

[1] Faculty of Mechanical Engineering, Technion – Israel
[2] Laboratory for Research in Reproductive Sciences, Department of Obstetrics and Gynecology, Emek Medical Center – Israel
[3] Faculty of Medicine, Technion – Israel

We perform bulge tests on live fetal membrane (FM) tissues that simulate the mechanical conditions prior to contractions. Experimental results reveal an irreversible mechanical behavior that appears during loading and is significantly different than the mechanical behavior that appears during unloading or in subsequent loading cycles. The irreversible behavior results in a residual strain that does not recover upon unloading and remains the same for at least 1 hour after the FM is unloaded. Surprisingly, the irreversible behavior demonstrates a linear stress-strain relation. We introduce a new model for the mechanical response of collagen tissues, which accounts for the irreversible deformation and provides predictions in agreement with our experimental results. Fittings of calculated and measured stress-strain curves reveal a well-defined single-value property of collagenous tissues, which is related to the threshold strain for irreversible transformation. Further discussion of several physio-mechanical processes that can induce irreversible behavior indicate that the most probable process, which is in agreement with our results for , is a phase transformation of collagen molecules from an a-helix to a b-sheet structure. A phase transformation is a manifestation of a significant change in the molecular structure of the collagen tissues that can alter connections with surrounding molecules and may lead to critical biological changes, e.g. an initiation of labor.

Keywords: Collagen, fetal membrane, irreversible transformation, phase transformation, mechanical behavior

*Speaker
†Corresponding author: yulia263@gmail.com

Constitutive modelling of collagen turnover towards the expansion of abdominal aortic aneurysms

Christopher Miller *† [1], T. Christian Gasser [1]

[1] Department of Solid Mechanics – KTH Royal Institute of Technology, Teknikringen 8, SE-10044 Stockholm, Sweden

Vascular tissue is endowed with a remarkable capacity to optimise its structure and organisation in response to its mechanical environment. Tissue growth and remodelling is achieved through a careful balance between the synthesis and degradation of its extracellular matrix (ECM) constituents; principally collagen, whose short half-life renders it integral to the tissues adaptive capabilities. Several cardiovascular pathologies are however characterized by a divergence away from normal healthy arterial remodelling. Specifically abdominal aortic aneurysms (AAA's), which are the result of an irreversible pathological alteration to the vessel wall, leading to a localized dilation of the Aorta at its infrarenal segment. As a result of the severe deterioration in Elastin content, fibrillar collagen is the predominant microstructural component of aneurysmatic tissue and is thus the main contributor to its mechanical functionality. It is postulated that a malfunction in collagen turnover prevents the tissue from reaching a homeostatic state and consequently is thought to be a contributing factor to AAA disease. Due to the inherent difficulties associated with the investigation of such phenomena, biomechanical modelling presents as a critical tool toward the evaluation of the underlying mechanisms associated with aortic expansion. Here we consider a multi-scale microstructural constitutive description of vascular tissue that accounts for the temporal adaption of the orientation dependent density and engagement probability of collagen fibrils, toward its impact upon the macroscopic stress state in patient-specific geometries. The present work builds upon the aforementioned model through a series of further refinements. Namely, the inclusion of a collagen fibril engagement stretch distribution concluded from in-vitro tensile testing data. Perhaps most significantly, we discuss the implementation of an updated engagement stretch distribution for newly synthesized collagen; where we introduce a dependency upon the current microstructural configuration of collagen and the pulsatile physiological deformation experienced by the vessel wall. The thought being that differences in strain pulsations in the circumferential and axial directions may influence the undulation at which vascular cells configure and incorporate fibrils into the ECM. Furthermore, a collagen degradation rate equation is introduced that accounts for the experimental observation that collagen is preferentially preserved at heightened strains.

Keywords: collagen turnover, remodelling, vascular tissue, aneurysm, growth, rupture, constitutive modelling

*Speaker
†Corresponding author: chrismi@kth.se

Engineered biomimetic nanopores: unravelling nuclear transport through coarse-grained molecular modeling

Ankur Mishra [1], Erik Van Der Giessen [1], Patrick Onck * [1]

[1] Micromechanics of Materials, Zernike Institute for Advanced Materials, University of Groningen – Nijenborg 4, 9747 AG Groningen, Netherlands

In eukaryotic cells the transport of biomolecules between the nucleus and the cytoplasm is enabled by the nuclear pore complex (NPC), a large protein complex embedded in the nuclear envelope. The NPC is lined with intrinsically disordered proteins that are rich in phenylalanine-glycine repeats (so-called FG-Nups). These FG-Nups not only form a permeability barrier for free diffusion of soluble macromolecules, they also provide the binding sites for active transport. Biomimetic nanopores have been engineered recently with the aim to understand nucleocytoplasmic transport by mimicking the essential transport features of the NPC. In these nanopores, single molecule events governing nucleocytoplasmic transport are detected by measuring the conductance of ions through the nanopore under an applied electric potential. It was found that individual transport receptors were able to pass through, whereas inert particles of similar size were effectively blocked. To gain a better fundamental understanding of these observations, we use a one-bead-per-amino-acid coarse grained molecular dynamics model to describe the dynamics of the FG-Nups. We studied the time-averaged protein density of nanopores coated with FG nups and related the density distribution to ionic conductance through the nanopores. Our results show a low conductance below a critical nanopore size and a near-linear conductance above it. We address the selectivity of inert particles (tCherry) and transport receptors (kap95) by calculating the potential mean of force (PMF) associated with these particles in pores coated with the FG-Nup Nsp1 and a mutated version, Nsp1-S, in which hydrophobic amino acids are replaced by neutral beads. The energy barriers obtained from the PMF curves are used to predict the experimentally-observed event rates.

Keywords: Molecular dynamics, nuclear pore complex, biological materials

*Speaker

Modelling perfusion in liver parenchyma using two-level homogenization

Eduard Rohan * [1,2], Vladimír Lukeš [3], Jana Turjanicová [3]

[1] University of West Bohemia in Pilsen, Faculty of Applied Sciences, NTIS (UWB) – Univerzitni 8, 30614 Pilsen, Czech Republic
[2] University of West Bohemia – Czech Republic
[3] University of West Bohemia in Pilsen, Faculty of Applied Sciences, NTIS (UWB) – Czech Republic

The liver parenchyma is formed by the lobular structure which can be approximated as a periodic array constituted by the honeycomb cells. Each such cell is formed by the sinusoidal porosity which separate so-called vertex and central veins. Although this picture is an idealization of the real structure, it is a convenient basis for modelling flow in the deforming liver tissue using the homogenization technique. In the paper we compare two homogenized models relying on different assumptions.

The first model is derived by the homogenization of the mesoscopic structure with the double-porosity medium represented by the Biot model with large contrasts in the permeability coefficients constituting the Darcy law. In the dual porosity associated with the sinusoids, the scaling of the permeability leads to the macroscopic model with two macroscopic pressure fields associated with the portal and hepatic vascular compartments. The poro-viscoelastic coefficients are obtained by the homogenization of the quasistatic Biot model. The macroscopic model is featured by the fading memory effects inherited from the time convolution integrals, see [1,2]

The second perfusion model is an extension of the previous work [3], where the rigid medium was considered. The new model is derived using the reiterated homogenization of the fluid-structure interaction. The first stage produces the homogenized Stokes flow problem associated with the sinusoids. The scaling of the viscosity enables to respect the double porosity effects characterizing flow in the liver lobulae. The macroscopic model is defined in terms of the pressure field associated with flow in the liver sinusoids, and the two velocity fields associated with the precapillary vessels of the portal and hepatic vein systems.

We illustrate and compare the properties of the two models using selected examples with the representative periodic cell describing the liver tissue lobulus. The numerical results are computed using the finite element method implemented in the SfePy software (see sfepy.org).

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*Speaker

Keywords: liver tissue, perfusion, periodic homogenization, double, porosity media

Influence of microstructure on tensile behaviour of unidirectional hemp composites under controlled humidity.

Samuel Réquilé * [1], Antoine Le Duigou [1], Alain Bourmaud [1], Christophe Baley [1]

[1] Institut de Recherche Dupuy de Lôme (IRDL - CNRS FRE 3744) – Université de Bretagne Sud, CNRS : FRE3744 – France

Ecological and environmental concerns have increased the interest in the use of natural fibers to substitute synthetic fibers for the development of composites. Hemp fibers are interesting candidates to fulfill the requirements of biocomposites with an interest driven by high performances as well as environmental factors. They offer many advantages over conventional reinforcements: they are abundant and renewable resources, present low density, high specific properties [1]–[3] and a low price which has been constant over the years [4]. These advantages justify their use in numerous composite applications such as the automotive industry, plastic processing and building applications.
In composite materials, high mechanical performances is mainly governed by the quality of the fiber/matrix adhesion as well as the mechanical properties and the aspect ratio of the reinforcement homogeneously distributed into the matrix [5]. Therefore, in the case of natural fibers, the state of division of the fiber bundles, as initially organized in the plant, gives rise to a complex definition of the microstructure as compared to man-made fibers [6]. The single fiber and bundle's proportion is driven by middle lamellae whose cohesion evolves according to the degree of retting. This operation enables its degradation by an enzymatic degradation mechanism. Thus, using hemp fibers as reinforcement highlights a mixing of elementary fibers and bundles into the laminate.

While the work carried out over the last few years reveals the high potential use of biocomposites, the lack of information regarding their behaviour in humid environments limits the extension of their use for various applications. It is now well-established that water in the form of vapor or liquid, penetrates preferentially into the fibers and induces reduction of laminate properties [7]. In addition, middle lamellae that controls bundle cohesion are composed of amorphous pectins which very sensitive to moisture [8].

A key question is therefore about the influence of composites' microstructure on the hygroscopic behaviour of biocomposites. We take the challenging question in this work and hence, study the influence of composite microstructure, *i.e.* reinforcement aspect ratio, and retting degree on the hygroscopic response (water uptake, swelling, diffusion mechanisms) of the composite as well as its induced mechanical properties.

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Keywords: Natural fibers, Biocomposites, Microstructure, Hygroscopic behaviour, Tensile testing

S12: Mechanics of interfaces and evolving microstructures

Microstructural characterization of an IN718 linear friction weld

Xavier Boyat * [1], Dorick Ballat-Durand [2], Salima Bouvier [2], Julie Marteau [2], Jérôme Favergeon [2]

[1] Université de Technologie de Compiègne [Compiègne] (UTC) – Université de Technologie de Compiègne [Compiègne] : UMRCNRS - 7337 – rue du Dr Schweitzer Compiègne, 60200 FRANCE +33 3 44 23 44 23, France
[2] Université de Technologie de Compiègne [Compiègne] (UTC) – Université de Technologie de Compiègne [Compiègne] – rue du Dr Schweitzer Compiègne, 60200 FRANCE +33 3 44 23 44 23, France

Linear Friction Welding is a solid-state joining process already in use as a niche technology for the assembly of bladed disks in aero-engines. The weld is obtained by the friction of a moving part in a reciprocating motion on a stationary part under a force. The local heat generation at the interface causes the materials to flow expelling along oxides and surface contaminants with plastically deformed material allowing parts coalescence in a thin metallurgical bond. Aerospace industry is showing a growing interest in the potential of LFW technology as a substitute in aircraft parts production to massive machining by material removal and is in concurrence with additive manufacturing processes. Moreover solid state welding is an interesting alternative avoiding solidification problems as grain boundary liquation, detrimental phase formation or micro-cracking problems in fusion zone.
In this study butt-weld test campaigns were carried out implying the joining of Ni-Fe-Cr superalloy Inconel 718 (10 x 80 x 70 mm3) solid blocks with a 10 x 80 mm2 weld surface dimensions. Alloy Inconel 718 is a γ" (Ni3Nb) precipitation hardenable material extensively used for service in extreme environments applications due to its good mechanical properties at high temperature and its excellent corrosion resistance. Two material heat treatment conditions were friction welded : ST and STA. The base material in ST condition consists in a microstructure composed of D=50 μm γ-fcc austenitic grains with δ-orthorhombic inter-granular Ni3Nb phase. Two successive annealing at 720◦C then 620◦C were applied to obtain the STA condition yielding to the strengthening of the initial γ-fcc austenitic matrix by the quasi-coherent precipitation of γ" (Ni3Nb) disc-shaped particles evenly distributed in the fcc matrix.

During the welding process, severe thermo-mechanical loads are applied resulting in local microstructure and mechanical properties modifications. The characterization of the post-welded microstructures has been carried out by SEM and EBSD analysis on cross sectioned weld samples. Local inspection of the welding zone revealed the presence of a thermo-mechanical affected zone (TMAZ) that consists in a thick band of uniform dynamic recrystallized grains with an equiaxed grain morphology around the welding line, then a partially recrystallized zone composed of fine recrystallized grains distributed along the grain boundaries of elongated grains followed by a zone made of deformed grains remaining from the initial microstructure. Phase and microstructure changes across the joint were shown to have influence on hardness properties by micro-hardness tests across the welds.
As many nickel based alloys controlling the microstructure and the grain size and distribution after hot processing of IN718 is a key factor in the optimization of the mechanical properties of the material. To that end, post weld heat treatments were applied in an attempt to recover a homogeneous microstructure across the weld with interesting mechanical properties for in-use applications.

Keywords: Linear friction welding, welding interface, recrystallization

*Speaker

Experimental investigation of Austenite-Martensite phase boundary motion in Ni-Mn-Ga

Emil Bronstein * [1], Eilon Faran† [1], Doron Shilo‡ [1]

[1] Technion – Israel

Martensitic and reverse martensitic phase transformations in shape memory alloys are considered to be "very fast", even supersonic, due to their diffusionless and athermal nature. However, how fast they really are, has yet to be resolved. Specifically, kinetic laws for the evolution of the phase transformation and in particular the kinetic relations between the thermodynamic driving force and the velocity of individual austenite-martensite (A-M) interfaces have yet to be revealed. To uncover the true kinetics of the phase transformation, experiments have to be performed under conditions at which the transformation rate is restricted neither by the rate of heat transfer nor by mechanical inertia. In this work, we present a novel experimental method for investigating the kinetics of the martensite phase transformation in single crystals through two complementary experimental setups: (1) slow (quasi-static) heating and (2) fast pulse heating. In both types of experiments, the tested sample is clamped at its ends such that there are no moving masses during the phase transformation. In addition, all experiments are conducted under an optical microscope equipped with a high-speed camera, enabling tracking the propagation of individual interfaces and the evolution of the twinned microstructure at the A-M interface during propagation of the phase boundary. Setup (1) can provide information on the quasi-static characteristics of the phase transformation through the visualization of the twinned microstructure at the A-M interface, as well as direct measurement of the stress-temperature phase diagram. In setup (2), a short heating pulse (at the time scale) is applied to the tested sample and promotes phase transformation under nearly isothermal conditions. In situ optical tracking enables the measurement of the temporary velocity of the phase boundary, while the corresponding stress is measured with a dedicated force sensor.

Keywords: Kinetics of phase transformation, Rapid heating

*Speaker
†Corresponding author: eilonfa@technion.ac.il
‡Corresponding author: shilo@me.technion.ac.il

Experimental and numerical study of allotropic transformation in iron

Nicolas Bruzy * [1], Michel Coret† [1], Laurent Stainier [2], Bertrand Huneau [1]

[1] Institut de Recherche en Génie Civil et Mécanique (GeM) – Ecole Centrale de Nantes, Université de Nantes, CNRS : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[2] GeM / Ecole Centrale de Nantes (GeM) – Ecole Centrale de Nantes – 1 rue de la Noë 44321 Nantes, France

Owing to the growing complexity of iron-based alloys microstructures and the high deformation levels involved in their industrial processing, the need for a better understanding of the intricacy between phase changes and plasticity at the mesoscale has emerged. As a first step towards this goal, this work focuses on ferrite-austenite transformation. Strain fields are obtained at a subgrain scale, thus allowing a characterization of the mechanical perturbations induced by the change of compacity between the two phases.
An experimental device is developed in-house to perform in situ observations. Experiments are conducted on nearly pure iron samples (with Carbon content of approximately 0.001%) whose characteristic grain size is 200 μm. Electron Backscattered Diffraction (EBSD) analyses are carried out before and after testing in an attempt to gain further insight into microstructure evolution. Heating up to phase change temperature is performed through Joule effect. A PID regulation is synthesized to impose temperature ramps to the samples. Typical heating rate is around 10$\circ$C/s. Images of the surface of the samples are captured by means of a high-resolution camera. Following previous works at high temperatures [1], special care is taken to avoid samples degradation and/or loss in image quality during heating. In particular, samples are put in an inert argon atmosphere and an optical illumination and filtering system in the blue wavelengths is implemented.

Samples are designed so that they present both a central zone - where temperature is homogeneous and transformation initiates - and an external zone in which the establishment of a temperature gradient allows the progression of a transformation front. Alumina painting is deposited on the sample to form a speckle pattern and strain fields are computed thanks to the Digital Image Correlation (DIC) technique. Calculations are performed using UFreckles software. Maximum shear strain is selected as an indicator of transformation occurrence. During phase change, it exhibits maxima that seem to correspond with the underlying grain boundaries, especially with triple junctions.

In parallel, a numerical model that assimilates the medium to a dissipative standard material is developed under the small strain assumption. In accordance with variational principles [2], thermal, mechanical and transformational contributions are gathered in the expression of a power functional whose stationarity conditions are equivalent to the considered thermo mechanical problem. Finite element calculations are performed on meshes built from experimental data. Boundary conditions aim at reproducing experimental solicitations. Heterogeneities induced by these latter are shown to strongly influence the onset of transformation and its subsequent evolution.

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*Speaker
†Corresponding author: michel.coret@ec-nantes.fr

Keywords: Iron, Allotropic transformation, Digital Image Correlation

An elastic phase field model of pressure-assisted sintering

Branislav Dzepina * [1,2], Daniele Dini [1], Daniel Balint [1]

[1] Imperial College London (ICL- Mech. Eng.) – United Kingdom
[2] Centre for Doctoral Training in Diamond Science and Technology (DST CDT) – United Kingdom

Pressure solution is a deformation mechanism experienced by non-hydrostatically stressed elastic bodies whose primary mode of material transport is diffusive mass transfer. Although originally investigated within the geology community to describe the enhanced compaction of rock and soil particles, the pressure solution mechanism is also applicable to the high pressure sintering of advanced metals and ceramics. During the ultra-high pressure liquid phase sintering of diamond grains, which is the focus of the study, it is estimated that inter-particle contact pressures can exceed 100 GPa at some of the contacts. Within the vicinity of these contacts, significant elastic strain energy is stored in the material. As a result of diffusive transfer, material is transported along energy gradients from the contact to the lesser stressed surrounding particle surface. Tracking of the particle interfaces due to this deformation mechanism is not trivial, especially when other processes such as bonding are considered. Thus a phase field model for this process is proposed. Elastic energy in phase field models have previously been reported in literature, however, these models are usually concerned with the strain energy resulting from elastic mismatch at the interfaces, phase transformation or strain fields applied to the entire simulation domain.
The presented work is an extension on the advective-diffusive sintering phase field model initially proposed by Wang [1]. Here, a free energy functional is composed of bulk, interface and grain boundary energy. The particles are initiated by scalar fields which represent their mass density within the simulation domain. Given a starting configuration, the diffuse interfaces of the particles are allowed to evolve in time in order to minimise the energy of the system. In addition to Wang's model, an elastic energy term is included in the free energy functional to accommodate the strain energy at the contacts. Contact pressure distribution within the contact is approximated by the overlap of the scalar fields that represent the respective particles. Rigid particle motion by advection velocity fields is used to maintain contact between the particles. The effect of pressure solution on the shape of a single particle pressed onto a non-interacting wall is presented. The proposed model is also applied to the demonstration of high pressure sintering between two particles and finally to a cluster of several interacting particles.

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Keywords: Contact, pressure solution, phase field

*Speaker

Dynamics of twin boundaries in FSMA Ni-Mn-Ga: mechanisms of motion, energy barriers, and kinetic relations

Eilon Faran * [1], Doron Shilo * † [1]

[1] Faculty of Mechanical Engineering, Technion – Israel

Twinning is a shear dominated material transition that plays a significant role in metal plasticity, geological processes, and actuation of shape memory and ferroelectric materials. In these materials, twinning transformation proceeds through the motion of twin boundaries as a result of a mechanical / electrical / magnetic driving force. The motion of a twin boundary is dictated by various energy barriers that resist boundary motion, which may have different intensities (amplitude) and widths (length scale). In addition, different barriers may be overcome by different mechanisms of motion, thus leading to the existence of different kinetic relations. The latter are basic material laws that correlate the velocity of a material interface to the thermodynamic driving force. In this work we employ combined theoretical and experimental approaches for studying the dynamics of sidewise twin boundary motion in a representative twinned ferromagnetic Ni-Mn-Ga crystal. Pulsed magnetic field tests coupled with direct optical tracking of individual interfaces lead to experimentally measured kinetic relations. Several mechanisms for the propagation of a twin boundary are considered, based on the topological description of the interface, and are validated against the experimental results. This approach leads to the identification of the dominant energy barriers for twin boundary motion and to the extraction of atomistic scale material properties that govern the dynamics of twinning. For example, we identify the intrinsic lattice barrier as a critical material property that determines the transition from slower, thermally activated twin boundary motion to faster, a-thermal motion. Finally, we discuss the potential of applying validated kinetic relations for modeling the dynamic macroscopic response of FSMA-based actuators.

Keywords: Twin boundaries, kinetic relations, Ni, Mn, Ga

*Speaker
†Corresponding author: shilo@technion.ac.il

Multilevel model of inelastic deformation of polycrystalline, including description of recrystallization process

Nikita Kondratev * [1], Peter Trusov [1]

[1] Perm National Research Polytechnic University (PNRPU) – Russia

The physical and mechanical properties of materials, the working characteristics of finished products, as is known, are determined by the current state of the internal structure of different scale levels [1]. In the processing of metals, the internal structure significantly changes. A correct description of the structure of the material makes it possible to optimize the existing and develop new methods for obtaining materials and products with enhanced performance characteristics. Consequently, in recent decades, models based on explicit consideration of mechanisms and carriers of inelastic deformation have evoked interest in the mechanics of a deformed solid [1]. In such models, as a rule, for the correct description of the existing mechanisms of plasticity, it is necessary to introduce several scale levels (two or more). The multilevel approach is universal and can be used to design structures from new, not yet existing materials, and to create technologies for their production [2].
The theoretical basis of this research method is mathematical modeling using procedures for identification and verification of the model. In the framework of a multilevel approach for describing the inelastic deformation of metals under thermomechanical effects at the macrolevel, a material point with a set of homogeneous characteristics is considered. In accordance with this point, a set of homogeneous regions of the underlying scale level [3]. The characteristics of the upper level are determined by averaging the "related" parameters of the lower level. The number of scale levels involved in consideration is determined by the aims, research tasks and the most important mechanisms of inelastic deformation. At lower scale levels, there is a fundamental possibility of correctly taking into account the mechanisms of inelastic deformation. An approach is used to construct the defining relations, based on the introduction of internal variables that reflect structural interactions and rearrangements of the meso- and microstructure. Thermomechanical effects are transferred from the macrolevel and lead to a change in the internal structure, which then determines the effective characteristics of the material.

A multilevel approach allows describing the response of a material with the same type of determining ratios at different scale levels. In the framework of this paper, Hooke's law is used in the arte relaxation form, written in terms of asymmetric measures of strain rates. At the meso level, crystallite (a homogeneous part of a polycrystalline material) is considered with a set of prescribed properties (anisotropic elastic moduli, lattice orientations, a set of slip systems). An important aspect of the model is a correct description of the evolution of the variables responsible for the indicated properties of the crystallite. The kinematic relations that describe inelastic deformations at the mesic level due to slipping of dislocations, evolution relationships for critical shear stresses (by different mechanisms), a description of the rotation of the crystallites, the effect of temperature changes, and the applied stresses on the development of the defect structure are included in the model.

The paper formulates a model of the physical theory of plasticity for describing the deformation of polycrystalline materials taking into account the evolving internal structure of the material. Elevated deformation temperatures lead to activation of relaxation processes of elastic stresses. They are recovery and recrystallization. The first process occurs due to reorganization of the dislocation substructure. The description of the second process requires consideration of changes in the morphology and structure of grains and their boundaries. In this paper, recrystallization is included, based on the mechanism of the motion of the initially existing boundaries of

*Speaker

the polycrystal due to plastic deformation. The basis of the grain boundary migration model is the ratio of Bailey and Hirsch [4], based on a comparison of the difference in the stored energy in neighboring grains and the surface energy of the boundary between them. When the criterion is satisfied, grain boundaries begin to move, and the kinetics of their growth is determined by the relationship between the theory of grain boundary mobility [5]. The normal growth of grains is associated with grain boundary steps, i.e. the normal component of the Burgers vector of orientation mismatch dislocation [6]. Within the framework of the two-level model, a method for describing the movement of the boundary is proposed.

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Keywords: crystal plasticity, recrystallization, grain structure, microstructure

Dynamic recrystallization and grain growth kinetics in Inconel 718 using cellular automata

Sushil Mishra * [1], Rajat Gujrati† [1], Jyoti Jha‡ [1]

[1] Department of Mechanical Engineering [IIT-Bombay] (ME-IIT) – IIT-Bombay, Powai, Mumbai 400 076, India, India

The hot deformation behavior of Inconel 718 with a homogenized microstructure is modeled in the temperature range 900–1100∘C and strain rate range 0.001–10s–1, for obtaining processing windows and achieving microstructural control during hot working. The processing map has been developed on the basis of flow stress data as a function of temperature, strain rate and strain. The map exhibited three different domains: (i) the equiaxed microstructure domain is identified to represent the fully recrystallized grain occurred at about 1000-1100∘C temperature and strain rate 0.001-0.01s–1. (ii) the equiaxed grain with pancake microstructure exhibited at the high temperature and high strain rate 1000-1100∘C temperature and strain rate 1-10s–1 respectively. (iii) Undeformed domain exhibits at the temperature range 900-1050∘C and strain rate close to 0.1s–1. (iv) Dynamic recrystallized domain at 900-950∘C and strain rate of 0.001-0.1s-1 respectively.
Further, interrupted compression tests at temperature 950∘C and strain rate of 0.01s-1 for 10%, 20%, 30% and 40% deformation have been carried out to understand the dynamic recrystallization and the microstructure evolution with the increase in the strain increment. Grain boundary serration, nucleation, and growth lead to the microstructure evolution. Kocks-Mecking plots and Avrami plots were plotted corresponding to flow stress data at the different forming condition of temperature and strain. Avrami constants were calculated to understand the kinetics of dynamic recrystallization. Cellular automata based model for the grain growth in DEFORM 3D was employed to simulate grain growth and its kinetics at required temperature and strain. In this study understanding of dynamic recrystallization and its prediction in Inconel 718 was established.

Keywords: Dynamic recrystallization, serration, nucleation, Kocks, Mecking, Avrami, Cellular Automata, DEFORM 3D

*Speaker
†Corresponding author: rajat.gujrati@iitb.ac.in
‡Corresponding author: jyoti.jha@iitb.ac.in

Monoclinic lath orientation choice and related local energy barriers for microstructure structure formation in zirconia

Mohan Kumar Rajendran *† [1], Michael Budnitzki [1], Meinhard Kuna [1]

[1] TU Bergakademie Freiberg, Institute of Mechanics and Fluid Dynamics (IMFD) – TU Bergakademie Freiberg, Institut für Mechanik und Fluiddynamik Lampadiusstraße 4 09596 Freiberg, Germany

In zirconia (ZrO 2) systems a martensitic phase transformation (MPT) ie. tetragonal (t-phase) to monoclinic phase (m-phase) transformation (t→m) is most commonly observed between room temperature 300K and martensitic start temperature 1305K. Such a martensitic transformation has a vital role in dissipating impact stresses during crash and providing fracture toughness at the crack zone. The crystallography of lattice structures and orientation of parent t-phase and the product m-phase lath structure plays an important role in dissipating impact stresses by phase transformation (t→m) in the system. The possible orientations of the monoclinic variants determine the orientation of monoclinic lamellas. In a simplest possible 2D case of such a transformation there remains two possible configurations for the choice of lamelar direction. The first most simplest and the least possible energy state is when the junction plane and habit plane align on each other. The second possible case is when the junction plane and habit plane has a angle mismatch which equals to shear angle experienced by crystal during transformation from tetragonal to monoclinic. In both configurations the junction plane is aligned to one of the monoclinic crystal lattice directions $< 100 >$. Both configuration has same transformation strain since crystal experiences a rigid body rotation, so they have a equal chance of formation but the choice mainly depends on geometrical influence by grain shape, nucleation site, external loading and boundary conditions. The junction plane of both configuration are perpendicular to each other. The difference with the second type of configuration with angle mismatch is, there remains some tetragonal phase untransformed (tetragonal wedges) mostly stabilized by elastic energy at the domain/grain boundaries. A study is conducted which illustrates these possible configurations and their local energy wells with finite element method (FEM) based framework used to describe the boundary value problem and Phase-field method utilized to describe the microstructure evolution. The study also illustrates that, it is possible to achieve specific orientation choice by introducing additional elastic energy by means of external mechanical loading conditions and force the system to attain a specific local minima.

Keywords: Zirconia, Phase transformation, microstructure, energy barriers

*Speaker

†Corresponding author: Mohan-Kumar.Rajendran@imfd.tu-freiberg.de

Rate-independent dissipation in phase-field modelling of evolving microstructures

Stanislaw Stupkiewicz * [1], Karel Tůma [2], Henryk Petryk [1]

[1] Institute of Fundamental Technological Research, Polish Academy of Sciences (IPPT PAN) – Poland
[2] Faculty of Mathematics and Physics, Charles University – Czech Republic

The phase-field method is a well-established approach to modelling of microstructure evolution. In this approach, a phase boundary is treated as a diffuse interface and is described using an order parameter that is spatially continuous. Evolution of microstructure and, specifically, propagation of diffuse interfaces is then typically described by an evolution equation of a viscous type. Consequently, interface motion can be triggered by a vanishingly small driving thermodynamic force, and the system asymptotically evolves towards an equilibrium state of vanishing driving forces. Furthermore, the hysteresis, e.g. in the stress-strain response, depends on the rate of external loading, and it tends to zero as the rate of loading tends to zero. The usual phase-field approaches are thus not capable of describing rate-independent dissipative effects, such as microstructure arrest and non-zero hysteresis in cyclic response at vanishing external loading rate. At the same time, the related effects are commonly observed, for instance, in materials undergoing displacive transformations, such as martensitic transformation and twinning.
In this work, rate-independent dissipation is introduced into the phase-field framework for modelling of microstructure evolution in displacive transformations. As the starting point, we take our recent finite-strain phase-field model [1,2] which employs a purely viscious dissipation. The corresponding variational formulation is then extended by including a non-smooth mixed-type dissipation potential that combines the viscous and rate-independent contributions. As a results the evolution problem is formulated in a concise form as a constrained, non-smooth minimization problem for a global rate-potential. The rate formulation is next transformed into an incremental finite-step formulation which is the basis for the finite-element implementation. Computational treatment of the incremental problem is based on the augmented Lagrangian method [3] in which a single field of scalar Lagrange multipliers is used to enforce the physical constraints on the order parameter and to handle the non-smooth dissipation potential. The model has been applied to solve two- and three-dimensional boundary value problems representative for shape memory alloys.

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Keywords: microstructure, diffuse interfaces, phase, field method, non, smooth minimization

*Speaker

Atomistic study of the reorientation behaviors in magnesium single crystals

Qun Zu *† [1], Yafang Guo [2]

[1] Hebei University of Technology – China
[2] Beijing Jiaotong University – China

The plastic deformation mechanisms in Mg nano-pillars under compression and tension of different orientations are investigated by molecular dynamics simulations. Multiple crystalline reorientations, *e.g.* basal/prismatic (BP) transformation, double twin-like lattice reorientation and shear band, are particularly studied. Particularly, under *c*-axis tension, the BP transformation plays an important role in plastic deformation. BP interfaces nucleate by a shuffling mechanism via local atomic rearrangement. Both two-layer disconnection and one-layer disconnection contribute to the migration of the BP interfaces. The three-dimensional analysis reveals that the junction between the free surface and BP interface is the source of one-layer disconnections, and that of the partial pyramidal dislocations and BP interface is the source of two-layer disconnections. The disconnections prefer to move towards the [1-210] direction rather than the [-1010]/[0001] direction since the accumulation of mismatches along the [-1010]/[0001] direction can impede the disconnections movement. Moreover, the boundary between the matrix and reoriented crystal is consisted of BP interface and {10-12} twin boundary or series of BP/PB interfaces. The transformation between each other can be fulfilled by the glide and accumulation of interfacial disconnections. Furthermore, Both BP transformation and {10-12} twinning can effectively accommodate the applied tensile strain along the *c*-axis. The co-existing BP interfaces and {10-12} twin boundaries allow for large deviations of a twin interface from the {10-12} twin plane.

Keywords: Molecular dynamics, Crystalline reorientations, Basal/prismatic interfaces, {1012} twin boundary, Mg

*Speaker
†Corresponding author: zuqun0322@163.com

S13: Mechanics of discrete systems

On the debris-level origins of adhesive wear

Ramin Aghababaei [1], Derek Warner [2], Jean-François Molinari *† [3]

[1] Aarhus University – Denmark
[2] Cornell University – United States
[3] Ecole Polytechnique Federale de Lausanne (EPFL) – Switzerland

Every contacting surface inevitably experiences wear. Predicting the exact amount of material loss due to wear relies on empirical data and cannot be obtained from any physical model. Here, we analyze and quantify wear at the most fundamental level, i.e., wear debris particles. Our simulations show that the asperity junction size dictates the debris volume, revealing the origins of the long-standing hypothesized correlation between the wear volume and the real contact area. No correlation, however, is found between the debris volume and the normal applied force at the debris level. Alternatively, we show that the junction size controls the tangential force and sliding distance such that their product, i.e., the tangential work, is always proportional to the debris volume, with a proportionality constant of 1 over the junction shear strength. This study provides an estimation of the debris volume without any empirical factor, resulting in a wear coefficient of unity at the debris level. Discrepant microscopic and macroscopic wear observations and models are then contextualized on the basis of this understanding. This finding offers a way to characterize the wear volume in atomistic simulations and atomic force microscope wear experiments. It also provides a fundamental basis for predicting the wear coefficient for sliding rough contacts, given the statistics of junction clusters sizes.

Keywords: Adhesive Wear, Discrete Modeling, Molecular Dynamics

*Speaker
†Corresponding author: jean-francois.molinari@epfl.ch

Extreme loading of Diamond-Like-Carbon Coatings: SEM and FIB Damage Characterization

Antonios Choleridis *† [1], Christophe Héau [2], Marie-Alix Leroy [2], Sergio Sao-Joao [1], Guillaume Kermouche [1], Christophe Donnet [3], Helmut Klöcker [1]

[1] Laboratoire Georges Friedel, UMR 5307 – Ecole Nationale Supérieure des Mines de St Etienne – France
[2] Institut de Recherche en Ingénierie des Surfaces – Groupe HEF – France
[3] Laboratoire Hubert Curien, UMR 5516 – Université Jean Monnet [Saint-Etienne] – France

Introduction

Diamond-Like-Carbon Coatings are widely used in mechanical applications for wear and friction reduction. Some severe loadings are sometimes observed for automotive components. In present work, DLC coatings have been produced by Plasma Enhanced Chemical Vapor Deposition [1]. An under layer followed by 20% hydrogenated DLC coatings were deposited on a M2 Steel substrate (Figure 1a). These coatings exhibit high residual compressive stresses. Classical characterization means indicate a good adhesion prior to tribological loading.

Extremely severe contact loading in an oil bath at 100◦C was achieved in the friction test facility shown in Figure 1b. It consists of a rotating ring rubbing against the surface of the DLC coated sample. At the same time, an oscillating in-plane movement of the specimen takes place.

The process induced residual stresses have been measured on FIB milled micro-beams and corroborated by FE simulations. The damage induced by the extreme loading conditions has been characterized by post mortem SEM and FIB observations and quantified by AFM measurements.

Results

Samples with several DLC coating thicknesses were tested. The compressive residual stresses [2,3,4] in the DLC coating vary from _˜1 to _˜2 GPa. The largest coating thickness leads to the highest stress.

The tribological loading (ring plane experiment) leads to significant wear. Figure 1c shows the macroscopic wear trace. Small blisters are observed close to the ring's exit.

The SEM observations in Figure 2a reveal cracks on blisters borders. The damage mechanism was analyzed thoroughly by FIB cross sections through particular blisters. Figure 2b shows a typical cross section revealing the substrate, the interface and the different layers of the coating. A thin layer of substrate material remains attached below the under layer. Moreover, it is found that its thickness is maximal in the center of the blister and decreases moving to its borders.

An EDX analysis was made in several zones of this film. As expected from the previous SEM observations the quantity of iron (Fe) detected is increased at the center of the blister and progressively decreases up to the borders.

Conclusions

*Speaker
†Corresponding author: antonios.choleridis@emse.fr

The high compressive residual stresses on perfectly adherent films prior any solicitation were quantified by micro-beam deflection measurements and FE simulations. Tribological loadings in the ring on plane friction test facility lead to film blistering and delamination. This damage has been characterized by SEM observations after FIB cross sectioning particular blisters.

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Keywords: Extreme loading, DLC Coatings, Damage Characterization

Poisson's ratio measurement by a combination of normal and lateral indentation

Thomas Chudoba * [1]

[1] ASMEC GmbH (ASMEC) – Maria-Reiche-Str. 1 01109 Dresden, Germany

High resolution normal force-displacement measurements are used since more than 30 years for nanoindentation experiments to investigate indentation hardness and modulus perpendicular to the surface. However conditions in an application are often more complex and the understanding of surface or coating failures also requires the consideration of lateral forces. Further the Poisson's ratio, internal stresses or lateral inhomogeneity cannot be extracted from normal measurements alone. The Poisson's ratio of coatings is mostly not known and only an assumption is used to convert the reduced modulus (that is measured by nanoindentation) to the indentation modulus.
Since few years a lateral force unit can be used in combination with nanoindentation technique to measure lateral force-displacement curves also with nanometer resolution. This unit is not only a tool for friction force measurements. An internal actor like in a nanoindentation head allows the application of lateral forces without any requirement of lateral movement between indenter and sample beside a small elastic deformation. The transition between full sticking, the reduction of the contact area due to increasing shear stresses and the begin of sliding can be fully resolved. This transition range between sticking and sliding friction, which is typically connected with a lateral elastic deformation below 100nm, can be used to measure the lateral contact stiffness. The ratio of lateral and normal contact stiffness was used by Lukas et al. in a publication from 2004 [1] to derive the Poisson's ratio for several materials, but the results could not be confirmed by another group.

It will be shown that it is possible to derive the Poisson's ratio for hard and smooth materials by a combination of fully elastic normal and lateral force-displacement measurements. A fit of the lateral curves in the reversal points of a lateral deformation of only some tenth of nanometer is used together with friction coefficient and contact area to calculate the shear modulus. The Young's modulus is obtained from the normal elastic deformation. Finally the Poisson's ratio can be derived from Young's and shear modulus. At the end, first results will be given where the Poisson's ratio is obtained from combined normal and lateral indentation measurements with a sharp Berkovich indenter.
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Keywords: Poisson's ratio, shear modulus, indentation

*Speaker

Surface roughness genomics: a new approach to multiscale modelling of roughness

Paolo Cinat [1], Marco Paggi [*†] [1]

[1] IMT School for Advanced Studies Lucca – Piazza San Francesco 19, 55100 Lucca, Italy

The modern nano-technology is becoming more and more sophisticated, requiring an efficient description of multi-scale roughness at different length scales to characterize interface properties such as the electric contact conductance. A new approach, called surface roughness genomics, is herein proposed to characterize surfaces at multiple length scales from the topological point of view. Similar to biological systems, where the biological information is encoded in DNA base pairs, surface roughness is decomposed in elementary waves, whose unique ensemble is the surface genome. The identification process of genomes, the sequencing procedure, is based on the solution of a constrained convex optimization problem. The reconstruction of a rough profile from its genomes is pursued following a top-down or a bottom-up approach, to understand and quantify the role of specific multi-scale features on the contact problem.

Keywords: Contact mechanics, surface roughness, convex optimization

[*]Speaker
[†]Corresponding author: marco.paggi@imtlucca.it

Galling characterization and classification in several stainless steels

Thibault Lesage [1], Salima Bouvier * [1], Yan-Ming Chen [2], Marion Risbet [1], Abdeljalil Jourani [1], Abdelali Oudriss [3], Pierre-Emmanuel Mazeran [1]

[1] Université de Technologie de Compiègne (UTC) – Université de Technologie de Compiègne – rue du Dr Schweitzer Compiègne, 60200 FRANCE +33 3 44 23 44 23, France
[2] CEntre Technique des Industries Mécaniques (CETIM) – CEntre Technique des Industries Mécaniques - Cetim (FRANCE) – France
[3] LaSIE UMR - 7356 CNRS - Université de La Rochelle – Université de La Rochelle – Av. Michel Crépeau, 17042 La Rochelle, France

Galling is a severe case of adhesive wear; it goes with the appearance of undesirable surface modifications leading to the deterioration of components in contact. It is problematic in a wide range of industrial applications, *e.g.* medical instruments, sheet metal forming or nuclear plants. Stainless steels are widely used in these industries due to their relative ease of manufacture, high strength and stiffness and excellent corrosion resistance. However, it has been found to be quite susceptible to galling. Several studies focus on galling resistance of stainless steels, nevertheless, one can notice that galling resistance is most often only defined by galling threshold, without any consideration of severity. We herein consider other factors than sole galling threshold in order to have a more accurate description of the galling state. By this mean, several unique post-mortem features can be detected.
We herein focus on 3 untreated stainless steel grades, namely AISI 316L, widely used in industrial applications, AISI 660 and a galling resistant grade, Nitronic60®. Samples are tested in unlubricated and untreated condition, with initial turned surface with Sa = 0,3 μm. Both AISI 316L and AISI 660 present after galling test following ASTM G98 a very low galling threshold (11 MPa) and are therefore usually considered as having equivalent galling resistance in the literature. Nitronic60®, however shows a high galling threshold (219 MPa).

In this paper, we consider both surface and microstructural evolution using 3D profilometry, SEM-FEG observation, EDX measurements and EBSD analysis. AISI 316L is characterized by a heavily deformed surface with adhesion marks almost hidden by smearing, with numerous third bodies on the surface. AISI 660 shows mainly adhesive wear with few smearing and relatively low amount of third bodies. Galling appears in these cases in the form of band of variable width and depth. As opposite, Nitronic60® presents localized galling initiation sites with no galling bands. Surface modifications is therefore visually very low and show very little evolution with pressure as long as pressure doesn't exceed a given threshold (320 MPa in this case).

EBSD analysis and KAM measurement through thickness cross section are carried out in order to determine the depth to which microstructure is affected by the galling test. Martensite formation and mechanical twinning are also investigated after galling test. The depth of the affected zone in the AISI 316L is very important, more than 1,2 mm at 350 MPa, while AISI 660 and Nitronic60 show smaller depth, respectively 485 μm and 336 μm at 350 MPa.
As a result, we propose the occurrence of three distinct classes of galling in stainless steels, namely catastrophic galling (AISI 316L), galling without smearing (AISI 660) and tolerant galling (Nitronic60®). Tolerant galling could be of great interest in industrial application since it leads to very little deformation upon galling occurrence and allows extended use in terms of both pressure and temperature.

*Speaker

Keywords: Galling, Stainless steel, Microstructure

Modelling of multiple impacts in granular chains

Ngoc-Son Nguyen * [1], Bernard Brogliato [2]

[1] GeM Institute – Universite de Nantes, CNRS: UMR6554 – 58 rue Michel Ange, BP 420, 44606, Saint-Nazaire Cedex, France
[2] BIPOP team – INRIA Greoble-Rhône Alpes, Univ. Grenoble-Alpes, Laboratoire Jean Kuntzman – 655 avenue de l'Europe, 38334 Saint-Ismier, France

Granular media are multi-body and multi-contact systems. When they are subjected to a shock, several collisions occur at the same time. This is the multiple impacts problem. The wave induced by the shock propagates through the contact network, and the induced energy is dispersed and dissipated. As a consequence, modeling multiple impacts is quite complex. Different approaches have been proposed to model multiple impacts. (i) Rigid-body models assume that collisions between particles are instantaneous and occur either at the same time (for Moreau's law [1]) or in a sequential manner (for binary collision model [2]). (ii) Second order dynamics models like Discrete Element Method (DEM) use compliant contact models with lumped flexibility like spring-dashpot models. (iii) The LZB approach [3] is intermediate between classes (i) and (ii). In this approach, the first-order Darboux-Keller dynamics equation is used and the impact dynamics is integrated with respect to impulse scale. This impact model incorporates the compliance effect at contact points by using a bi-stiffness compression/expansion model. The energy dissipation is taken into account by an energetic restitution coefficient. In this presentation, we present the LZB model and a comparison of this model with Moreau's law and the binary collision model. For this comparison, the impact dynamics in granular chains of balls is simulated and different parameters such as the elasticity coefficient, contact stiffnesses, restitution coefficient, particle mass distribution are varied. The wave propagation during the impact process, the energy dispersion and dissipation properties of granular chains are then analyzed.

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Keywords: granular chain, multiple impacts, rigid body model, binary collision model, LZB approach, wave propagation

*Speaker

Discrete element modeling of concrete under high confinement

Ahmad Omar * [1]

[1] AZM University (AZM) – Fouad Chehab Boulevard, Tripoli, Lebanon, Lebanon

The design of concrete protective structures is a real challenge for engineers nowadays. Under severe loadings coming from different sources, like natural hazards such as rock falls or industrial accidents such as explosions, consequences can be disastrous. Then, it is very important to be able to anticipate the structure behavior in order to strengthen it where it is needed. Different types of concrete structures may be subjected to severe loadings and require a particular attention such as nuclear power plants, bridges or dams. This will lead to discontinuities and fragmentation within the concrete structure. Therefore, to represent a highly nonlinear local behavior of a structure in the impacted zone and to obtain a detailed description of the fracture and fragmentation mechanisms a 3D Discrete Element Method (DEM) has been used. This developed method is adapted for the modeling of cohesive materials and take into account a moment transfer law (MTL) which is essential in order to model properly the quasi-static ductile behavior of concrete in compression. Moreover, the local interaction laws between discrete elements have been modified to model the irreversible compaction due to the closure of concrete porosity under high stresses. The numerical implementation and simulations have been carried out using Europlexus software. The DEM model has been validated by modeling oedometric and hydrostatic tests involving high-confining pressures (500 MPa). In this regard, the numerical results showed a very good agreement with the experimental tests carried out on a R30A7 dry concrete.

Keywords: Discrete element method, Concrete, Compaction, Impact Loading, High Triaxial Confinement.

*Speaker

S14: Experimental mechanics

Cardiovascular devices: Mechanical characterization of coronary stents

Mickaël Bonin [1], Jean-Marc Olive [2], Patrice Guérin [3], Fabienne Jordana [*† 4]

[1] INSERM U1229 – Institut National de la Santé et de la Recherche Médicale - INSERM – INSERM U1229 UFR d'Odontologie 1 Place Alexis Ricordeau BP 84215 44042 Nantes cedex 1, France
[2] Institut de Mécanique et d'Ingénierie – CNRS : UMR5295 – I2M (UMR CNRS 5295) Université de Bordeaux Bât A4 RDC 351 Cours de la Libération 33405 Talence Cedex, France
[3] Centre hémodynamique et vasculaire interventionnel – CHU Nantes, Université de Nantes, Université de Nantes – Hôpital Nord Laennec Boulevard Jacques-Monod Saint-Herblain 44093 Nantes Cedex 1, France
[4] University of Nantes – Université de Nantes, CHU de Nantes, INSERM U1229 – UFR d'Odontologie, 1 Place Alexis Ricordeau, BP 84215, 44042 Nantes cedex 1, France

Background: Coronary stents participate to limit cardiovascular death but are associated with some complications. Matching stent biomechanical characteristics with specific coronary lesions could limit these complications. Objectives: Development of a standardized and global bench test protocol and evaluation of most currently used coronary stents to improve stent choice in cathlab.

Materials: We evaluated biomechanical characteristics of coronary stents (Absorb^{TM}-ABBOTT®, Xience Alpine^{TM}-ABBOTT®, Resolute Integrity^{TM}-MEDTRONIC®, Resolute Onyx^{TM}-MEDTRONIC®, Orsiro^{TM}-BIOTRONIK®, Synergy^{TM}-BOSTON SCIENTIFIC®, Optimax^{TM}-HEXACATH®) in an in vitro study: radial elastic recoil, foreshortening, crimped stent with balloon flexibility and deployed stent flexibility. We also evaluated maximal resistance, elastic strength limit and elastic deformation limit for radial and longitudinal compression. Stents were deployed in a saline solution at 37$\pm$0.5$\circ$C. 9 stents were used to evaluate elastic recoil and foreshortening. Then, 3 among them were used to evaluate radial resistance between parallel plates, 3 were used to evaluate longitudinal resistance and 3 others were used to evaluate deployed stent bending stiffness. Before stent inflation 3 stents, among the 9 devices dedicated to biomechanical evaluation, were used to evaluate the uninflated stent with balloon bending stiffness. For a maximum comparability between stent models, we chose the most used stent size in our clinical practice (3.0 mm diameter and the nearest to 20 mm length). For these evaluations, all devices were inflated with them own balloon, at nominal pressure, according to manufacturer's recommendations. Nominal pressure was maintained for 30 seconds. We studied coating with field emission gun scanning electron microscope after POT-SIDE-POT (PSP) simulation to evaluate coating resistance to angioplasty. Bifurcation performances were evaluated by microcomputed tomography imaging of PSP stented silicon bifurcation models. Statistical analyses were performed using XLStats 2017 (Addinsoft).

Results: Elastic recoil, deployed stent flexibility and crimped stent flexibility were significantly different between groups (all $p < 0.0001$); as were radial and longitudinal maximum resistance ($p < 0.0001$). Synergy^{TM}, Orsiro^{TM} and Xience Alpine^{TM} had the lowest elastic recoil. Synergy^{TM} and Resolute Onyx^{TM} were the most flexible. Optimax^{TM} had the highest radial and longitudinal resistance. Coating lesions after PSP were not significantly different, excepted for Optimax^{TM} which had no coating lesion. In bifurcation model, side branch ostium coverage and malapposed strut ratio were significantly different between groups (respectively, $p = 0.01$ and $p = 0.004$). Strut fractures were founded only in Absorb^{TM}.
Conclusion: Currently used stents have very different biomechanical and bifurcation performance profiles. Their choice had to be adapted to each coronary lesion particularity to improve coronary interventions results.

*Speaker
†Corresponding author: fabienne.jordana@univ-nantes.fr

Keywords: Medical devices, Coronary stents, Bench test, Biomechanical tests

Method to extract stress-strain relations from pure torsion or pure bending experimental tests

Nathanael Connesson *† [1], Denis Favier [1], Gabriel Antherieu [1]

[1] Techniques de lÍngénierie Médicale et de la Complexité - Informatique, Mathématiques et Applications [Grenoble] (TIMC-IMAG) – Centre National de la Recherche Scientifique : UMR5525, IMAG, Université Joseph Fourier - Grenoble 1, Université de Lyon – Domaine de la Merci - 38706 La Tronche, France

Stress-strain relations are usually experimentally determined during tests where the applied stress is uniform over the specimens. Such tests are pure traction, pure compression or pure shear tests. Each of these tests presents its own experimental challenges. For compression test for example, buckling prevents reaching a wide range of uniform stress on slender specimens: identifying the compression stress-strain relation on a satisfying range is difficult and requires specific apparatus, usually involving additional friction during the test and corrective analyzes.
The aim of this work is to present an original method to experimentally identify stress-strain relations during tests involving no additional friction. It is proposed to extract (1) shear stress-shear strain and (2) compressive stress-strain relations from pure torsion or pure bending tests, respectively, which are tests during which the applied strain field is not anymore uniform in the specimen section.

As an originality, pure bending results obtained on slender specimens thanks to the experimental setup developed in [G. Antherieu et al, (2015), Exp. Mech. DOI: 10.1007/s11340-015-0102-5] have been analyzed. As the developed system allows to reach curvature radius smaller than 10mm, high compression strain can be reached locally even with wire specimen of diameter smaller than 0.5mm.

This work describes thus a noise robust method to identify the compression stress-strain relation form pure bending tests. The proposed method is also adapted to identify shear stress-shear strain relation from pure torsion tests.

In this abstract, only the extraction method of the shear stress-shear strain relation from the torsion torque versus the twist angle is summarized to provide an overall idea of the method: first the sought shear stress-shear strain relation is expressed as a linear combination of n splines. This thus defines qn unknowns to be identified. A theoretical torsion torque versus twist angle function can then be directly related to this shear stress-shear strain function and its associated qn unknowns. Eventually, these qn unknowns are sought so as to minimize (in the least square sense) the difference between the experimental and theoretical torques.
The method has also been developed to identify the compressive stress-strain relation from pure bending experimental results provided the tensile stress-strain relation has been previously measured. The method ability will be validated first on noisy numerical simulation and secondly on experimental data while analyzing the elastic and plastic domain of steel and pure copper wire specimens.

Keywords: Pure bending, Pure torsion, inverse method, experimental characterization

*Speaker
†Corresponding author: nathanael.connesson@univ-grenoble-alpes.fr

Experimental validation of a stress identification algorithm without constitutive equations

Marie Dalemat *† [1], Michel Coret [1], Adrien Leygue [1], Erwan Verron [1]

[1] Institut de Recherche en Génie Civil et Mécanique (GeM) – Université de Nantes, Ecole Centrale de Nantes, Centre National de la Recherche Scientifique : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France

Measurements of displacements, done with well-established technics such as Digital Image Correlation, usually allow the determination of kinematical fields. Generally, stress fields cannot be measured directly. They are computed with the help of constitutive equations, using common numerical schemes such as the Finite Element Method. Thus, constitutive models have to be calibrated with reliable solutions. The primary identification method consists in using stress and strain fields from simple testing, for which the analytical response is known (uniaxial, shear and/or equibiaxial loading conditions [1, 2]). More advanced identification approaches use heterogeneous fields; a common one is called Finite Element Model Updating (FEMU) [3]. It performs iterations of FE simulations to match these experimental data in order to determine the parameters of a given constitutive model.
A contrasting method is under development, called Data-Driven Identification. The algorithm allows finding the stress fields that satisfy equilibrium considering a large and redundant database of strain fields and applied forces. Its particularity is to deal with strain-stress couples without underlying constitutive equations. The method has already been validated with synthetic data [4]. The purpose of this work is to validate it experimentally. Hyperelastic materials are first considered (further developments for dissipative behaviours are to be done).

In practice, a multi-perforated silicone sheet subjected to several loading conditions is considered. Strain fields are measured with DIC. Stress fields are obtained with classical methods (direct identification with uni/bi-axial testing and FEMU) and with the DDI approach. This demonstrates the ability for DDI to deal with real data (affected by noise). Moreover, the importance of both quantity and quality of input data is discussed.

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Keywords: Data Driven Computational Mechanics, Digital Image Correlation, Constitutive Equation, Material response

*Speaker
†Corresponding author: marie.dalemat@ec-nantes.fr

Using correlative HRDIC, EBSD and ECCI to answer questions of microstructure-specific plasticity

Allan Harte *† [1], Alistair Garner [1], Alberto Orozco-Caballero [1], João Quinta Da Fonseca [1], Michael Preuss [1]

[1] School of Materials, The University of Manchester, UK – United Kingdom

High-resolution digital image correlation (HRDIC) is quickly becoming an essential tool for quantifying strain localisation in a wide range of materials. We aim to understand the origin of the strain distributions in Ni-based superalloys using a correlative approach. Strain distributions from HRDIC are correlated with electron backscatter diffraction (EBSD) for lattice rotation and diffraction- controlled electron channelling contrast imaging (ECCI) for the analysis of single dislocations and slip bands in the scanning electron microscope. This allows for the investigation of the effect of grain size, annealing twins and slip incompatibility at grain boundaries on strain localisation. It is observed that the presence and size of gamma prime precipitates in both the polycrystal and the single crystal affect strain localisation and the underlying defects. To understand surface vs. bulk behaviour, HRDIC strain maps are correlated with serial ECCI and also 3D EBSD serial sectioning in a Xe plasma focussed ion beam microscope.

Keywords: Nickel, based superalloys, gamma prime, plasticity, HRDIC, EBSD, ECCI

*Speaker
†Corresponding author: allan.harte@manchester.ac.uk

Cardiovascular devices: Mechanical characterization of aortic valves

François Huchet * [1], Patrice Guérin [2], Fabienne Jordana [3]

[1] Centre hémodynamique et vasculaire interventionnel – CHU Nantes, Université Nantes Angers Le Mans – Hôpital Nord Laennec Boulevard Jacques-Monod Saint-Herblain 44093 Nantes Cedex 1, France
[2] Centre hémodynamique et cardiovasculaire interventionnel – CHU Nantes, Université Nantes Angers Le Mans – Hôpital Nord Laennec Boulevard Jacques-Monod Saint-Herblain 44093 Nantes Cedex 1, France
[3] Université de Nantes – Université Nantes Angers Le Mans, CHU Nantes, INSERM U1229 – UFR d'Odontologie 1 Place Alexis Ricordeau BP 84215, 44042 Nantes cedex 1, France

Background: Perioperative manipulations of the devices in the cathlab may lead to morphologic and biomechanical evolution possibly involved in clinical adverse events. The new devices available in the cathlab, like or percutaneous aortic valves, lead to new clinical issues.
Objectives: Development of a standardized and global bench test protocol and evaluation of most currently used coronary stents to improve stent choice in cathlab. The main objective was to define the consequences of intra-operative manipulations of the prosthesis as well as the consequences of post-dilatation on valve function.

Materials and Methods: Before valve inflation, we built a database to assess the impact of inflation volume on the size of the balloon used to deploy the prosthesis. For each volume of inflation, 3 balloons were tested. The measurements were made at 3 locations on the balloon: proximal site, median site and distal site. We studied two current percutaneous aortic valves (Edwards Lifescience© valves, Sapien-XT and Sapien-3 models). We analyzed three experimental conditions, close to current practice situations: non-manipulated prosthesis: control group (n=1); prostheses undergoing inflation at nominal volume then conventional manipulations (n=2); prostheses undergoing inflation at nominal volume then conventional manipulations then a post-dilation maneuver (n = 2). Stents were deployed in a saline solution at 37±0.5◦C. The biomechanical analyses were performed with in a mechanical test bench. Repeated analyzes were practiced. Groups were defined regarding the deployment conditions: inflation volume for the bioprosthesis. We determined the recoil (diametric reduction between inflation and balloon shrinkage) and the foreshortening (longitudinal reduction between inflation and balloon shrinkage) for each value of volume of inflation. Statistical analyses performed were Mann-Whitney, Kruskall-Wallis and Chi2 tests.

Results: The only statistically significant difference between the nominal and post-dilated bioprostheses was the effective diameter of the bioprosthesis after stabilization, with a larger diameter for post-dilatation bioprostheses ($p < 0.001$). No significant differences were found for recoil, foreshortening, length, or compression strength. There was no significant difference in diameter, recoil or foreshortening according to the model of prosthesis. The Sapien-3 prostheses were significantly longer than the Sapien-XT prostheses ($p < 0.001$), and had a greater radial force ($p < 0.001$) and in compression strength ($p < 0.001$). This difference persisted when the force response was standardized according to the height of the prosthesis, with a larger radial force for the Sapien-3 model ($p < 0.001$).
Conclusion: Our results on the radial force of the stents, in this case that the stent of the Sapien-3 model was more resistant than that of the Sapien-XT model, are the first available in academic research.

Keywords: Medical devices, Aortic valves, Bench test, Biomechanical tests

*Speaker

Study of the tensile anisotropy of extruded ODS steel tubes using notched rings

Thibaud Jaumier *† [1], Sébastien Vincent [2], Rodrigue Desmorat [3], Ludovic Vincent [1]

[1] DEN – DEN- Service de Recherches Métallurgiques Appliquées, CEA, Université Paris-Saclay, F-91191 GIF-SUR-YVETTE, France. – 91191 Gif sur Yvette cedex, France
[2] DEN – DEN- Service de Recherches Métallurgiques Appliquées, CEA, Université Paris-Saclay, F-91191 GIF-SUR-YVETTE, France. – France
[3] LMT – LMT, ENS Cachan, CNRS, Université Paris Saclay – 94235 Cachan, France

Oxide dispersion strengthened (ODS) steels are suitable candidates for cladding applications in sodium cooled fast nuclear reactors. Obtained by means of cold rolling, ODS steel tubes can exhibit microstructural anisotropies, which translate into different mechanical properties in the hoop and axis directions. Assessing these properties and potential anisotropies is necessary should these materials be used.
To this end, tensile tests are performed in the temperature range 400-750∘C on two specimen geometries: tiles for the axial properties and notched rings for the hoop properties. Simple tooling is used for the latter, consisting of two half mandrels to apply tension to the ring with the two symmetrical gauge sections set at the edges of the mandrels. Tests were not performed with any lubricant even at the higher end of the temperature range, resulting in potential undesirable effects of friction. The coefficient of friction, temperature dependent, was not evaluated by direct means. Instead, 2D digital image correlation (DIC) was used to evaluate the strain evolution in the gauge section. 3D finite-element simulations were performed with material parameters identified on the results of tension tests performed on tile specimens manufactured with an isotropic 9%Cr ODS steel tube. Comparison between experimental and numerical strain fields on the surface of the ring allows the extrapolation of the coefficient of friction and the inverse identification of the stress-strain mechanical behavior of the material in the range 400-750∘C.

Using the same methodology on an anisotropic 14%Cr ODS steel tube, the apparent anisotropy introduced by the specimen geometry can be adjusted and the relevant data be interpreted for the determination of the material-dependent anisotropy between the axial and hoop directions.
Better assessment of the hoop properties using these notched rings, in particular the strain distribution in the width of the gauge section, can be further used with creep tests performed in similar loading conditions.

Keywords: ODS steel, tube, hoop, anisotropy, ring, DIC, identification

*Speaker
†Corresponding author: thibaud.jaumier@cea.fr

Data-Driven Identification and analysis of mechanical response through heterogeneous experiments

Adrien Leygue *† [1], Michel Coret [2], Julien Réthoré [1], Laurent Stainier [1], Erwan Verron [3]

[1] Institut de Recherche en Génie Civil et Mécanique (GeM) – Université de Nantes, Ecole Centrale de Nantes, Centre National de la Recherche Scientifique : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[2] Institut de Recherche en Génie Civil et Mécanique (GeM) – Ecole Centrale de Nantes, Université de Nantes, CNRS : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[3] GeM / Ecole Centrale de Nantes (GeM) – Ecole Centrale de Nantes – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France

Identifying the mechanical response of a material from full fields measurements is a delicate task that usually requires the parameterization of the stress fields through a constitutive model. Strategies such as Finite Element Updating [1] search the model parametric space to match the measured fields.
In this work, we propose a novel method for the non-parametric identification of the mechanical response of materials from heterogeneous full field measurements. The method, called Data Driven Identification (DDI) [2], is based on the Data-Driven Computational mechanics recently introduced by Kirchdoerfer and Ortiz [3,4] that is extended to the case of a priori of unknown mechanical response. In this approach, the mechanical response is simply described as a finite set of states in the (strain,stress) space thereby not introducing the a priori bias of a constitutive model.

We illustrate the ability of the method to identify complex and non-homogeneous stress fields in both the infinitesimal and finite strain cases. Finally we discuss the results interpretability in the absence of constitutive model.

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Keywords: Data, Driven, Digital Image Correlation, Constitutive model

*Speaker
†Corresponding author: adrien.leygue@ec-nantes.fr

Bayesian inference to determine elastoplastic parameter distributions

Hussein Rappel * [2,1], Lars Beex [1], Ludovic Noels [2], Stephane Bordas† [4,3,1]

[2] Department of Aerospace and Mechanical Engineering, University of Liege, Belgium (ULg) – Belgium
[1] Faculty of Science, Technology and Communication, University of Luxembourg, Luxembourg (UL) – Luxembourg
[4] Adjunct Professor, Intelligent Systems for Medicine Laboratory School of Mechanical and Chemical Engineering, The University of Western Australia, Australia – Australia
[3] School of Engineering, Cardiff University, Wales, UK – United Kingdom

Material parameters identified by mechanical tests can vary from one specimen to another. This variability is often caused by the variability of the small-scale structures of the different specimens. Examples are geometrical variations, the variations of crystallographic orientations, and the variations of the number amount of defects present.

The variability of material parameters can be described as a probability density function (PDF) as a function of the parameters. One possible way to identify such a PDF is to test numerous specimens but this entails a substantial amount of experimental efforts.

In this contribution, we employ Bayes' theorem [1] to only test a relatively small number of specimens and use their results to infer the parameters of an initially assumed distribution [2]. Besides avoiding an enormous amount of experimental work, a convenient result of this approach is that the distribution comes with an uncertainty in terms of the parameters. This entails that it is relatively clear how certain the obtained distribution is and how the uncertainty must be propagated, if of interest.

The use of Bayesian inference results in a probability density function (PDF), a so-called posterior distribution, as a function of the quantity of interest (i.e. the parameters that describe the distributions for the material parameters). The statistical properties of the PDF, e.g. the mean parameter values, the values at which the PDF is maximum and their correlations, can be obtained by analysing the posterior distribution [1, 2].

In this presentation we demonstrate the approach for both elastic and elastoplastic materials which harden nonlinearly. As elastoplastic materials are characterised using several material parameters, the coupling between these parameters in the PDF will receive special attention. This coupling is incorporated via a so-called copula [3], which will receive special attention in this work. We will for instance present how our results change when the assumed copula is different from the one used to create the experimental measurements.

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*Speaker
†Corresponding author: stephane.bordas@uni.lu

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Keywords: Bayesian inference, Bayes' theorem, copula, parameter distribution, parameter identification, elastoplasticity

Modelling and Simulation of Shear Rheometry on Soft Cohesive Soils

Sumith S *† [1], Kannan K [1], Shankar K [1]

[1] Indian Institute of Technology Madras – Machine Design Section, Department of Mechanical Engineering Indian Institute of Technology Madras Adyar Chennai, Tamil Nadu 600036, India

With the increasing demand for mineral resources and their fast depletion on land, deep-sea resources become a promising resources substitution. For exploitation of deep-sea resources, some deep-sea mining systems have been designed and this has to operate in ocean floor having soils of very low shear strength. There are empirical relations for soft cohesive soil which has been extensively used in modeling the terrain vehicle interaction. However these relations vary significantly with the types of testing. The deep-sea sediments has a larger void ratio, higher water content, and more obvious rheological properties than land-soil[1].Due to the difficulty in obtaining deep-sea sediments from insitu, bentonite-water mixture have been used as a substitute by many researchers and its preparation is based on the shear strength of deep sea sediment insitu[2]. In this study Shear Rheometry experiment is performed on sea bed soil simulacrum (bentonite water mixture) using standard parallel plate rheometer to study its rheological behavior. The variation of torque versus time characteristics at various constant rates is investigated. To investigate the rate type mechanical response of soft cohesive soil observed from experiment, a non-linear viscoelastic fluid model is proposed based on a thermodynamic framework which includes the concept of natural configuration in our setting that can be obtained from the current configuration upon removing the external loading[3],[4]. When a body is subject to external stimuli, it undergoes a thermodynamic process and its evolution depends on thermodynamic criterion. This evolution of the natural configuration leads to rate type constitutive relations. In a solid all the energy that is stored can be recovered whereas in a viscous fluid a part of mechanical working is converted to thermal energy and thus the body produces entropy. It assumes that from amongst the processes that are possible the body proceeds in such a manner so as to maximize rate at which entropy is produced. This model is tested against the same shear rheometry experiments, and reasonable agreement with both torque overshoot and relaxation regimes is observed. The agreement is better at low shear rates.

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*Speaker

†Corresponding author: sumithsree@gmail.com

Keywords: Rheometry, Thermodynamic approach, Viscoelastic fluids

Modeling of puncture-cutting forces of a soft material based on fracture mechanics

Ennouri Triki * [1], Francois Barthelat [1], Chantal Gauvin [2]

[1] McGill University – Canada
[2] IRSST – Canada

Adding cutting motion to puncture process can significantly reduce the puncture-cutting resistance of protective gloves. This paper presents experimental and analytical investigations of the combined puncture and cutting resistance of elastomer-like materials. A model describing the combined puncture and cutting of soft material by a pointed blade is developed using force distribution analysis and basic concepts of fracture mechanics. Result shows that the penetration and cutting force (*FP/C*) required for a completely insertion of a pointed blade into a soft material is a result of a synergistic contribution between a pushing force, *FP*, (corresponding to fracture mode I) and a cutting force, *FC*, (corresponding to fracture modes II + III). Fracture mechanics theory is then used to determine the relationship between the penetration and cutting force, *FP/C*, and the total puncture/cutting energy, *GTotal*, that includes fracture toughness of material and friction energy between pointed blade and material. The presented model is well verified by comparing the predicted value of *FP/C* with experimental data obtained from neoprene rubber punctured by three pointed blades having tip angles of 22.5 °, 35 ° and 56°.

Keywords: fracture energy, soft material, tip, sharp object, puncture, cutting, force

*Speaker

An Image-Based Impact Test for the High Strain Rate Properties of Tungsten Carbide

Lloyd Fletcher *† [1], Fabrice Pierron [1]

[1] University of Southampton (Southampton, UK) – United Kingdom

The properties of tungsten carbide make it an ideal material for machine cutting tools. This usage of tungsten carbide exposes the material to high strain rate loading. Unfortunately, it is difficult to obtain experimental data for the high strain rate properties of tungsten carbide. Existing high strain rate data for tungsten carbide has been obtained using the split Hopkinson pressure bar (SHPB) technique. The SHPB method relies on the assumption of 'quasi-static equilibrium' such that the material properties of the specimen can be inferred from point measurements taken on the bars of the apparatus. Neglecting inertial effects makes it impossible to obtain reliable data for the elastic properties or tensile strength of tungsten carbide using the SHPB.
Recently, a new image-based impact test has been developed for analysing the high strain rate properties of brittle materials. This test method uses ultra-high speed full-field measurements to derive acceleration and strain fields from an edge-on impact test. The acceleration and strain fields are then processed with the virtual fields method to identify the stiffness and tensile strength of the material. The aim of this study is to use the image-based impact test methodology to analyse the high strain rate properties of tungsten carbide.

Explicit dynamics simulations were used to design the test configuration and validate the material property identification procedures. The optimal test configuration was then used to conduct impact tests on tungsten carbide samples using a purpose-built gas gun. The impacted samples were imaged at 5 MHz using a Shimadzu HPV-X camera. Full-field displacement measurements were taken throughout the impact test using the grid method.
Preliminary results showed that it is possible to use the image-based impact test to identify both the elastic modulus and strength of tungsten carbide at strain rates on the order of 1000 s. For a tungsten carbide with 13% cobalt binder the elastic modulus was identified to be 518 GPa and the tensile strength was found to be 1400 MPa at 1000 /s. Additional experiments are planned which will analyse and compare the high strain rates properties of various tungsten carbide grades. Specific compositions to be analysed include: tungsten carbide with 13% cobalt binder, tungsten carbide with 6% cobalt binder and tungsten carbide with 6% nickel binder.

Keywords: full, field measurement, tungsten carbide, high strain rate, tensile strength

*Speaker
†Corresponding author: L.C.Fletcher@soton.ac.uk

Image-based stress field reconstruction in complex media

Rian Seghir * [1], Fabrice Pierron [1], Lloyd Fletcher [1]

[1] University of Southampton (USo) – Highfield Campus, Southampton, S017 1BJ, Hampshire, U.K., United Kingdom

In many instances in life, materials around or within us suffer deformation at high rates. This is the case when engineering structures undergo impact, crash, blast, etc. but also when forming materials like stamping or assembling them like magnetic pulse welding. Another important area concerns biological tissues. Characterizing and accurately modelling materials and/or structures subjected to high deformation rates is therefore crucial.
Nevertheless, the transience and the inhomogeneous aspect of such loadings make both: (1) the experimental capture of the mechanical response very challenging, especially due to current difficulty to accurately measure the force in presence of inertia, and (2) make all the potential assumptions regarding the constitutive relation of the deforming material extremely hazardous. Indeed, while a significantly time-dependent material transforms immediately, in the presence of transient dynamic loading, in a complex and constantly changing composite, some polycrystalline materials will undergo for instance strong wave-structure interactions, strain localisation, high dissipation thus local softening, dynamic recrystallization etc. Hence, the local thermomechanical state depends on gradients of loading, superimposed on, and coupled to, varying gradients of behaviour, produced along deformation paths necessarily multiaxial and neither constant in strain-rate nor temperature. In other words, the definition of a constitutive law, local or homogenized, is at the crossing of many different cutting-edge research topics and remains a very open question. While, the progress in complex numerical simulations allow researcher for estimating still unmeasurable quantities and the progress in field measurements and inverse methods, like FEMU or the VFM, allow for feeding more and more complex constitutive equations, both techniques are in the present case powerless since they both rely on the *a-priori* input of a constitutive law. A very new way to experimentally estimate the local mechanical response of complex media has, therefore, to be defined.
We demonstrate in the following contribution that experimental full-field measurements of accelerations can be directly used to inverse the local equilibrium equation and reconstruct fields of stress tensor with no assumption at all on the constitutive relation and its potential spatial and temporal variations. Spatially and temporally resolved displacement fields are obtained using ultra-high speed camera and the grid-method while strain and acceleration fields are subsequently obtained by spatial and double temporal differentiation. The methodology is firstly validated on simulated data then applied to an instrumented spalling test where the local failure strength is identified. While such a direct estimation of the local stress state would be useful by itself in many instances, e.g. definition of a failure strength or energy-based recrystallization criteria, it is also demonstrated that both experimental stress and strain fields can be recombined to eventually identified the local secant mechanical property tensor of the material. The latest constitute a first step in what could be named as "true model identification", as opposed to parameters' model identification.

Keywords: dynamic, high speed imaging, stress, identification, equilibrium

*Speaker

S15: Experimental nanomechanics

Robust architectured materials: deformation and failure under cyclic loading

Schroer Almut [1], Jeffrey M. Wheeler [2], Ruth Schwaiger * [1]

[1] Institute for Applied Materials (IAM), Karlsruhe Institute of Technology (KIT) (IAM-WBM) – Hermann-von-Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
[2] Department of Materials, ETHZ – Swiss Federal Institute of Technology – Vladimir-Prelog-Weg 5, 8093 Zurich, Switzerland

Specifically designed micro and nanolattices are able to combine outstanding mechanical and physical properties and, thus, expand the current limits of the material property spaces. By combining mechanical size effects with lattice architecture extraordinary strength values are observed. The highest resolution in manufacturing is currently achieved by 3D direct laser writing, resulting in highly customized polymeric architectures, which are often coated or annealed in order to increase the strength of the structures. As demonstrated by push-to-pull nanotensile tests, annealing can increase the material strength by up to a factor of 10. While a ceramic coating with a thickness in the range of 10 – 100 nm results in improved strength, at the same time the failure mechanisms change. When comparing 10 nm and 100 nm thick alumina coatings, a transition from buckling to brittle fracture is observed. Understanding deformation and failure under repeated loading is key to further optimizing these high-strength architected materials. Cyclic tests showed energy dissipation, which is a function of progressively failing ligaments. Post-yield softening induced by plastic buckling or crushing of individual ligaments, limit the performance under cyclic loading as revealed by in situ experiments. Deformation and failure as well as the strategies to improve the properties of architectured materials will be discussed.

Keywords: in situ nanomechanical testing, nanolattice materials

*Speaker

In situ nano-mechanical tests on individual metal nanowires in the light of synchrotron X-ray diffraction

Thomas Cornelius * [1]

[1] Institut des Matériaux, de Microélectronique et des Nanosciences de Provence (IM2NP) – Aix Marseille Université, CNRS : UMR7334 – Aix-Marseille Universités 13937 Marseille Université de Toulon 83957 La Garde, France

In the recent past, the mechanical properties of low-dimensional materials have attracted enormous attention. The yield strength for defect free nanostructures was shown to approach the ultimate limit of the respective material [1, 2]. Despite numerous experimental and theoretical works the mechanical behavior and the onset of plasticity on the nanoscale such as the influence of surface stress on defect nucleation is still not fully understood. To shed additional light on this topic, *in situ* experimental setups are being designed for monitoring the evolution of the structures during mechanical deformation.
Compared to electron microscopy, X-ray diffraction has the benefit of being non-destructive, penetrating (hence no special need for pre-thinning the sample) and extremely sensitive to elastic strains and defects. Thanks to the development of new synchrotron sources, increasingly efficient focusing optics, and advanced 2D detectors X-ray diffraction is becoming a major tool for investigating the structure of nano-objects *in situ* during mechanical testing. In particular, Bragg coherent X-ray diffraction imaging (BCDI) which is a novel lensless imaging technique with a spatial resolution of about 10 nm and a displacement field sensitivity of 1 pm [3] and Laue microdiffraction with a high sensitivity on crystal orientation and geometrically necessary dislocations are pre-destined methods for *in situ* nano-mechanical testing [4,5]. Here, recent developments on *in situ* tensile and three-point bending tests on individual metal nanowires coupled with BCDI, respectively, Laue microdiffraction will be presented [6,7,8]. These *in situ* tests allow for visualizing the elastic as well as the plastic deformation of the nanostructure under load and for characterising the induced defects.

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Keywords: in situ nanomechanical testing, three point bending, tensile test, metal nanowire, Laue microdiffraction, Bragg coherent X, ray diffraction

*Speaker

Hydrogen Embrittlement of Tungsten Induced by Deuterium Plasma: Insights from Nanoindentation Test

Xufei Fang *† [1], Arkadi Kreter [2], Marcin Rasinski [2], Christoph Kirchlechner [1], Steffen Brinckmann‡ [1], Gerhard Dehm [1]

[1] Max-Planck-Institut für Eisenforschung GmbH, Structure and Nano-/ Micromechanics of Materials – Germany
[2] Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung – Plasmaphysik, Partner of the Trilateral Euregio Cluster (TEC) – Germany

Hydrogen exposure has been found to result in embrittlement in metals. We use nanoindentation experiments to study the mechanical properties of single crystalline and polycrystalline tungsten subjected to deuterium plasma. The results exhibit a decrease in the pop-in load and increase in hardness on exposed tungsten sample due to the presence of deuterium. The defactant theory is adopted to explain the decrease of the load required for dislocation nucleation. The result suggests hydrogen embrittlement of tungsten with the underlying mechanism of hydrogen enhanced localized plasticity. In addition, the maximum shear stress for tungsten is found to be irrelevant of the grain orientations.

Keywords: Hydrogen embrittlement, Tungsten, Deuterium plasma exposure, Nanoindentation

*Speaker
†Corresponding author: x.fang@mpie.de
‡Corresponding author: s.brinckmann@mpie.de

Nanoindentation cartography method to map the mechanical properties of the cell walls of an Al-Si aluminum foam

Jean-Baptiste Giouse *† [1,2], Christophe Tromas [1], Ken White [2]

[1] Institut Pprime (PPRIME) – Université de Poitiers, ENSMA, Centre National de la Recherche Scientifique : UPR3346 – Institut P: Recherche et Ingénierie en Matériaux, Mécanique et EnergétiqueSP2MI Téléport 2Boulevard Pierre et Marie CurieBP 3017986962 FUTUROSCOPE CEDEX, France

[2] Department of Mechanical engineering [Houston] – N207 Engineering Bldg 1, 4726 Calhoun Rd, Houston TX 77204-4006, United States

Metallic foams and more specifically aluminum foams are widely used in layered composites materials. They are light and offer very good energy absorption properties due to their unique structure made of interconnected cells. Their main applications include structural components for the aeronautic and automotive industries as well as core for sandwich beams and panels. The macroscopic mechanical properties of foams depend mainly on two parameters which are the cell morphology (size, shape, distribution) and the cell wall material. Hence, it is very important to characterize the mechanical properties of the cell wall to understand the macroscopic response of the foam. However, while several studies focused on this topic, few were actually interested in the very local properties of the material. The material is a hypoeutectic Al-Si alloy reinforced with silicon carbide particles to stabilize the material during the fabrication of the foam.

This paper offers a multi scale characterization of the cell wall mechanical properties of aluminum foam using the nanoindentation cartography in order to reveal the difference in mechanical properties between the different phases. The method is applied on the cross section of the foam in order to characterize the cell wall properties. It was first used to increase the resolution of nanoindentation measurements in multiphase materials with high mechanical properties discrepancies. It relies on the statistical analysis of a large amount of indentations. Firstly, a large regular array of indentation is performed, then using an interpolation algorithm, a map of hardness and Young modulus is reconstructed revealing the gradient of hardness and/or modulus in the material.

As expected from the Al-Si phase diagram and confirmed by SEM imaging, the microstructure is heterogeneous with an aluminum dendritic phase and an Al-Si eutectic phase in which the silicon crystallizes in fibrous splats. The SEM observations also show a non-negligible presence of precipitates from the other alloying elements (mainly Mg, Mn and Fe). The early results suggest a drop of hardness in the aluminum near the dendrite/eutectic phase interface. It also seems that the eutectic aluminum has lower hardness than the dendritic one. Those observations will be linked to the atomic composition of the alloy using energy dispersive spectroscopy (EDS).

Keywords: Nanoindentation, Mechanical properties, Aluminum foam

*Speaker

†Corresponding author: jean.baptiste.giouse@etu.univ-poitiers.fr

New dedicated methods for the improvement of quantitative in-situ TEM nanomechanical testing

Hosni Idrissi *† [1], Vahid Samaeeaghmiyoni [2], Caroline Bollinger [3], Francesca Boioli[4], Patrick Cordier [5], Dominique Schryvers [2]

[1] Institute of Mechanics, Materials and Civil Engineering. Université Catholique de Louvain – Belgium
[2] EMAT, University of Antwerp (UA) – Belgium
[3] Bayerisches Geoinstitut, University of Bayreuth – Germany
[4] Unité Matériaux et Transformations - UMR 8207 (UMET) – Université de Lille, Sciences et Technologies – France
[5] Unité Matériaux et Transformations - UMR 8207 (UMET) – Université de Lille, Sciences et Technologies – Université Lille 1, France

Recently, the development of a new generation of advanced instruments for quantitative in-situ TEM nanomechanical testing has allowed establishing a one-to-one relationship between load-displacement characteristics and stress-induced microstructure evolution in the transmission electron microscope (TEM). In the present work, it will be demonstrated that a step forward in the investigation of the small-scale plasticity mechanisms and size effects can be made by using original sample preparation methods. Recently, we used an original method to revisit the plasticity of olivine single crystals at low temperature. Microscopic tensile samples with pre-defined crystallographic orientation were prepared by focused-ion-beam (FIB) from macroscopic olivine single crystals oriented with X-rays. This allowed preparing samples with ideal conditions for the activation of dislocations and for the imaging of these dislocations. Furthermore, in order to facilitate the nucleation of dislocations in such hard and brittle material, the samples have been prepared on small scratches (from the last polishing stage of the bulk sample) located at the surface of the macroscopic sample. Cyclic deformation was thus applied in the load control mode using the PI-95 TEM picoindenter holder and the Push-to-Pull (PTP) device (Bruker.Inc). Load was increased to a given value, which is maintained constant for several minutes before unloading. During the plateau, dislocation motion is observed and characterized (hence, under a known and constant applied stress). Using this method and dislocation dynamic (DD) simulations, we found that the intrinsic ductility of olivine at low temperature is significantly lower than previously reported values which were obtained under strain-hardened laboratory conditions. More generally, we demonstrated the possibility of characterizing the mechanical properties of specimens which could be available in the form of sub-millimetre sized particles only. More recently, very clean single crystal and bi-crystal Ni samples with desired crystallographic orientations and microstructures have been prepared for quantitative in-situ TEM tensile tests. The preparation included twin jet electro-polishing, FIB as well as an extra annealing step in TEM to remove FIB damages. The results revealed that, this method could significantly improve our understanding of the relationship between the intrinsic deformation mechanisms and the mechanical behaviour of small-sized systems.

Keywords: Quantitative in, situ TEM nanomechanical testing, fundamental deformation mechanisms, size effect

*Speaker
†Corresponding author: hosni.idrissi@uclouvain.be

Imaging the structural evolution in nanocrystalline metals during mechanical deformation

Christian Kuebel [1], Ankush Kashiwar * [2], Aaron Kobler [4,3], Horst Hahn [4,2]

[1] Karlsruhe Institute of Technology (KIT) – Institute of Nanotechnology & Karlsruhe Nano Micro Facility, Hermann-von-Helmholtz Platz 1, 76344 Eggentein-Leopoldshafen, Germany
[2] Karlsruhe Institute of Technology (KIT) – Institute of Nanotechnology, Hermann-von-Helmholtz Platz 1 76344 Eggentein-Leopoldshafen, Germany
[4] Technical University Darmstadt – Germany
[3] Nanoscribe – Germany

Most of our current understanding of the deformation mechanisms active in nanocrystalline (nc) metals stems from *in situ* deformation experiments on bulk materials using x-ray diffraction (XRD). However, XRD cannot directly resolve the local deformation processes. For a local analysis, these processes are traditionally investigated using BF/DF-TEM, but varying contrast due to local orientation changes, bending and defects during *in situ* BF-TEM straining experiments make an accurate interpretation for nanometer sized grains difficult. Therefore, we have developed a combination of *in situ* studies with 4D-STEM imaging, in particular using automated crystal orientation (ACOM) [1] mapping in a scanning electron microscopy (STEM) setup, to not only follow morphological changes of a statistically meaningful sample volume but to retrieve the crystallographic information of structural changes using both local and statistical analysis of the resulting crystal orientation maps [2, 3]. With a spatial resolution of around 1 nm, this allows to identify the crystallographic orientation of crystallites with sizes down to around 10 nm, well below the limit of electron back scatter diffraction (EBSD). This approach was key to a detailed data evaluation. By tracking individual crystallites through the straining series, the change of their orientation can be evaluated in order to distinguish between local crystallite rotation and sample tilting/bending [2, 3]. In addition, twinning/detwinning and grain growth can be directly followed (Fig. 1, 2) and the automatic data evaluation leads to a user independent quantitative statistical information such as grain size distribution and grain rotation statistics [3].
While ACOM-STEM is a powerful approach for *in situ* experiments on nanocrystalline materials, a major disadvantage is that the acquisition of one statistically meaningful orientation map takes around 30-60 min, putting serious limits on the stability of the *in situ* deformation setup. In particular, a detailed analysis of the mechanical data is difficult. In current experiments, we therefore combine BF/DF-STEM with ACOM analysis at a few selected states to increase the speed of the *in situ* straining experiments. This approach seems to be promising in order to study e.g. the Bauschinger effect in nanocrystalline metals, to obtain both reliable structural and mechanical data.

In this presentation, we will discuss the possibilities and challenges of reliable structural and mechanical characterization and illustrate it using *in situ* straining of nc PdxAu1-x thin films as example, looking at twinning, S9 boundary formation, grain rotation and dislocation activity with respect to the Bauschinger effect.

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*Speaker

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Keywords: In situ TEM, automated crystal orientation mapping (ACOM), nanocrystalline metals

On chip study of the irradiation creep behavior of copper films

Pierre Lapouge [1], Fabien Onimus * [2], Michael Coulombier [3], Jean-Pierre Raskin [4], Thomas Pardoen [3], Yves Brechet [5]

[1] PIMM Arts et Métiers ParisTech – Centre National de la Recherche Scientifique - CNRS – 151 bd de l'Hôpital, 75013 Paris, France

[2] Service de recherches métallurgiques appliquées, CEA, Université Paris-Saclay (CEA) – Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA) - Saclay, Université Paris-Saclay,Sorbonne Universités – 91191, Gif-sur-Yvette, France

[3] Institute of Mechanics, Materials and Civil Engineering, Université catholique de Louvain – 1348, Louvain-la-Neuve, Belgium

[4] Institute of Information and Communication Technologies, Electronics and Applied Mathematics, Université catholique de Louvain – 1348, Louvain-la-Neuve, Belgium

[5] CEA Saclay (CEA) – Commissariat à l'énergie atomique et aux énergies alternatives – 91191 Gif-sur-Yvette cedex, France

Structural materials used in the pressurized water reactor cores, such as austenitic stainless steels or zirconium alloys, are exposed to neutron flux and, at the same time, to stresses from various mechanical loadings. At the macroscopic scale, the mechanical behavior under irradiation is well characterized. However, at a microscopic scale, the deformation mechanisms under irradiation still remain unknown. Many irradiation creep mechanisms have been proposed from a theoretical point of view but the available experimental data have not permitted the identification of the relevant mechanisms at the origin of the deformation behavior.
The objective of this work is precisely to improve our understanding of the irradiation creep mechanisms of metals by the development of a novel experimental method. The irradiation is emulated by heavy ions with the advantage of a fast damage rate without activation of the material. However, the irradiated depth is confined within a layer of a few hundreds of nanometers. Such small depth of penetration requires a specific experimental device in order to deform and measure stress on specimens with the appropriate corresponding small thickness. This device is based on the release of internal stress in a silicon nitride beam to deform a metallic thin film which is attached to the silicon nitride "actuator" beam.

After proving the feasibility of the study and adapting the device to the irradiation environment, the method has been used to reproduce an irradiation creep experiment at room temperature on copper. A single creep power law with a stress exponent of 5 has been found under irradiation on 200 and 500 nm thick films. The SEM and TEM observations suggest that the deformation mechanism rely on the irradiation assisted glide of dislocations.
This law seems to be independent of the microstructure and the loading history. The dislocation climb, if it occurs, would not be controlled by diffusion process acting over long distance but instead by direct interaction between displacement cascades and dislocations.

Keywords: thin film, small, scale test, copper, irradiation, creep

*Speaker

Composition dependence of mechanical properties of cubic and hexagonal NbCo2 Laves phases

Wei Luo *† [1], Christoph Kirchlechner [1], Gerhard Dehm [1], Frank Stein [1]

[1] Max-Planck-Institut für Eisenforschung GmbH – Germany

Transition metal-based Laves phases have high melting point, high strength and good creep resistance which make them potential candidates for high-temperature applications. On the other hand, they exhibit pronounced brittleness at low temperature. Due to their brittleness, the difficulty of producing sufficiently large and flaw-less bulk samples for conventional mechanical testing limits the study of their mechanical properties. Interestingly, the existing literature indicates that the mechanical properties of transition metal-based Laves phases significantly depend on their composition but the reported results are quite contradictory. While some authors reported that the hardness of Laves phase increases as the composition deviates from the stoichiometric composition due to defect hardening, other studies show that the hardness decreases at off-stoichiometric composition. It is unknown whether this dependence is also reflected in their fracture toughness values. Our knowledge about the mechanical properties of Laves phases is still quite limited. The underlying mechanism of the composition effect is not yet understood.

Laves phases with AB2 stoichiometry can have three structure types, cubic C15 (MgCu2-type), hexagonal C14 (MgZn2-type) and hexagonal C36 (MgNi2-type). All three types of Laves phases exist as stable phases in the Co-Nb system and the C15-NbCo2 Laves phase has a large composition range of 26.0±0.5 – 35.3±0.3 at.% Nb. It makes the NbCo2 Laves phases a perfect candidate to study not only the mechanical properties of transition metal-based Laves phases but also the influence of composition and crystal structure. To circumvent the difficulties in preparing large flaw-less samples, we combine the diffusion couple technique with the micromechanical testing. The idea is to grow diffusion layers of the cubic and hexagonal NbCo2 Laves phases with concentration gradients using the diffusion couple technique and cut a series of micro-sized, single-crystalline samples with different compositions in the diffusion layers using the focused ion beam (FIB) technique. And finally their mechanical properties are studied by micromechanical testing.

In the present work, the hardness, fracture toughness and critical resolved shear stress at room temperature of the cubic and hexagonal NbCo2 Laves phases were studied and the influence of composition and crystal structure on their mechanical properties was analyzed. Hardness was measured at different positions in the diffusion layers along the concentration gradient by nanoindentation. Single-crystalline micro-cantilevers of cubic and hexagonal NbCo2 Laves phases with different compositions were fabricated by focused ion beam (FIB) and *in-situ* bending tests were performed to study the influence of chemical composition and crystal structure on the fracture toughness. Micropillar compression tests were performed to study the deformation mechanism at room temperature and the critical resolved shear stress. Electron back-scatter diffraction (EBSD) and high-resolution scanning electron microscopy were used to identify the activated slip systems. The deformation mechanism of the cubic and hexagonal NbCo2 Laves phase and the effect of orientation, composition and crystal structure will be discussed in the presentation.

Keywords: Laves phase, Composition effect, Hardness, Fracture toughness, Micropillar compression, Diffusion couple

*Speaker

†Corresponding author: w.luo@mpie.de

3D Laue Micro-Diffraction characterization of local microstructure and strain with submicron resolution

Loïc Renversade *† [1,2], Odile Robach [1,2], Olivier Ulrich [1,2], Jean-Baptiste Marijon [3], Olivier Castelnau [3], Samuel Tardif [1,2], François Rieutord [1,2], Christoph Kirchlechner [4], Jean-Sebastien Micha [1,2]

[1] Institut Nanosciences et Cryogénie (INAC) – Commissariat à l'énergie atomique et aux énergies alternatives : DRF/INAC, Université Grenoble Alpes – Grenoble, France
[2] Ligne de lumière synchotron CRG-IF BM32 à l'ESRF (CRG-IF BM32) – CNRS, Commissariat à l'Énergie Atomique et aux Énergies Alternatives (CEA) - Grenoble – ESRF-The European Synchrotron CS40220 CRG-IF-BM32 38043 Grenoble Cedex 9 France, France
[3] Procédés et Ingénierie en Mécanique et Matériaux [Paris] (PIMM) – Conservatoire National des Arts et Métiers [CNAM], Centre National de la Recherche Scientifique : UMR8006, Arts et Métiers ParisTech – 151 boulevard de l'hôpital, 75013 Paris, France
[4] Max-Planck-Institut für Eisenforschung GmbH, Structure and Nano-/ Micromechanics of Materials – Germany

Laue microdiffraction is a powerful technique that uses a white micro-focused X-ray beam from a synchrotron source to characterize local microstructural properties and micromechanical behaviours in a wide range of crystalline and polycrystalline materials [1]. Allowing fast two-dimensional mapping of local crystal structure, orientations and deviatoric elastic strains, the method operates without sample rotation to reach sub-micron spatial resolution and angular resolution of 10-4, therefore making it well suited to in situ studies of mechanical testing on small objects [2].
Due to the penetration of X-rays into the sample, from a few microns to millimeters depending on the material, Laue microdiffraction provides in practice depth-integrated diffraction patterns, which superimpose the intensity diffracted by all the grains along the penetration course of the incident beam. The 3D Laue microdiffraction, or " Differential Aperture X-Ray Microscopy ", was therefore proposed to extend the capabilities of conventional micro-Laue and resolve the dimension along the incident beam. To this end, a wire (e.g, made of tungsten) is used as an absorption profiler and placed between the sample surface and the detector. The scattered intensity is scanned by translating the wire in micron steps parallel to the incident beam and a laue pattern is recorded at each wire position. Analyses of the intensity variations between succesive images, combined with geometrical considerations, allow then to reconstruct the scattered intensity profiles as a function of depth and obtain depth-resolved Laue patterns.

Over the past few years, significant efforts were made to implement 3D Laue microdiffraction on the french CRG beamline IF-BM32 at ESRF. Recent results have demonstrated the capabilities of the currently available setup and analysis tools to characterize microstructural and mechanical features in micro-scale objets [3]. The depth resolution, usually considered as being of the order of the scan step (i.e, 1 μm), remains however largely limited by the partial attenuation at the edges of the wire, on thicknesses ranging up to several microns depending on the scattering energy. In the present work, we sought to account for this partial absorption and proposed therefore a new reconstruction scheme based on an inverse problem formulation that allows for a more accurate and direct data treatment. This was accompanied by the development of a new software package, designed for the beamline users to analyze wire scan datasets. We describe these recent advances and illustrate them with application examples.

*Speaker
†Corresponding author: loic.renversade@esrf.fr

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Keywords: Laue microdiffraction, synchrotron, imaging, orientation, strain

Hysteretic mechanical behavior of the MAX phase Ti2AlN studied by nanoindentation and micropillar compression tests

Christophe Tromas *† [1], Wilgens Sylvain [1], Anne Joulain [1], Ludovic Thilly [1], Patrick Villechaise [1], Marc Legros [2,3]

[1] Institut Pprime (PPRIME) – CNRS : UPR3346, Université de Poitiers, ISAE-ESMA – Département de Physique et Mécanique des Matériaux, SP2MI, Téléport 2, Boulevard Marie et Pierre Curie, BP 30179, 86962 Chasseneuil-Futuroscope Cedex, France

[2] Centre d'élaboration de matériaux et d'études structurales (CEMES) – CNRS : UPR8011 – 29 Rue Jeanne Marvig - BP 4347 31055 TOULOUSE CEDEX 4, France

[3] Université de Toulouse (UPS) – Université Paul Sabatier-Toulouse III - UPS (FRANCE) – F-31055, Toulouse, France

MAX phases combine properties of metals and ceramics, which give them a high potential for technological applications. These materials are nano-lamellar ternary carbides and nitrides, with a hexagonal crystallographic structure. Their mechanical properties are characterized by a high stiffness and a relatively low yield strength. More surprisingly, deformation tests on MAX phases reveal a mechanical hysteresis. At a macroscopic scale, in polycrystalline samples, several studies have shown that this behavior could be related to load transfers from grain to grain. However, a mechanical hysteresis is also observed in single crystals.

In this work, the mechanical hysteresis and the plasticity of the MAX phase Ti2AlN has been studied at small scale by using nanoindentation tests with a spherical tip and micro-pillar compression tests. In both cases, cyclic loadings have been applied in single grains, for different crystallographic orientations, previously determined by EBSD. These cyclic loadings, with partial unloadings have revealed a same behavior in nanoindentation tests and in micro-pillars compression test. In both cases, the unloading curves show an elastic behavior followed by a plastic recovery at low load. Furthermore, this mechanical hysteresis is related to the crystallographic orientation since the energy dissipated during the cycles is shown to be minimum when the basal plane is perpendicular or parallel to the indentation (or compression) axis.

The dislocation structure associated with this hysteretic behavior has been investigated by surface slip lines analysis by AFM (for the indents) and by SEM (for the pillars). The different configurations between nanoindentation and micro-pillar compression tests (in terms of stress field, free surface, deformed volume...) have provided complementary information to explain the mechanical hysteresis in terms of dislocation mechanisms.

Keywords: MAX phase, nanoindentation, mechanical hysteresis, Ti2AlN, micro, pillar compression

*Speaker

†Corresponding author: christophe.tromas@univ-poitiers.fr

Local mechanical properties and plasticity of a Zn-Al-Cu-Mg alloy

Zhicheng Wu *† [1], Jing Rao [1], James Gibson [1], Stefanie Sandlöbes [1], Sandra Korte-Kerzel [1]

[1] Institute of Physical Metallurgy and Metal Physics [RWTH Aachen University] (IMM) – Templergraben 55, D-52056 Aachen, Germany, Germany

In multiphase Zn-Al alloys, the mechanical behaviour and activated deformation mechanisms are controlled by both the properties of individual microstructural constituents as well as the joint effect of these constituents as an aggregate. In the present study, the local mechanical properties and deformation mechanisms of individual microstructural constituents in a ZnAl4Cu1Mg0.31 alloy are studied using nanoindentation tests at room temperature (25∘C) and 85∘C. The primary η-Zn phase is softer than η-Zn+α-Al eutectic/eutectoid structures and deforms plastically by compression twinning and dislocation slip, while η-Zn+α-Al eutectic/eutectoid structures deform predominantly by phase boundary sliding. Further, the strain partitioning between individual microstructural constituents and their roles in macroscopic tensile deformation at 85∘C is investigated using quasi in-situ digital image correlation (DIC). The DIC measurements show that eutectic/eutectoid colonies carry higher strain than the primary η-Zn phase grains and confirm strain transfer across Zn/Al phase boundaries and eutectic/eutectoid colony boundaries.

Keywords: Zinc alloys, nanoindentation, plasticity, digital image correlation (DIC)

*Speaker
†Corresponding author: wu@imm.rwth-aachen.de

On a chip fracture mechanics test method

Sahar Jaddi *† [1], Michael Coulombier‡ [1], Jean-Pierre Raskin§ [2], Thomas Pardoen¶ [1]

[1] Institute of Mechanics, Materials and Civil Engineering, Université catholique de Louvain – 1348, Louvain-la-Neuve, Belgium

[2] Institute of Information and Communication Technologies, Electronics and Applied Mathematics (ICTEAM) – Place du Levant, 3, B-1348 Louvain-la-Neuve, Belgium

A new testing method based on an on-chip concept has been developed to measure the fracture toughness of freestanding submicron films. Fracture mechanics models have been developed to address various types of crack configurations occurring in thin films on substrates. These models have been applied to a wide range of systems, providing relevant fracture toughness data that are important for the design and integrity assessment of coatings and microelectronics applications, for instance. Still, it is sometimes very complicated to deconvolute the constraint exerted by the substrate on the cracked film especially when it involves viscoelastic or plastic deformation. Furthermore, freestanding films allow, if sufficiently thin, direct observation in transmission electron microscopy (TEM). The design of this new test configuration consists of two long actuator beams undergoing large internal stress. A specimen is attached to these two actuators, incorporating a notch patterned by means of e-beam lithography. The geometry resembles a double cantilever beam geometry classically used in fracture mechanics testing. At the start, both actuators and specimen lie on a sacrificial layer. Nothing happens. A chemical release step is then performed through the etching of the sacrificial layer. During the release of the test, the actuators contract pulling on the specimen. A crack is initiated from the notch tip, propagates and finally stops after the energy release rate decreases down to its critical value. This is thus a crack arrest measurement. For the sake of a proof of concept, 55 nm thick silicon nitride films were successfully tested using this new method. Analytical equations that describe the stress intensity factor (energy release rate) were developed and assessed towards the finite element analysis (FE). The experimental results lead to a fracture toughness of these SiN films between 1.6-1.73 GPa$\sqrt{\mu}$m.

Keywords: Thin films, on, chip, fracture, toughness, internal stress, silicon nitride, finite element (FE).

*Speaker

†Corresponding author: sahar.jaddi@uclouvain.be

‡Corresponding author: michael.coulombier@uclouvain.be

§Corresponding author: jean-pierre.raskin@uclouvain.be

¶Corresponding author: thomas.pardoen@uclouvain.be

An analysis of the effect of Al content on the critical resolved shear stress for basal slip in Mg by means of micropillar compression

Jingya Wang * [1], Jon Molina-Aldareguia [1], Javier Llorca† [1,2]

[1] IMDEA Materials Institute. C/ Eric Kandel 2, 28906 Getafe, Madrid, Spain – Spain
[2] bDepartment of Materials Science. Polytechnic University of Madrid. 28040 Madrid, Spain – Spain

Mg-Al alloys with different Al content were obtained from diffusion couples. High purity Mg and Mg-9 at.% Al alloys were casted in an induction furnace in the (VSG 002 DS, PVA TePla) under a protective Ar atmosphere. The ingots were homogenized at 673K for 15 days and cut into discs of 12 mm in diameter and 7.5 mm in length. The Mg and pure Mg-9Al discs were diffusion-bonded using the Gleeble 3800 thermomechanical for 1h at 673K in vacuum under a uniaxial pressure of 30 MPa. Then, the diffusion couples were sealed into quartz capsules within a protective Ar atmosphere. The samples were annealed in a furnace for different times (up to 352h) at 673K before water quenching. The microstructure around the diffusion interface was analyzed by electron -backscatter diffraction in a dual-beam FIB-FEG electron microscope (Helios Nanolab 600i FEI) and the Al concentration (as a function of the distance to the diffusion interface) was measured by electron probe microanalysis (JEOL Superprobe JXA-8900M) in grains with different orientation. Micropillars with different diameters (in the range 3 μm to 10 μm) were machined from grains suitable oriented for basal slip and with different Al content using a dual-beam FEG-FIB microscope (FEI Helios 600i) and the critical resolved stress was determined by means of micropillar compression tests carried out in a nanoindentor (Hysitron TI950). It was found that the initial critical resolved shear stress was dependent on the micropillar diameter for micropillars below 7 μm and that the slip localization within the micropillar also depended on the micropillar diameter. The results of the mechanical tests showed the influence of the Al in solid solution on the critical resolved shear stress for basal slip and further applications of this technique to analyse the effect of solid solution atoms and precipitates on twinning were explored.

Keywords: critical resolved shear stress, basal slip, micropillar compression, diffusion couples

*Speaker
†Corresponding author: javier.llorca@imdea.org

S16: Mechanics of highly porous materials - Experiments and models

Compression behaviour of cellular structures produced by selective laser beam additive manufacturing: X-ray tomography based finite element and experimental appraoches

Yasin Amani *† [1], Sylvain Dancette [1], Eric Maire [1], Pauline Delroisse [2], Aude Simar [2]

[1] INSA de Lyon, MATEIS CNRS UMR5510 – Université de Lyon – France
[2] Institute of Mechanics, Materials and Civil Engineering (iMMC), Louvain-La-Neuve – Belgium

Selective laser melting is a novel additive manufacturing technique to produce cellular structures with desired shape and pattern provided by a computer-aided design software. During the process, series of layers consisting of metal powders are molten and solidified on top of each other using a laser beam. Two face-centred cubic structures with the same shape and repetitive pattern but different beam and node thicknesses were produced for this work using this technique. Deformation of the structures under compression is imaged by in situ and ex-situ X-ray tomography scanning. The initial state of the structures is scanned using the stitching tomography method to capture high-resolution 3D images illustrating micro and macro porosities. A 3D image-based conformal finite element model is then built for the simulation of the compression test using porous plasticity. The local porosity of each element is directly informed from high resolution tomography. Simulations considering a homogeneous matrix with an average initial porosity everywhere are compared to the new inhomogeneous model. A fairly good agreement is found between the inhomogeneous model and experiments.

Keywords: Selective laser melting, Finite element, X ray tomography, Image analysis, GTN model

*Speaker
†Corresponding author: yasin.amani@insa-lyon.fr

Multi-scale study of compression mechanical behaviour of very-low-density polymeric foams: Development of an eX-Poro-HydroDynamic system

Erwan Fourt * [1], Jean Bouyer [1], Pascal Doumalin [2], Aurelian Fatu [2], Serguei Kunik [1]

[1] Institut Pprime (PPRIME) – CNRS : UPR3346, Université de Poitiers, ENSMA – 11 Bd Marie & Pierre Curie BP 30179 86962 Futuroscope Cedex, France
[2] Institut Pprime (PPRIME) – CNRS : UPR3346, Université de Poitiers, ENSMA – France

The Ex-Poro-HydroDynamic (XPHD) system is a new mechanism for pressure distribution. This new system consists of integrating a porous foam imbibed by a lubricating fluid between a stator and a runner, called dislocator. The rotation of the dislocator will create a pressure field to support the load. Unlike its hydrodynamic equivalent, the XPHD thrust bearing supports up to 100 times more load, even at low speeds [1].
Based on the work demonstrating the feasibility of this new system [1], the objective of the present work is therefore to increase the knowledge about the relationship between foam's configuration (added fluid, porosity, pore size...) and mechanical behaviour during compression tests. We are interested by uniaxial compression of very-low-density open-cell foams made of polyurethane. Three foams were studied imbibed by three different fluids (water, oil and air) and samples with different sizes were tested. Optical non-contact techniques of full-field measurement have been employed to extract the mechanical response of foams at different scales of the microstructure. The results of macroscopic tests have be completed by 2D strain field measurements obtained by Digital Image Correlation at the surface of foams. A tridimensional study based on the coupled use of X-ray microtomography and Digital Volume Correlation has been performed in order to evaluate and validate the relation between microstructure and mechanical behaviour of dry and imbibed foams.

The first results demonstrate that the geometry of samples does not affect the mechanical behaviour under compression, however to imbibe a sample change significantly some characteristics of this behaviour such as his Young's modulus, the plateau strain or the energy dissipated. In the same way, those results show that porosity is a parameter which modifies the global mechanical behaviour of dry foams. A relation between porosity and global deformation has been established considering a Poisson's ratio of 0 (no radial deformations) and has been verified by the experimental study with X-ray microtomography. The 2D or 3D measured strain fields in dry foams have revealed that the local strain micromechanisms lead to a strain localisation by bands perpendicular to the compression direction. We show that these strain mechanisms associated to local buckling are not driven by pore size but by local geometrical instabilities of the microstructure. The 3D study of an imbibed sample is under analyse and allows us to evaluate the influence of a fluid on these micromechanisms.

This first work allows us to understand the mechanical behaviour of studied foams, to evaluate their performances and to select a couple fluid/foam to be tested on our XPHD system.
[1] D. Pascovici, "Lubrication by dislocation : A new mechanism for load carrying capacit," Bucharest.

Keywords: Foam, Porosity, Very, low, density, Tridimensional

*Speaker

The peculiar mechanical behavior of silica aerogels revealed by Molecular Dynamics simulations on large volumes

William Gonçalves [1], Christophe Martin * [2,3], Julien Morthomas [1], Michel Perez [1], Patrice Chantrenne [1], Geneviève Foray [1]

[1] Matériaux, ingénierie et sciences [Villeurbanne] (MATEIS) – Institut National des Sciences Appliquées de Lyon, Centre National de la Recherche Scientifique : UMR5510, Université Claude Bernard Lyon 1 – Bâtiment Blaise Pascal 7, avenue Jean Capelle 69621 VILLEURBANNE CEDEX, France
[2] Science et Ingénierie des Matériaux et Procédés (SIMaP) – CNRS : UMR5266, Institut National Polytechnique de Grenoble - INPG, Université Grenoble Alpes – 1130 rue de la Piscine, BP 75 38402 Saint Martin D'Hères, France
[3] CNRS – Centre National de la Recherche Scientifique - CNRS – France

Silica aerogels are highly nanoporous materials structured into a tortuous three-dimensional silica network. This high porosity may reach up to 99% with hypercritical drying. Typically, 80% of the nano-size of pores is below 30nm in size. This nanoporosity is at the origin of the exceptionally low thermal conductivities, acoustical insulation properties and low densities of silica aerogels. Such properties offer unparalleled application opportunities for building insulation, electronics, aerospace, chemistry, pharmacy and many other sectors. However, super-insulation properties come at the price of poor mechanical properties. In this context, the understanding and optimization of the mechanical behavior of silica aerogels is paramount to their future use in applications. This is challenging as their complex structure exhibits different sizes of porosity ranging from the nano to the mesoscale.
Here, we study the mechanical properties of silica aerogels by molecular dynamics (MD) simulations on large samples. In order to investigate the mechanical behavior of such aerogels with high surface area, an interatomic potential able to reproduce both bulk and surface properties of amorphous silica with a significantly reduced computation time is needed. We use a simple pair potential optimized in computation time that reproduces surface and bulk properties very satisfactorily, while leading to a 3000 gain factor on the CPU time per atom per step [$goncalves2016$]. With this optimized pair potential, our atomistic simulations are able for the first time to reproduce samples that are large enough to contain an adequate number of pores together with a pore size distribution, centered on 10 nm size that matches experiments. These nanoporous structures are investigated in detail for their mechanical behavior from elasticity down to fracture. The unprecedented combination used here of large volumes, large strains, and small strain-rates, offers direct evidence of the peculiar mechanical behavior of silica aerogels at the nanoscale.

We show that the surface stress that silica filaments experience produces an unusual discontinuity in the Poisson effect and a dissymmetry in tension and compression. The ductility of highly porous silica aerogels arises from an interplay between a significant amount of reorganization in filaments and surface stress. Taking advantage of the large volumes accessible here, the very heterogeneous nature of low-density silica aerogels is reproduced, with an impact both on their elasticity and on their strength. In particular, we show that the strength of silica aerogels, at the length scale of secondary particles, is a volume dependent property.
[$goncalves2016$] Gonçalves, W., Morthomas, J., Chantrenne, P., Perez, M., Foray, G., & Martin, C. L. (2016). Molecular dynamics simulations of amorphous silica surface properties with truncated Coulomb interactions. Journal of Non-Crystalline Solids, 447, 1–8.

*Speaker

Keywords: silica aerogels, Molecular Dynamics, fracture

Effect of porosity on mechanical response of a functionally graded beams

Lazreg Hadji * [1], Nafissa Zouatnia *

[2], Zoubida Khelifa *

[3], Abdelkader Safa *

[4]

[1] Ibn Khaldoun university of Tiaret – BP 78 Zaaroura, Tiaret, Algeria
[2] Hassiba Benbouali University of Chlef – BP 151, Hay Essalam, UHB Chlef, Algeria
[3] Ibn Khaldoun university of Tiaret – BP 78 Zaaroura, 14000 Tiaret, Algeria
[4] University Center of Relizane, Relizane – Bourmadia, Rélizane, Algérie, Algeria

This work presents a static and free vibration analysis of functionally graded metal–ceramic (FG) beams with considering porosities that may possibly occur inside the functionally graded materials (FGMs) during their fabrication. A new displacement field containing integrals is proposed which involves only three variables. Based on the suggested theory, the equations of motion are derived from Hamilton's principle. This theory involves only three unknown functions and accounts for parabolic distribution of transverse shear stress. In addition, the transverse shear stresses are vanished at the top and bottom surfaces of the beam. The Navier solution technique is adopted to derive analytical solutions for simply supported beams. The accuracy and effectiveness of proposed model are verified by comparison with previous research.
A detailed numerical study is carried out to examine the influence of the deflections, stresses and natural frequencies on the bending and free vibration responses of functionally graded beams.

Keywords: Bending, Free vibration, Functionally graded materials, integral, Hamilton's principle.

*Speaker

Micromechanical properties of metal foam by in-situ and ex-situ testing on the meso and micro scale

Anne Jung * [1], Thomas Bleistein [1], Jutta Luksch [1], Martin Reis [1], Stefan Diebels [1], Jerome Andrien [2], Eric Maire [2]

[1] Saarland University – Germany
[2] INSA LYON - Université de Lyon – Institut National des Sciences Appliquées de Lyon – France

Metal foams are a relatively new class of cellular materials with structural features resembling to lightweight load-bearing materials such as cancellous bones and wood. Their high stiffness-to-weight ratio coupled with their typical long flat stress-strain response make them ideal candidates as cost-effective shock energy absorbers. Cellular materials such as foams offer a tripartite hierarchical structure. The macro scale comprises the entire component or specimen, the meso scale only deals with a couple of pores and the micro scale describes individual struts and their microstructure. The macroscopic mechanical properties of foams are strongly influenced by both the mechanical behaviour of single pores at the mesoscopic level and the struts and their structure at the microscopic length-scale based on a strong structure-property relationship.
Whereas macroscopic mechanical characterisation is widespread, micromechanical characterisation and assessment of micromaterial parameters on single struts is very limited. A robust micromechanical understanding and knowledge of micromaterial parameters is essential to design components made of foams e.g. supported by numerical simulations. However, up to now, micromechanical characterisation of individual struts is very challenging but an emerging field of research.

The present contribution deals with the mechanical characterisation of open-cell aluminium foams on the meso and micro scale. In-situ and ex-situ micro compression and micro tensile tests respectively were conducted on individual pores as well as individual struts of open-cell aluminium foams. X-ray computed tomography (CT) and a photogrammetric method were used to create 3D finite element models of the pores as well as the struts in order to perform numerical simulations. The accuracy of the photogrammetric method is compared to the more precise CT measurements. In-situ experiments in scanning electron microscope and ex-situ micro compression tests were performed on individual pores to determine micro material parameters of the strut material by parameter identification using inverse modelling. Furthermore, in-situ X-ray CT micro tensile tests and ex-situ micro tensile tests were conducted on individual struts. There is a large scattering in the micro material parameters deduced from individual strut. X-ray CT scans during micro tensile testing and ex-situ micro tensile tests performed on struts, where the local microstructure (blowholes, pores, cracks and intermetallic inclusions) was previously determined in CT scans, were performed. The scattering in the material parameters is largely connected to the occurring defects in the microstructure of individual struts.
The unique combination of in-situ and ex-situ mechanical characterisation as well as numerical simulation and parameter identification on the strut level and pore level gives a deep insight in the structure-property relationship of open-cell aluminium foams. This information is important for the design of components made of metal foams.

Keywords: metal foams, microtensile testing, X, ray CT, in, situ testing, pores, struts

*Speaker

Plastic Poisson's Ratio of Nanoporous Metals: A Macroscopic Signature of Tension–Compression Asymmetry at the Nanoscale

Lukas Lührs * [1], Birthe Zandersons [1], Norbert Huber [1,2], Jörg Weissmüller† [1,2]

[1] Institute of Materials Physics and Technology, Hamburg University of Technology (TUHH) – Germany
[2] Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht (HZG) – Germany

At small length scales atomistic simulations as well as observations by zero-creep experiments suggest a surface-induced tension–compression of the strength and flow stress of metallic bodies. As experimental evidence supporting this notion is still missing, we study the impact of capillary forces on small-scale plasticity.
Nanoporous metals can take the form of macroscopic bodies that consist of a bicontinuous network of "ligaments" with sizes that can be tuned from a few nanometers to several microns. Among these materials nanoporous gold (NPG) appears as an ideal model material due its high chemical stability and tunable surface area. Here, we study the transverse plastic deformation of NPG under uniaxial compression in electrolyte. This affords *in situ* variation of the surface state, specifically the surface tension, γ, during plastic flow. We find that decreasing γ results in an increase of the macroscopic plastic Poisson's ratio, ν_P. We show that γ promotes the compression while hindering tensile elongation of individual ligaments. Transverse deformation during compression of the network structure is partly caused by the stretching of ligaments oriented perpendicular to the load axis. Here, the surface-induced tension–compression asymmetry acts to reduce ν_P. Finite element simulations on randomized strut networks with surface tension support experimental observations and confirm the significant contribution of the surface tension to small-scale plasticity.

L. Lührs, B. Zandersons, N. Huber, J. Weissmüller *ACS Nano Letters* (2017) doi: 10.1021/ acs.nanolett.7b02950

Keywords: Nanoporous metal, mechanical properties, tension–compression asymmetry, small, scale plasticity, Poisson's ratio, surface tension

*Speaker
†Corresponding author: weissmueller@tuhh.de

In situ tests on architectured metallic materials

Eric Maire * [1], Jerome Adrien [2], Xavier Boulnat [3], Morgane Mokhtari [3], Christophe Le Bourlot [3], Mahmoud Kachit [3]

[1] Matériaux, ingénierie et sciences (MATEIS) – CNRS : UMR5510, Institut National des Sciences Appliquées (INSA) - Lyon – Bâtiment Blaise Pascal 7, avenue Jean Capelle 69621 VILLEURBANNE CEDEX, France
[2] MATEIS INSA (MATEIS) – Université de Lyon, INSA de Lyon, Laboratoire MATEIS CNRS UMR 5510 – France
[3] mateis insa lyon – Université de Lyon, INSA de Lyon, Laboratoire MATEIS CNRS UMR 5510 – France

Architecture of porous materials is difficult to capture experimentally. X ray computed tomography helps us to do this nowadays with a better precision and in a non destrcutive manner. It has thus become an ideal method to analyze the deformation process of these complex materials. This lecture will examplify this with different architectured highly porous materials.

Keywords: X ray computed tomography

*Speaker

Finite Element Modeling and Geometrical Analysis of Nanoporous Gold Based on Skeletonization of 3D FIB-SEM Tomography Data

Claudia Richert * [1], Kaixiong Hu [1], Norbert Huber [1,2]

[1] Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht (HZG) – Max-Planck-Straße 1, 21502 Geesthacht, Germany
[2] Institute of Materials Physics and Technology, Hamburg University of Technology (TUHH) – Eißendorfer Straße 42, 21073 Hamburg, Germany

Nanoporous Gold (NPG) made by dealloying takes the form of macroscopic millimeter- to centimeter-sized porous bodies with a solid fraction around 30 %. The material exhibits a uniform, bicontinuous network of nanoscale pores and solid ligaments. For its promising functionality and applications spanning from fuel cells to electrochemical sensors, the mechanical behavior is a critical aspect. One main observation of various experimental studies is the anomalously high elastic compliance and early yielding.
In the most recent studies, Liu et al. (Acta Mat., 2016), Hu et al. (Phil. Mag., 2016) and Ziehmer et al. (Acta Mat., 2016) examined the geometrical network structure of NPG, by analyzing SEM images, or carrying out tomographic reconstructions of NPG samples using a dual-beam FIB and SEM, respectively. Furthermore, the ligament diameter distribution and the local curvature were statistically analyzed for varying sample sizes. Examining the network structure, a large percentage of the ligaments are found to be disconnected. The authors attribute the observed mechanical behavior to this lowered network connectivity, because those ligaments are dangling ligaments and thus cannot carry external load.

For deeper understanding of the mechanical behavior and the occurring deformation mechanisms, various modeling approaches are suggested in literature, which simplify the complex NPG network to unit cell structures such as cubic, diamond or three point bending beam. This significant simplification and yet lack of satisfactory understanding of the underlying structure-property relationship brings the risk of losing detailed insight into the real NPG structure, and thus, possibly important aspects of its mechanical behavior.

This study presents a skeleton FEM beam model, which is based on skeletonization of such actual 3D FIB-SEM tomography data of NPG, to achieve an as realistic as possible FEM model of the NPG microstructure. The resulting macroscopic properties are compared to a solid FEM model created from the very same 3D tomographic data, as well as to results obtained from idealized diamond unit cell structures, and the nodal correction for beam models proposed by Jiao et al. (Int. J. Mech. Sci., 2017). In contrast to our expectations, the skeleton FEM beam model shows higher macroscopic stiffness and strength in direct comparison with the solid FEM model. Possible reasons will be discussed.
Besides the generation of a skeleton beam model for any tomography data set, the program routine allows for the statistical evaluation of the skeleton network also non-locally, e.g. the diameter variation along a ligament axis, or the nodal connectivity. The results show that most junctions are three-fold and not four-fold, as assumed by the diamond structure proposed by Huber et al. (Acta Mat., 2014). Furthermore, the relation between nodal connectivity and projecting ligament geometry is analyzed. The investigation of the ligament shapes confirms the assumption of quite massive nodes in comparison to the ligaments. In addition, the ligaments of the analyzed structure show on average a concave shape, with a non-negligible number of convex ligaments though.

*Speaker

Keywords: Nanoporous gold, Finite element method, Mechanical behavior, Structure property relationship

Nanoporous Metals as Actuators: Modelling of Chemoelectromechanical Coupling on Interfaces

Jana Wilmers * [1], Andrew Mcbride [2], Swantje Bargmann [3]

[1] Chair of Solid Mechanics, School of Mechanical Engineering and Safety Engineering, University of Wuppertal – Germany
[2] The University of Glasgow, School of Engineering, Division of Infrastructure and Environment – United Kingdom
[3] Chair of Solid Mechanics, School of Mechanical Engineering and Safety Engineering, University of Wuppertal – Germany

Electromechanical coupling in actuators and sensors arises from various physical processes in the material, e.g., charge re-orientation or surface modification. Depending on the material system at hand, different mechanisms are activated and superimposed.
Nanoporous metals stand out due to their exceptionally high surface-to-volume ratio which makes them react sensitively to any electrically induced surface modification. By filling the interconnected pore space with a liquid or polymeric electrolyte, these nanoporous metals become promising sensor and actuator materials with a wide range of possible applications.

To model the chemoelectromechanically coupled behaviour of such nanoporous actuators, one has to account for interface modifications arising from the build-up of charges in the metal-electrolyte interface and electroadsorption of electrolyte ions onto the interface. In this work [1], a continuum model is utilized that couples large deformations with electrostatics and
charge carrier transport to model the bulk behaviour. This framework is further extended using the principles od surface elasticity theory [2] to establish a model for the unique electromechanical behaviour of the metal-electrolyte interface.
The developed framework utilises the concept of interface stresses to model the different coupling mechanisms occurring on the interface, that is, interface charging and electroadsorption, in addition to the coupled behaviour in the bulk material arising from mass transport in the pore space. The framework allows to study the different phenomena and their interaction with each other and gives insights into the underlying physical mechanisms.
Numerical examples are presented to elucidate the capabilities of the proposed model.

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Keywords: nanoporous metals, actuation, chemoelectromechanical coupling, interface elasticity

*Speaker

S18: Advanced modelling techniques: higher-order continua

Elastic second-strain gradient beams

Fabien Amiot *† [1]

[1] Institut FEMTO-ST – Université Bourgogne Franche-Comté, Université de Franche-Comté, CNRS : UMR6174, Ecole Nationale Supérieure de Mécanique et des Microtechniques, Université de Technologie de Belfort-Montbeliard – France

Because of their high surface over volume ratio, the mechanical behavior of micrometer-sized structures differs from that of usual macroscopic objects. Their surface plays a key role, and this property has been proposed to devise micromechanical sensors of environmental changes. In particular, a significant effort has been put on the development of biological sensors, based on cantilevers operated in static mode, and the published results are highlighting the need for a more basic understanding of coupled surface phenomena [1].

It has been shown that the use of an Euler-Bernoulli beam theory for isotropic second strain gradient elastic materials may provide a framework describing these results, at the cost of additional modeling parameters which are yet to be identified [2]. The available higher-order beam theories are however only based on kinematic assumptions, so that they cannot render Poisson effect for instance [3]. The correct beam stiffness for vanishing higher-order elasticity parameters is however sometimes recovered in a somehow arbitrary way, so that the consistency with the usual Cauchy material-based beam theory is questionable [4]. Refined higher-order beam theories are therefore desirable, keeping their complexity as low as possible.

The approach proposed herein is based on the minimization of the constitutive equation gap in order to simultaneously satisfy kinematic and static conditions. It is shown that the resulting beam equations are consistent with the usual ones obtained with Cauchy materials and are yet tractable. The differences with first-strain gradient theories and the usual (kinematic) second-strain gradient approach are highlighted for several representative load cases, so that the scale range such refined theory is required is identified. Additionally spanning the range of thermodynamically admissible materials, it is shown that the predicted behaviors cluster in few, rather different, families, depending on the higher-order parameters. This could trigger the development of innovative MEMS devices and paves the way for the experimental approach of these materials.

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Keywords: Beam theory, second, strain gradient elasticity

*Speaker
†Corresponding author: fabien.amiot@femto-st.fr

Non-local modeling: macroscopic behavior of a randomly voided material and influence of void morphology on the elastic properties gradient.

Sami Ben Elhaj Salah *† [1], Azdine Nait-Ali‡ [1], Mikaël Gueguen§ [1], Carole Nadot-Martin¶ [1]

[1] Pprime – ENSMA – Téléport 2, 1 Avenue Clément Ader, 86360 Chasseneuil-du-Poitou, France

Abstract

The asymptotic expansion analysis was developed in the framework of homogenization technique, which is applicable for three-dimensional composites made up of inclusions randomly embedded within a matrix. The so-called asymptotic expansion homogenization (AEH) method was developed by Francfort [1] for the case of linear thermoelasticity in periodic structures. The AEH method has been employed to calculate the homogenized thermomechanical properties of composite materials (elastic moduli and coefficient of thermal expansion) [2, 3]. This technique of homogenization enables to replace heterogeneous materials by a homogeneous equivalent medium including second-order displacement gradients [4].

The displacement vector and the stress tensor are considered as functions of macroscopic (x) and microscopic (y) variables. They may be expanded in a series of powers of small (material) parameter , which is the ratio between macroscopic and microscopic scales:

More precisely, the present work is devoted to linear stochastic homogenization and $Gamma$-convergence [5] problems for variational functional. This $Gamma$-convergence allows us to study the corresponding variational problem and to prove the convergence of the minimums and of the minimizers. By combining variational convergence with ergodic theory, we study the macroscopic behavior of linear elastic heterogeneous materials. The inclusions are randomly distributed within a matrix, their size is of order η. The variational limit functional energy obtained when η tends to 0 is deterministic and non-local [6, 7]. By including the characteristic displacement vectors, or correctors, the problem can be solved in order to evidence some links with second gradient theory. The extended form of our variational formulation can be expressed as follows

In this equation, the functional models the overall elastic energy, the functions Un represent the displacement fields within the structure subjected to a given load, denotes the first gradient of the (symmetric) macroscopic strain tensor and Ω denotes the volume of the structure. In addition, the dual quantities of the first and second () gradients of the displacement field, represent the simple and double force stress tensors, respectively. Computational results in periodic and stochastic cases will be exposed and discussed.

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*Speaker
†Corresponding author: sami.ben-elhaj-salah@ensma.fr
‡Corresponding author: azdine.nait-ali@ensma.fr
§Corresponding author: mikael.gueguen@ensma.fr
¶Corresponding author: carole.nadot@ensma.fr

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Keywords: homogenization theory, non local theory, second gradient theory

Continuum modelling of size effects in unstable mechanical metamaterials

Claudio Findeisen * [1], Samuel Forest [2], Jörg Hohe [3], Peter Gumbsch [4,5]

[1] Fraunhofer Institute for Mechanics of Materials (IWM) – Germany
[2] Centre des Matériaux (MAT) – MINES ParisTech - École nationale supérieure des mines de Paris, PSL Research University, Centre National de la Recherche Scientifique : UMR7633 – Centre des matériaux P. M. Fourt RN 447 - BP 87 91003 EVRY CEDEX, France
[3] Fraunhofer-Institut für Werkstoffmechanik (IWM) – Wöhlerstr. 11 79108 Freiburg, Germany
[4] Karlsruhe Institute of Technology (KIT) – Institute for Applied Materials (IAM-CMS), Kaiserstr.12, 76131 Karlsruhe, Germany
[5] Fraunhofer Institute for Mechanics of Materials (IWM) – Wöhlerstr. 11, 79108 Freiburg, Germany

Metamaterials are characterized by effective properties which are mainly driven by the topology of the microstructure, instead of the properties of their constituents. Exploiting the capabilities of structural instabilities, a variety of unusual and interesting effective material properties can be achieved especially with respect to energy dissipation [1,2].
In this contribution we focus on the different kinds of size effects of such materials which can be related to the stability behavior of the microstructure and the finite localization width. By means of a discrete model, we will first present the different kinds of size effects which can be observed in unstable metamaterials and give a physical explanation of their origin. Using an enhanced gradient continuum together with a simple constitutive law, we investigate in the capabilities of such a model to capture the observed size effects. From the solution of an eigenvalue problem we derive an analytical relation between the gradient stiffness and the size of the localization width. By this we are able to capture the finite localization width rather well, which is the necessary condition to describe the related size effects. By a numerical solution of the gradient model, together with a stability analysis we present and discuss the capabilities of the model to capture the observed size effects.

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Keywords: metamaterials, gradient continuum, instabilities, size effects

*Speaker

On revisiting size-dependent beam theories in gradient elasticity

Sergey Lurie *† [1], Yury Solyaev [1], Natalia Tuchkova [2]

[1] Institute of Applied Mechanics of Russian Academy of Science (IAM RAS) – Leningradsky ave., 7, Moscow, Russia
[2] Dorodnicyn Computing Centre of Russian Academy of Science (CC RAS) – Vavilova, 40, Moscow, Russia

The problem of the size-dependent Bernoulli-Euler beam models development in the frame of strain-gradient elasticity theories is considered. General Mindlin's Form I and Form II [1], Gusev-Lurie theory [2] and simplified strain gradient elasticity theory [3] are considered. It is shown the deviation between several known size-dependent beam models and analytical and numerical three-dimensional solutions found for a beam bending problems.
Semi-inverse solutions of a beam pure bending problem in the frame of three-dimensional statement of gradient elasticity with correct satisfaction of natural boundary conditions on the beam surfaces are presented. In particular, it is shown that in the semi-inverse analytical solutions the inverse squared dependence of normalized bending stiffness on the beam thickness could arise only due to non-correct formulation of the boundary conditions. In correct analytical solutions, the finite values of normalized bending stiffness for ultra-thin beams are realized. These results are also check based on 3D FE modelling in the frame of gradient elasticity formulation. It is shown that FE modelling also predicts the independence of normalized bending stiffness on the beam thickness in a pure bending problem. However, in cantilever bending test it predicts a strong dependence of a beam apparent bending stiffness on its length and thickness due to influence of the fixed end of the beam.

Thus, it is shown, that there exist only one correct approach for a beam models developing in the frame of gradient elasticity that is assume a uniaxial stress state of the beam. Corresponding variational approach for a correct beam models formulation is proposed. It is shown, that these size-dependent models are in line with three-dimensional solutions and with known molecular dynamic simulations and they do not contradicts with known experimental data for micro-sized beams.

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Keywords: gradient elasticity, size dependent beam models, semi inverse solution, pure bending, FE modelling

*Speaker
†Corresponding author: salurie@mail.ru

Modeling surface effects and size-dependent hardening in single crystals

Xiang-Long Peng *† [1,2], Edgar Husser [3], Gan-Yun Huang [1], Swantje Bargmann [2]

[1] Department of Mechanics, School of Mechanical Engineering, Tianjin University (TJU) – Yaguan Road, Jinnan District, 300350 Tianjin, China
[2] Chair of Solid Mechanics, School of Mechanical Engineering and Safety Engineering, University of Wuppertal (BUW) – Gaußstr. 20, 42119 Wuppertal, Germany
[3] Institute of Continuum Mechanics and Material Mechanics, Hamburg University of Technology (TUUH) – Eißendorfer Str. 42, 21073 Hamburg, Germany

Crystalline materials at small scale usually possess plastic behavior quite different from those of their bulk counterparts, such as the size-dependence of the yield or flow stress and strain hardening, which are beyond the predictability of conventional plasticity theories. Since macroscopic crystal plasticity mainly results from the microscopic dislocation gliding on crystallographic slip planes, the unusual plastic behavior in small-scaled crystals should be closely relevant to the distinctive dislocation activities therein. On the one hand, geometrically necessary dislocations (GNDs) more likely to accumulate in small-sized crystals are found to be responsible for size-dependent hardening. On the other hand, as the volume to grain boundary (GB)/surface ratio is extremely larger in small-scaled crystals, the interactions between dislocations and GBs/surfaces such as dislocations absorption and/or emission by GBs/surfaces significantly affect the plastic behavior. To construct predictive theories aimed at plastic behavior in small-scaled crystals, those dislocation-relevant mechanisms both in the bulk and at GBs/surfaces should be decently considered on the continuum level. So far, although various higher-order or lower-order strain gradient theories constructed by incorporating the influence of GNDs are able to capture size effects on strain hardening, more attentions should be paid on modeling GBs/surfaces. In this work [1], we focus on modeling the interaction between dislocations and surfaces in single crystals, in particular, dislocation absorption by surfaces. A surface model with energetic and dissipative surface effects is proposed within the framework of higher-order strain gradient crystal plasticity theories [2-8]. The physically motivated energetic surface effect results from the change of surface energy due to the formation of surface steps after dislocation absorption [5]. The dissipative surface effect accounts for the resistance against dislocation absorption by surfaces. The key feature of the surface model is an evolution equation for the slip rate at the surface for each slip system, which governs surface yielding and hardening. The theory is implemented into an in-house finite element code based on a dual-mixed finite element solution strategy [2]. A thin film under shear deformation serves as a benchmark problem for validation of the proposed model. It is found that both the energetic and dissipative surface effects significantly affect the plastic behavior. The predicted film thickness-dependence in terms of the stress-strain response is qualitatively consistent with experimental results.

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*Speaker
†Corresponding author: xlpeng@tju.edu.cn

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Keywords: strain gradient, crystal plasticity, surface effects, size effect, surface yielding

A micromorphic computational homogenization framework for heterogeneous materials in finite deformation

Leong Hien Poh *† [1]

[1] National University of Singapore – Singapore

The first-order computational homogenization approach is restricted to problems where the macro characteristic length scale is much larger than the underlying RVE. In this contribution, focusing on matrix-inclusion composites, a novel computational homogenization framework is proposed such that *standard* continuum models at the micro-scale translate onto the macro-scale to recover a micromorphic continuum. Departing from the conventional FE2 framework where a macroscopic strain tensor characterizes the average deformation within the RVE, our formulation introduces an additional macro kinematic field to characterize the average strain in the inclusions. The two macro kinematic fields, each characterizing a particular aspect of deformation within the RVE, thus provide critical information on the underlying rapid fluctuations. The net effect of these fluctuations, as well as the interactions between RVEs, are next incorporated naturally into the macroscopic virtual power statement through the Hill-Mandel condition to recover a micromorphic continuum at the macro-scale. The length scale parameter associated with the higher-order term characterizes the nonlocal interaction between neighbouring micro-mechanisms, which in turn provides a regularization effect and enables an accurate prediction of the size-effect. The excellent performance of the proposed homogenization approach is illustrated by benchmarking its predictions against reference DNS solutions. Considering a shear wave loading problem, it is shown that the homogenized micromorphic model accurately captures the material responses, even in the *absence of a clear separation* between the loading wavelength and the RVE size. Specific choices for the decomposition of kinematic fields, as well as the boundary conditions adopted, will also be elaborated.

Keywords: homogenization, micromorphic, higher, order continua, generalised continua, size effect

*Speaker
†Corresponding author: leonghien@nus.edu.sg

Interface modelling by a nonlocal interphase – a comparison of approaches

Luv Sharma [1], Ron Peerlings * [1], Marc Geers [1], Pratheek Shanthraj [2], Franz Roters [2]

[1] Eindhoven University of Technology – Netherlands
[2] Max Planck Institute for Iron Research – Germany

In this work, a method to incorporate interface softening in a FFT based crystal plasticity framework is presented. The method is developed keeping in mind the application to multiphase polycrystalline materials. In FE based methods, the multiscale nature of the interface mechanics can be collapsed into subdimensional (interface) elements. In FFT based methods, elements do not conform to the interfaces. Therefore it is not possible to develop interface elements for FFT based methods. This limitation is circumvented using the idea of an interfacial band – an interphase band is introduced along the sharp interfaces. This band consists of the Fourier sampling points in the vicinity of the interfaces. It is this volumetric region which takes up the role of dissipation of fracture energy, as opposed to a surface in cohesive zone methods. This also allows to capture the full three-dimensional state of stress inside the damaging zone. Within the band, the plastic constitutive behavior is inherited from the respective adjacent grains. In addition, to model the anisotropic kinematics of the cracking process, a damage eigen strain is introduced. The eigen strain is constructed by appropriately mapping the opening strains (in tangential and normal modes) relative to the interfacial planes. The driving forces for these openings are the resolved tractions which act against a monotonously degraded resisting force. In order to avoid the localisation associated with softening, various nonlocal strategies – integral based averaging, gradient based non-local damage and phase field methods are explored. The boundary conditions at the two interfaces of the band also become important from the point of view of possible interaction with the intragranular damage physics. Application of these boundary conditions in the context of these different regularization techniques is discussed. The effective length scale of dissipation is controlled by the length scales of the nonlocal regularisation and the interface bandwidth. We consider the interface bandwidth as the numerical parameter with respect to which the results should be objective. Scaling relations for the work of separation and the peak load are obtained for a 1D case and then for a propagating crack in 2D. Suggestions to scale the constitutive parameters (critical strength and critical opening strain) are given. The performance of the different regularisation strategies from the view point of numerical stability and ease of implementation is also discussed. Finally, an application to cluster of grains is presented.

Keywords: Damage, Nonlocality, Regularization, Interfaces, Interphases

*Speaker

A thermodynamic consistent strain gradient cyclic plasticity model: A case study on cyclic torsion behavior

Xu Zhang *† [1], Jianfeng Zhao [1]

[1] School of Mechanics and Engineering, Southwest Jiaotong University – China

A thermodynamic consistent strain gradient cyclic plasticity model with combined isotropic hardening and kinematic hardening were developed. In this framework, the plastic work were assumed to be composed of two parts: the energetic part and the dissipative part. Then, the isotropic hardening is due to the dissipative part while the kinematic hardening is attributed to the energetic part. Based on a rigid-plastic approximation, the closed-form of monotonous and cyclic torsion responses was obtained, the numerical results showed that the size effect in initial yielding was due to the gradient related with the dissipative part, whereas the energetic gradient part leaded to the size effect in subsequent flow as well as the Bauschinger effect. Comparing with the torsion experiments, the established model captured the observed phenomena, e.g. the normalized backstress evolution, cyclic hardening, and especially, an abnormal plasticity phenomenon that the reverse plasticity even occurs before unloading.

Keywords: microscale wire, cyclic torsion plasticity, backstress, energetic, dissipative, strain gradient plasticity, abnormal plasticity phenomenon

*Speaker
†Corresponding author: xzhang@swjtu.edu.cn

Finite second and third-order gradient elasticity and plasticity

Albrecht Bertram * [1]

[1] Otto-von-Guericke University Magdeburg (OVGU) – Universitätsplatz 2 D-39106 Magdeburg, Germany

Within the context of finite deformations, an extension of the classical continuum theory to gradient media is by no means straightforward or unique. In fact, already the choice of appropriate variables for material models becomes difficult and controversial. Moreover, the derivation of the boundary conditions is gets extremely complicated for higher order materials.
We first introduce material variables which serve for invariant forms of the material laws. Once having established a reduced form for the constitutive equations, one wants to introduce symmetry properties for the further reduction. So one has to introduce symmetry transformations for this class of materials.
By putting such a theory into a thermodynamic format, one is able to derive necessary and sufficient conditions for the thermodynamic consistency.
This will be done for the second and third order gradient elasticity and elastoplasticity.

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Keywords: Keywords, third, order gradient elasticity, gradient plasticity, second, strain gradient

*Speaker

S19: Advanced modelling techniques: scale bridging

Argillaceous rock microstructure considering variability and heterogeneity for double scale modelling with hydro-mechanical coupling

Pierre Bésuelle * [1], Benoît Pardoen [1], Jacques Desrues [1], Stefano Dal Pont [1], Philippe Cosenza [2]

[1] Univ. Grenoble Alpes / CNRS / Grenoble INP, 3SR Lab. (3SR) – Université Grenoble Alpes, CNRS : UMR5521, Institut polytechnique de Grenoble - Grenoble Institute of Technology : UMR5521 – Grenoble, France
[2] Institut de Chimie des Milieux et Matériaux de Poitiers (IC2MP) – Université de Poitiers, Centre National de la Recherche Scientifique : UMR7285 – 4 RUE MICHEL BRUNET BAT B27 - CHIMIE 86022 POITIERS CEDEX, France

In the context of radioactive waste management, clay rocks are considered as favourable media for deep geological repositories. Questions have risen on how microstructural characteristics of heterogeneous rocks can enrich the constitutive behaviour at macroscale. Consequently, the modelling of the hydro-mechanical behaviour of a clay rock is considered by taking into account its microstructural characteristics and their variabilities. Furthermore, the principle of deep geological repositories relies among others on the low permeability of the host rock. As the permeability is influenced by mechanical damage of the material, the coupling between hydraulic and mechanical behaviour of the host rock is of importance.
In this context an approach is investigated for the modelling of the hydro-mechanical coupled behaviour of Callovo-Oxfordian claystone, a potential host rock for repositories in France. The approach presented is a double-scale finite element method (FEM2) using an elementary volume (EV) to model the material behaviour at the microscale. The global response of the EV serves as a homogenised numerical constitutive law for the macroscale. At macroscale, a poro-mechanical continuum is defined with fully coupled hydro-mechanical behaviour. At microscale, the microstructure of the material in the EV contains elastic deformable solids separated by damageable cohesive interfaces. Cohesive forces are described by a damage law, allowing softening of the material due to deformation. Additionally, the interfaces form a porous network allowing fluid transport prescribed by the variation in interface opening which leads to a variation of the material permeability. With fluid pressure acting on the solid parts, this gives a coupled hydro-mechanical system at the micro level. [1]

The work focuses on the definition of the EV in a clay rock, in order to be both a realistic and simple representation of the material. Experimental observations and characterisations of the rock's microstructure are considered to define the material in a realistic manner [2]. The representativeness of the microstructure in the elementary volume depends on its size which is limited due to numerical constrains for double-scale approach. The weakness of the representativeness can be partially solved by the spatial variability of the EV at Gauss points of the macro-FE-model. Moreover, the natural heterogeneity of clay rock at intermediate scales between the macro and micro scales can be taken into account by a spatial variability of the EV. A sensibility analysis on the choice of the EV and consequences on the macro response is investigated.

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*Speaker

Keywords: double scale model, FEM2, clay rocks, microstructure, variability

Variational homogenization for modeling the bending behavior of graphene

Antonino Favata * [1]

[1] Department of Structural and Geotechnical Engineering - SAPIENZA University of Rome – Via Eudossiana 18, 00184 Rome, Italy, Italy

Graphene is a two-dimensional carbon allotrope, in the form of a hexagonal lattice whose vertices are occupied by C atoms. It has recently attracted a huge interest of the scientific community, due to its extraordinary mechanical, electrical and thermal conductivity properties, that make graphene a candidate for a great variety of technological applications; actually, its potentialities, and those of graphene-based materials, are far from being fully understood, and many studies are carried out in order to develop new technological applications. In particular, understanding the bending behavior of graphene represents a challenge of significant interest because of possible applications in the field of flexible devices.
In this contribution, we present an atomistic-to-continuum model. The main results are based on the application of the notion of Gamma-convergence and the variational homogenization technique.

Under the assumption that the atomic interactions are governed by a harmonic approximation of the 2nd-generation Brenner REBO (reactive empirical bond-order) potential, involving first, second and third nearest neighbors of any given atom, we determine the variational limit of the energy functionals. It turns out that the Gamma-limit depends on the linearized mean and Gaussian curvatures. If some specific contributions in the atomic interaction are neglected, the variational limit turns out to be non-local.

This is a joint work with Cesare Davini and Roberto Paroni.

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Keywords: Graphene, homogenization, Gamma convergence

*Speaker

Multiscale homogenization schemes for the construction of second order gradient anisotropic continuum media of architectured materials

Jean-François Ganghoffer * [1], Yosra Rahali [2], Francisco Dos Reis [3]

[1] Jean-François GANGHOFFER (LEM3 - Université de Lorraine) – CNRS : UMR7239 – 7 rue Félix Savart BP 15082 57073 METZ CEDEX 03, France
[2] Unité de recherche de mécanique des solides, structures et développements technologiques. ESSTT. Université de Tunis, BP56, Bab Mnara 1008, Tunisie (ESTT) – Tunisia
[3] LPMT - Université de Mulhouse (LEM3) – LPMT – France

We presently construct effective second order grade anisotropic continuum models equivalent to initially discrete periodic beam lattices. This entails the construction of a second order grade continuum with effective mechanical properties at the first and second order, accounting for the impact of the underlying microstructure on the overall effective mechanical response of the effective continuum. Starting from the weak form of the equilibrium equations of the lattice and writing the expansion of the discrete displacement up to the second order gradient of the continuum displacement field, the expressions of the Cauchy stress and the hyperstress tensors of the effective second order grade continuum are identified versus the first and second order gradients of the displacement field. Three models of increasing complexity of the beam kinematics are presented: a first model relying on the displacement as the sole kinematic variable, a second model is incorporating a local microrotation in addition to the displacement as kinematic descriptors, and a third model accounting for the network curvature considering a general parameterization of the material points with curvilinear coordinates, and two hierarchical scales of the microstructure. The consideration of the local microrotation is shown to strongly improve the quality of the homogenized second order gradient continuum, when comparing the effective first and second order moduli with the corresponding FE computed moduli. The relevance of the third more complex model is illustrated by two examples showing a strong effect of the microstructured beams on the evaluated second order effective elastic properties.

Keywords: multiscale methods, second gradient, architectured materials, network materials, internal length scales, curvature effects

*Speaker

Homogenized response of mechanical metamaterials with microstructures revealing patterned fluctuation fields

M.g.d. Geers *† [1], M.m. Ameen [1], O. Rokoš [1], R.h.j. Peerlings [1]

[1] Eindhoven University of Technology (TU/e) – Netherlands

Classical engineering materials typically have microstructures for which the effective response can be easily predicted by standard homogenization schemes or more advanced computational homogenization schemes. This class of materials typically shows scale separation, whereby the fine scale fluctuations in the deformation fields can be condensed out through proper upscaling. This paper focuses on a class of materials which does not satisfy this scale separation property. Particular microstructures may develop fine scale fluctuation fields influencing the coarse scale behaviour directly. This typically occurs when a fluctuation pattern arises that has a direct influence on the fluctuation fields and patterns in its immediate neighbourhood. The emerging patterns tend to correlate and reveal long range order in the fine scale fluctuation field. This phenomenon has its direct consequences on the macro-scale mechanical response, for which it is no longer sufficient to extract the average deformation and stress state only. As a result, these materials are typically classified as mechanical metamaterials.
This paper addresses a particular example of such a pattern-transforming material, i.e. a periodically voided hyperelastic elastomer in which geometrical instabilities give rise to long range patterning in the fine scale deformation field. The elastomer is modelled as a classical Mooney-Rivlin material, with constitutive parameters based on experimental work by Bertoldi and co-workers. Two typical loading cases are considered, compression and bending, revealing the influence of the gradient in the macroscopic deformation field.

The homogenized reference solution is here constructed by ensemble averaging, by analysing a whole family of shifted microstructures relative to the macroscopic domain. The emergence of boundary layers and accompanying size effects is studied and discussed. The applicability and limitations of classical homogenization schemes are scrutinized and quantitatively assessed. Finally, some reflections towards advanced homogenization methods, applicable to this class of materials, are presented.
Acknowledgement: The research leading to these results has received funding from the European Research Council under the European Union's Seventh Framework Programme (FP7/2007-2013) / ERC grant agreement n○ [339392].

Keywords: Homogenization, metamaterials, microfluctuations, instabilities

*Speaker
†Corresponding author: m.g.d.geers@tue.nl

A statistical approach to characterize dislocation microstructures

Nina Gunkelmann *† [1], Markus Stricker [2], Iyad Alhafez [3], Dominik Steinberger [4], Herbert Urbassek [3], Stefan Sandfeld [4]

[1] Chair of Computational Material Sciences/Engineering, Institute of Applied Mechanics (TU Clausthal) – Germany
[2] Institute for Applied Materials, Computational Materials Science (Karlsruhe Institute of Technologie (KIT)) – Germany
[3] Physics Department and Research Center OPTIMAS (TU Kaiserslautern) – Germany
[4] Chair of Micromechanical Materials Modelling (MiMM), Institute of Mechanics and Fluid Dynamics (TU Bergakademie Freiberg) – Germany

For any simulation realistic initial dislocation structures must be modeled to adequately describe the dynamics of a system. The field of dislocation dynamics is especially challenging because the deformation behavior for small samples strongly depends on the initial configuration. In DDD a large amount of initial dislocation networks are used. Although realistic dislocation setups consist in general of complex networks most often a distribution of isolated Frank-Read sources (FRS) exhibiting different lengths and orientations has been applied as initial dislocation configuration. One drawback of this method – in particular for small samples – is the introduction of persistent pinning points, which permanently immobilize/stabilize parts of the dislocation network and artificially stabilize the dislocation network. More realistic structures can be obtained from relaxation processes which lead to complex statistical properties of the dislocation microstructure. To describe these structures, a concise method for detailed quantitative analysis of dislocation microstructures is necessary.
We present the conversion method D2C which can be used for computationally analyzing discrete dislocation microstructure from various methods, e.g. MD simulations, TEM microscopy or tomography, continuum or DDD simulations. We quantitatively analyze several different dislocation microstructures which are generated with a DDD framework in terms of continuum field variables. These fields have the benefit that they allow to easily compute ensemble averages to get statistically reliable data. Our data shows that FR sources lead to artificial statistical properties of the dislocation density fields. The statistical properties of the structures obtained from relaxation processes can be described by a Poisson point process.
DDD requires also input from lower scale methods as MD, for example in form of nucleation criteria of dislocations. In the second part of the presentation, we show how D2C can help to analyze data obtained from atomistic simulations. We are able to provide properties of the dislocation microstructure which cannot directly be captured by molecular dynamics data. As an example we apply the methodology to atomistic simulations of nanoscratching in iron. By characterizing the curvature nucleation rate of dislocation loops versus scratching length we find that for large scratching lengths the nucleation of dislocations is accommodated by annihilation processes leading to an almost constant averaged curvature of the dislocations.

Keywords: dislocation dynamics, data compression, continuum theory of dislocations, microstructure, molecular dynamics, nanoscratching

*Speaker
†Corresponding author: nina.gunkelmann@tu-clausthal.de

Dislocations as force distributions: theory and applications

Benat Gurrutxaga-Lerma *† [1]

[1] University of Cambridge – United Kingdom

This talk concerns the way in which dislocations can be represented as force distributions in an elastic, generally anisotropic continuum. The force representation of dislocations provides a simple description of dislocations, which may be employed in lieu of the traditional eigenstrain theory in both theoretical and computational models of dislocations. In this talk, we begin by recalling the Burridge-Knopoff force representation theorem [1], of wide use in seismology, and which enables any internal discontinuity to be represented as a body force.
For illustrative purposes, we first apply this theorem to straight edge and screw dislocations. We show that the elastic fields of these force representations match the expected static and dynamic elastic fields. We show that screw dislocations are self-equilibrated defects, whilst individual edge dislocations entail a force imbalance, and that dipoles of edge dislocations entail a torque. We then derive the force distribution for general closed loops, from which we prove the classical Volterra and Mura formulae, further showing the consistency of the approach.

We showcase how the force representation of dislocations may be employed in a number of numerical applications, including phase field models, boundary elements, and variational principle formulations such as the finite element method. As an example, we apply the former to study the scattering of elastic waves across a welded interface emanating from a moving dislocation. We also use the force representation of dislocations to study the thermoelastic fields of a dislocation.

We then go on to examine the meaning of the force distribution from an atomistic perspective. We employ the harmonic lattice formalism to study the way dislocations may be represented in a lattice in terms of forces, and we derive the harmonic lattice equivalent of the force representation in the continuum. We show that using the long wave argument [3], one achieves the continuum force representation of dislocations derived in this talk from the Burridge-Knopoff theorem, thereby giving a physical meaning to the force representation of dislocations.

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Keywords: Dislocations, atomistic, continuum, harmonic lattice

*Speaker
†Corresponding author: bg374@cam.ac.uk

A lattice Green function method for atomistic/continuum coupling: theory and data-sparse implementation

Max Hodapp *† [1], William Curtin [1], Guillaume Anciaux [1], Jean-François Molinari [1]

[1] Ecole Polytechnique Fédérale de Lausanne (EPFL) – Swiss Federal Institute of Technology EPFL-FSTI IEL-LTS2, Station 11 Lausanne 1015 - Switzerland, Switzerland

Treating atoms individually in material science applications comes along with high computational cost with increasing simulation size. However, many problems require atomic scale resolution only in small parts of the computational domain to resolve the nonlinear behavior of isolated defects, e.g. crack tips, dislocations, voids etc. Commonly these problems are treated using homogeneous Dirichlet conditions on the outer boundary (or the elastic field of the defect). However, if the Green function of the defect is long range, the problem sample has to be sufficiently large to reach a desired accuracy.
In the 1970's Sinclair and co-workers proposed so-called flexible boundary conditions which minimize inhomogeneous forces appearing in the pad domain after each atomistic relaxation by means of lattice Green functions [1]. However, this problem is of $O(N^2)$, where N is the number of pad atoms, which becomes quickly unfeasible with increasing problem size. Moreover, the form of the incremental update equation can be shown to be equivalent to a gradient descent iteration with respect to a weighted inner product space which is known to converge rather poorly. Therefore the method appears unsuitable for problems beyond the scope of studying isolated defects.

We show that Sinclair's method indeed converges to a solution which solves a linear system. This linear system is nothing but the discrete analog to the boundary integral equation for exterior problems [2]. Similar formulations were derived in [3] but ours is more general since it is not bound to a specific geometry or lattice type (the same is true for the formulation in [4] but the system matrices were not reduced to boundary matrices).

In order to overcome the bottleneck of memory consumption we exploit the fact that the system matrices can be represented as hierarchical matrices [H-matrices, 5]. H-matrices are block-wise representations of the original matrix, where suitable (off-diagonal) blocks can be efficiently stored in a data-sparse format with O(log(N)N) complexity using low-rank approximations, thanks to the asymptotic smoothness of the lattice Green function. This allows us to consider larger atomistic domains, more precisely, we may study arrangement of defects – on moderate computer clusters. Moreover, linear algebraic operations (e.g. matrix-vector multiplications) become considerably more efficient.

We have integrated our method into the open source atomistic code LAMMPS. The matrix assembly and linear algebraic operations via H-arithmetics are performed using the library from [5]. We give some details on the implementation aspects. Further, we present some numerical examples for two- and three-dimensional problems, i.a. probably a dislocation and a crack problem.

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*Speaker
†Corresponding author: max.hodapp@epfl.ch

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Keywords: atomistic/continuum coupling, lattice Green functions, domain decomposition, model reduction, dislocations

Atomistically Informed Dislocation Dynamics Computations: Application to the Simulation of Interactions between Dislocation and Radiation-Induced Loops in Zirconium

Wassim Kassem *† [1], Laurent Dupuy‡ [1], Fabien Onimus [1]

[1] Service de recherches métallurgiques appliquées, CEA, Université Paris-Saclay (CEA) – Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA) - Saclay, Université Paris-Saclay,Sorbonne Universités – 91191, Gif-sur-Yvette, France

Zirconium alloys are used for the cladding of the nuclear fuel of pressurized water reactors. The neutron irradiation, occurring inside the reactor core, affects the mechanical properties of the material. Since the cladding is the first barrier against the dissemination of radioactive nuclei, it is important to have the most reliable simulation tools able to predict the effect of irradiation.

At the microscopic scale neutron irradiation leads to the formation of point defects clusters in the form of small dislocation loops in very high density. The strong radiation-induced hardening and the loss of macroscopic ductility is related to the interactions between gliding dislocations and these dislocation loops. This is the reason why we have undertaken multi-scale numerical simulations of the interactions between dislocations and loops.

Starting from the atomic level, Molecular Dynamics simulations have been used (LAMMPS code) to study the details of the interactions, following the work done by Serra and Bacon [1]. However, Molecular Dynamics (MD) simulations remain limited to short time scale and small simulation box. In order to go towards higher length and time scales, we performed Dislocation Dynamics (DD) simulations using the NUMODIS code. These simulations require several inputs such as the crystallographic structure, the elastic constants, but also the dislocation self-energy and the dislocation mobility. A suitable parametrization is therefore obtained by a detailed and systematic comparison of MD and DD simulations performed at the same time and length scales on a limited set of elementary configurations.

Based on this parameterization, interactions between dislocation and loops are eventually computed with the two numerical tools and compared both qualitatively and quantitatively. A very good agreement is obtained between the two types of simulations, allowing the use of the mesoscale DD simulation for massive computations involving many loops and many dislocations. In future prospect these large scale computations could lead to the determination of constitutive laws that can be implemented in continuum crystal plasticity models.

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Keywords: dislocation dynamics, molecular dynamics, zirconium, dislocations

*Speaker
†Corresponding author: wassim.kassem@cea.fr
‡Corresponding author: laurent.dupuy@cea.fr

Approximating the fluctuations in random heterogeneous problems

Frederic Legoll * [1,2]

[1] Ecole des Ponts ParisTech (ENPC) – École des Ponts ParisTech (ENPC) – École des Ponts ParisTech 6-8 avenue Blaise-Pascal Cité Descartes 77455 Champs-sur-Marne Marne-la-Vallée cedex 2, France
[2] MATHERIALS (INRIA Paris - Rocquencourt) – INRIA, École des Ponts ParisTech (ENPC) – France

Computing the homogenized properties of random materials is often very expensive. The full-field approach consists in considering a large RVE, and solving the equilibrium problem on that RVE, submitted to e.g. periodic boundary conditions. Because the RVE is finite, the obtained apparent effective properties are random, and therefore fluctuate from one realization of the microstructure to another. We have recently introduced several efficient numerical approaches to reduce the statistical noise. These approaches allow to compute the expectation of the effective coefficients (for a given RVE size) in a more efficient manner than brute force Monte Carlo methods.

Beside the (averaged) behavior of the material response on large space scales (which is given by its homogenized limit), another question of interest is to understand how much this response fluctuates around its coarse approximation, before the homogenized regime is attained. More generally, we aim at understanding which parameters of the distribution of the material coefficients affect the distribution of the response, and whether it is possible to compute that latter distribution without resorting to a brute force Monte Carlo approach.

This talk, based on joint works with P.-L. Rothé, will review the recent progresses made on these questions.

Keywords: Random heterogeneous materials, Fluctuations

*Speaker

Multiscale Modeling of Discrete Mesomodels for Dry-Woven Fabrics

Marco Magliulo * [1], Lars Beex [2], Andreas Zilian [3]

[1] University of Luxembourg – Luxembourg
[2] Université du Luxembourg – Luxembourg
[3] University of Luxembourg, Research Unit in Engineering Science (RUES) – Luxembourg

Fabrics are frequently used in industry to enhance the mechanical behavior and reliability of plastic components such as membranes. To manufacture parts with such reinforced plastics, the dry-woven fabric is often placed in a preform and subsequently covered by the bulk material (for example plastic or rubber) as a liquid before it hardens. For the mechanical performances of the final product, it is of importance how the dry-woven fabric deforms during the placement in the preform. Local strains, as well as relative displacements of the yarns, may indeed occur thus modifying the mechanical response of the woven locally.
The material behavior of dry-woven fabrics is largely governed by the contact between yarns undergoing large displacements and rotations. Representing these local interactions accurately with a constitutive model is a non-trivial task.
This is why we have formulated a model that captures the behavior of individual yarns where each yarn is modeled by an assembly of finite elements with a slender geometry. Frictional contact between these assemblies using a simple Coulomb's law is also incorporated.
To enlighten the computational burden associated with such discrete mesomodels for application-scale simulations, we use a multiscale method, called the quasicontinuum (QC) method. This method has mostly been used to alleviate the burden of atomistic lattice computations and has recently been reformulated to deal with dissipation in structural models and to deal with irregular structures. We build on these extensions and show that the multiscale framework is substantially faster than the direct numerical simulation, whilst the additional numerical error remains substantially small.

Keywords: Woven, Quasicontinuum, Multiscale, Contact, Discrete Model

*Speaker

Conformal discretization of complex hetereogeneous RVEs

Thierry Massart * [1,2], Karim Ehab Moustafa Kamel [2], Bernard Sonon [2]

[1] Université libre de Bruxelles (ULB) – Belgium
[2] Université libre de Bruxelles (ULB) (ULB) – Belgium

The behavior of heterogeneous materials is often highly dependent on their micro-morphology. Models attempting to establish a link between experimental observations and the physical underlying mechanisms governing the behavior of heterogeneous materials therefore must incorporate explicitly the morphology of the microstructures of interest.
To this end, computational homogenization techniques have been developed over the last decades. These methods require the availability of Representative Volume Elements (RVEs) of a material under investigation, which can be obtained either experimentally (e.g. CT scans) or numerically generated by algorithms aiming to reproduce the main micro-morphological features [1].

In all cases, this results in complex geometries that need to be discretized to simulate the RVE response using various discretization techniques. The complexity of heterogeneous geometries has been accommodated by developing XFEM approaches based on the concept of partition of unity over the last decade [2]. Yet, there remains an interest to further allow the use of available conventional finite packages for multi-scale analyses, which allows benefiting from all the available tools related to advanced constitutive models, large strain or coupled formulations.

To achieve this, a mesh generation procedure based on previous works by Persson [3] is developed. It is based on a hierarchical Delaunay mesh generator, based on an extended Persson-Strang truss analogy optimization process using an input level set function to build confrming tetrahedral meshes. It allows for a local control of the element sizes, with an ad-hoc analogy with the equilibrium of a bar truss system. Desired bar lengths evaluated from a constructed element size function, and distances from the interface evaluated from the underlying level set function, are used to formulate forces acting on nodes of the truss to steer them to an equilibrated situation. A surface mesh conforming with the material interfaces is first obtained by starting from an initial Delaunay surface mesh, and by constraining the normal movement of nodes. A good shape factor for elements is ensured by controlling elements size with a tension/compression force field in the bars to reach the targeted lengths. A 3D mesh is subsequently obtained based on same optimization principles, using a constrained Delaunay generation based on the internal interfaces mesh.

This approach will be illustrated for RVEs generated computationally for various materials such as porous media, closed-cell metallic foams or irregular masonry. The application of the discretization methodology on microstructural geometries obtained experimentally by CT scans will also be assessed to illustrate the versatility of the approach.

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Keywords: Multiscale modelling, Computational modelling, Complex Microstructures

High frequency modulation in periodic systems. Analytical asymptotic study of reticulated structures

Antoine Rallu [1], Stephane Hans [2], Claude Boutin * [2]

[1] Centre d'Etude des Tunnels (CETU) – Centre d'Etude des Tunnels – , 25 avenue François Mitterand, 69674 Bron Cedex, France
[2] École Nationale des Travaux Publics de l'État (ENTPE) – Ecole Nationale des Travaux Publics de l'Etat, Ministère de l'Ecologie, du Développement Durable, des Transports et du Logement – 3 rue Maurice Audin - 69518 Vaulx-en-Velin cedex, France

This paper addresses the modelling of large scale modulations of high frequency mechanical waves propagating in periodic structures. By means of an asymptotic method implemented using a multi-cell approach, we derive (i) the equations governing the large scale modulations, (ii) the specific features of the modulation propagation, (iii) the domain of validity of the description.

This approach provides additional information on the physics of large scale modulations that are not directly accessible from neither the Bloch wave decomposition nor from a multi-scattering approach. The theoretical formulation enables (i) the identification of the frequency range for which wave motions are correlated over long distances, and (ii) simple calculations of high frequency wave field based on a two step procedure separating the (multi)cell scale and the large modulation scale.

The method is applied to the description of the high frequency modulations in reticulated beams. The dispersion equation for longitudinal and transversal vibrations are first established. Then, from the asymptotic analysis, the equations governing the structure behaviour in the standard homogenization regime and in the modulations regimes are derived. These results are illustrated and supported by numerical simulations. General comments on the correspondence between the modulation phenomena and the classical approaches of homogenization and Floquet-Bloch waves are developed in the conclusion

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Keywords: Dynamics, Structures, High frequency modulation, Multi, cell period, Asymptotic method.

Validation and constitutive closure of continuum plasticity models through data-mining of Discrete Dislocation Dynamics simulations

Stefan Sandfeld *† [1], Giacomo Po [2], Nina Gunkelmann [3]

[1] Chair of Micromechanical Materials Modelling (MiMM), Institute of Mechanics and Fluid Dynamics (TU Bergakademie Freiberg) – Germany
[2] UCLA – United States
[3] TU Clausthal – Germany

We present a data-mining approach that is based on the Discrete-To-Continuum (D2C) method. D2C allows to extract a large variety of informations from Molecular Dynamics or Discrete Dislocation Dynamics (DDD) simulations, such as defect energies, dislocation densities and other dislocation-related properties. DDD simulations are of particular interest for the small scale plasticity community because they offer full information about the dislocation microstructure together with internal stresses and strain energies and therefore can be considered as a perfect reference method for continuum plasticity models. In this work, large data sets obtained from DDD simulations will be used to perform the constitutive closure for so-called Continuum Dislocation Dynamics models and to validate existing constitutive laws in commonly used continuum plasticity models. Additionally, we will demonstrate the versatility of our scale-bridging approach by a number of numerical benchmark simulations, such as indentation tests, which elucidates the role of different terms contained in the defect energy functional.

Keywords: dislocation, plasticity, data mining

*Speaker
†Corresponding author: stefan.sandfeld@mimm-tubaf.de

Aspects of RVE topolgy, mesh discretization and boundary conditions in practical multiscaling for particulate composites

Konrad Schneider * [1], Benjamin Klusemann [2], Swantje Bargmann [3]

[1] Institute of Continuum Mechanics and Material Mechanics, Hamburg University of Technology – Germany
[2] Institute of Product and Process Innovation, Leuphana University of Lüneburg – Germany
[3] Chair of Solid Mechanics, University of Wuppertal – Germany

The identfication of effective material responses or macroscopic constitutive laws is on of the major goals in computational micromechancis.
State of the art are FE^2-methods or homogenization approaches that utilize representative volume elements (RVEs) which incorporate the microstructural information.
In this regard, periodic model setups featuring a fully periodic RVE topology and discretization are known to perform the best.
However, generating such RVEs and setting up a proper model might become a cumbersome task.
Therefore, it is highly questionable if the tremendous effort of generating such complex RVEs is justified over other simplification current in an engineering analysis.
In the present work we investigate the effect of utilizing simpler RVE model setups to determine effective material parameters and responses.
Especially the influences of different RVE topologies, discretizations and boundary conditions are studied.
The case of a fully periodic RVE with exact periodic boundary conditions will act as a reference solution for the evaluations.
Special emphasis is paid to so called matrix-inclusion composites, widely found in industrial applications.
General trends for linear and non-linear material behavior will be presented.

Keywords: homogenization, periodic boundary conditions, representative volume elements, effective material properties

*Speaker

Modeling the physical aging and yielding of glasses

Mykhailo Semkiv [1,2], Markus Hütter * [2]

[1] Dutch Polymer Institute (DPI) – Dutch Polymer Institute (DPI) P.O. Box 902, 5600 AX Eindhoven, Netherlands
[2] Eindhoven University of Technology (TUE) – Eindhoven University of Technology Den Dolech 2 5612 AZ Eindhoven, Netherlands

Abstract:
Physical aging, which originates from slow ongoing microstructural rearrangements, has a pronounced effect on the yielding-response of glassy materials. This presentation addresses the modelling of physical aging and mechanical rejuvenation in such materials. To that end, finite-deformation non-isothermal mechanics [1] is enriched by the concept of two distinct thermal subsystems, namely kinetic and configurational [2-6]. In this way, one can distinguish in a collective manner between the rare transitions (leading to aging) and the rapid vibrations on the microstructural level. Formulating such a two-subsystem mechanics model along the principles of nonequilibrium thermodynamics, one reaches the following conclusion [6]: Since the two thermal subsystems are in general coupled during deformation, the stress tensor is not simply related to the derivative of the thermodynamic potential with respect to the deformation measure. Rather, there can be non-potential contributions (akin to hypoelasticity) that vanish as the system tends to thermal equilibrium. It is also discussed in what sense the non-potential contributions to the stress tensor can be rationalized in terms of a microscopic toy model. In other words, the coupling of the two thermal subsystems during deformation is examined for a simplified microscopic model.

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Keywords: aging, yielding, two, scale modeling, nonequilibrium thermodynamics, microscopic model

*Speaker

A General Homogenization Framework for the Emergent Elastodynamics of Acoustic Metamaterials and Phononic Crystals

Ashwin Sridhar *† [1], Varvara Kouznetsova [2], Marc Geers [3]

[1] Eindhoven University of Technology (TU/e) – PO-box 513 5600 MB Eindhoven, Netherlands
[2] Eindhoven University of Technology (TU/e) – Netherlands
[3] Department of Mechanical Engineering (TUE) – P.O box 513 5600 MB Eindhoven, Netherlands

This work presents a powerful, general homogenization framework towards the computation of complex emergent elastodynamics of acoustic metamaterials and phononic crystals. The generality of the framework is exemplied by two key aspects. First, inspired from the works of Willis [1], the underlying formalism utilizes the Floquet-Bloch theory to obtain a robust definition of scale relaxed of any assumptions on scale separation. Second, the scale transition is defined as the projection with respect to a family of periodic vector shape functions, instead of the standard, uniform volume average. The resulting continuum at the macro-scale is therefore highly generalized. Combined, the two aspects enable the homogenization of complex dispersive phenomena resulting from Bragg scattering and local resonance. Furthermore, a high order asymptotic procedure is introduced to obtain accurate linear elastic corrections to the residual fine scale displacements, yielding a non-local macro-scale constitutive model. The shape functions defining the scale transition relations are synthesized for an arbitrary unit cell using the
Floquet-Bloch eigenvectors obtained at high symmetry points in the desired frequency regime, thereby capturing the essential emergent phenomena of interest in a compact form. The convergence of the homogenization scheme is demonstrated for the limit case where the set of shape functions approaches completeness. In this limit, the macro-scale continuum recovers the full dispersion spectrum of the ne scale system. The finite element method is used to discretize and solve the unit cell problem. The methodology is validated by comparing the dispersion spectra computed using the homogenized model
against standard Bloch analysis on example unit cell designs.
Acknowledgment
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Keywords: acoustic metamaterials, phononic crystals, computational homogenization, multiscale modeling, generalized continuum

*Speaker
†Corresponding author: a.sridhar@tue.nl

Modeling source and multiplication mechanisms in a dislocation based continuum formulation of plasticity

Markus Sudmanns * [1], Katrin Schulz [1], Peter Gumbsch [1,2]

[1] Karlsruhe Institute of Technology (KIT) – Institute for Applied Materials (IAM-CMS), Kaiserstr.12, 76131 Karlsruhe, Germany
[2] Fraunhofer Institute for Mechanics of Materials (IWM) – Wöhlerstr. 11, 79108 Freiburg, Germany

The need for predicting the behavior of crystalline materials on small-scales has led to the development of physically based descriptions of the motion of dislocations. Several dislocation-based continuum theories have been introduced, but only recently rigorous techniques have been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a dislocation density tensor, see [1]. Those evolution equations provide a physically based framework in describing the motion of curved dislocations in three-dimensional systems. However, an open question is still the initialization and multiplication of dislocation density in the considered systems and the description of reasonable macroscopic limits of complex mechanistic models.

Regarding dislocation density initiation and multiplication mechanisms in continuum models of plasticity in general, an area of conflict exists between the need for a mechanistic modeling of the involved physical mechanisms and a reasonable reduction of model complexity. This leads to phenomenological models on larger scales and at larger strains. The discussion, in which configurations and situations a simplified model leads to an oversimplification of the physical mechanisms is a central aspect for the analysis considered in this presentation.

We introduce a source formulation mimicking Frank-Read sources of dislocations complemented by a local dislocation multiplication model. This includes mechanisms as cross-slip and glissile reactions in fully three-dimensional systems. The results are evaluated by discrete dislocation dynamics and discussed in the context of a more macroscopic, phenomenological approach exposing the limits between different models.

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Keywords: dislocation dynamics, continuum theory, dislocation multiplication, dislocation sources, model limitations

*Speaker

Stochastic simulations of discontinuous dynamic recrystallization in HCP metals under large deformation

Abbas Tutcuoglu *† [1,2], Ananthan Vidyasagar [1,2], Kaushik Bhattacharya [3], Dennis Kochmann [1,2]

[1] Department of Mechanical and Process Engineering, Eidgenössische Technische Hochschule Zürich (D-MAVT, ETH Zurich) – Leonhardstrasse 21 LEE K 8092 Zurich Switzerland, Switzerland
[2] Department of Aerospace, California Institute of Technology (GALCIT, Caltech) – Graduate Aerospace Laboratories California Institute of Technology Mail Code MC 105-50 Pasadena, CA 91125, United States
[3] Engineering & Applied Science, California Institute of Technology (EAS, Caltech) – California Institute of Technology Division of Engineering and Applied Science 1200 E. California Blvd., MC 155-44 Pasadena, California 91125-2100, United States

Optimal control of yield strength through grain size reduction is commonly acknowledged to be the sole strengthening mechanism by which a simultaneous rise in ductility can be accomplished. Recently gaining increased attention based on their favorable specific strength, magnesium alloys predominantly achieve the aforementioned grain refinement through discontinuous dynamic recrystallization (DDRX) due to their low-to-moderate stacking fault energy. Numerous numerical models have attempted to gain insight into DDRX, but frequently assume conditions misrepresentative of what is observed during thermomechanical processing including the inherent finite deformations characteristic of e.g. equal channel angular extrusion (ECAE) as well as alternative strain accommodating mechanisms. This in return significantly limits the applicability of such models to capturing the microstructural evolution in HCP metals, where twinning is a frequently observed phenomenon at large strains. Motivated by the multitude of scales involved in DDRX, we pursue a vertical homogenization approach in which we solve the microscopic initial boundary value problem (IBVP) on a representative volume element (RVE) capable of capturing the micro and sub-micro effects inherent to the inelastic deformation mechanisms in magnesium. The governing equations are solved using a spectral method based on the Fast Fourier Transform (FFT) which readily implements the periodic boundary conditions derived from the homogenization assumptions. The time evolution of the inelastic state is captured via a variational constitutive model for slip-twinning interactions. Both mechanisms underlying DDRX, namely grain boundary migration as well as nucleation are modeled using a unified Monte-Carlo scheme, where the associated state switch definitions for both phenomena are motivated by experimental observations. The natural treatment of recrystallized grains allows to capture phenomena such as the characteristic multi-peak stress-strain behavior observed for DDRX at low strain rates. The results from these high-fidelity investigations are compared to results obtained through the Taylor model to assess their replicability using significantly less computational resources thus enhancing feasibility for industrial applications.

Keywords: Recrystallization, DDRX, Magnesium, Spectral Method, Homogenization, Thermomechanical Processing, Twinning

*Speaker
†Corresponding author: tabbas@ethz.ch

Variationally consistent computational homogenization of transient heat conduction using Craig-Bampton mode synthesis

Abdullah Waseem *† [1], Thomas Heuze [2], Laurent Stainier [3], Varvara Kouznetsova [4], Marc Geers [5]

[1] Institut de Recherche en Génie Civil et Mécanique (GeM) – Université de Nantes, Ecole Centrale de Nantes, Centre National de la Recherche Scientifique : UMR6183, Technische Universiteit Eindhoven – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[2] Institut de Recherche en Génie Civil et Mécanique (GeM) – Ecole Centrale de Nantes, CNRS : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[3] Institut de Recherche en Génie Civil et Mécanique (GeM) – Université de Nantes, Ecole Centrale de Nantes, Centre National de la Recherche Scientifique : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[4] Eindhoven University of Technology (TU/e) – Netherlands
[5] Eindhoven University of Technology (TU/e) – PO-box 513 5600 MB Eindhoven, Netherlands

Modeling and simulating heterogeneous media is a challenging and computationally expensive task especially if the contrast between material properties of constituents is high and loading conditions are significantly transient. Among many techniques, computational homogenization (CH) has proven to be a powerful method to solve static (Kouznetsova_et_al 02), quasi-static (Ozdemir_et_al 08) and also transient (Larsson_eta_al 10, Pham_et_al 13) problems for heterogeneous materials in a multi-scale setting. For linear problems, CH essentially consists in the construction of effective constitutive tensors from the micro-scale onwards, usually taken as a unit-cell or a representative volume element. In contrast to static and quasi-static problems, a transient analysis necessitates to evaluate these effective tensors at each macroscopic material point for each time increment, which makes these type of problems quite expensive.

In this work, we propose a computationally tractable method to solve such problems. First, different transient regimes were recognized for heat conduction problems in heterogeneous media. A theory based on CH and Craig-Bampton mode synthesis (CBMS) (Sridhar_et_al 16) was developed. This technique can be applied to transient problems with a weak separation of scales, in which the size of the unit-cell has a definite effect on the macroscopic response. Assuming linear material properties and a matrix having weak transient effects (relative to inclusions), the total microscopic response can be split into its steady-state and transient parts. Static condensation was used to obtain the steady-state solution, while CBMS was used to evaluate the transient response. The mode synthesis lowers the computational cost of a micro-problem with coupled N degree of freedom (d.o.f) to only k decoupled d.o.f, which lowers the computational cost significantly at each time step. Finally, the steady-state and transient solutions are used for deriving macroscopic tangent operators.

As compared to the formulations of (Ozdemir_et_al 08) and (Larsson_et_a 10) significant modeling and computational benefits have been achieved.

Keywords: Computational Homogenization, Transient Heat Conduction, Craig Bampton mode synthesis, Periodic Media

*Speaker
†Corresponding author: abdullah.waseem@ec-nantes.fr

Self-consistent estimates for the thermoelastic response of cracked polycrystals with hexagonal symmetry

François Willot * [1], Hervé Trumel [2], Dominique Jeulin [3], Jean-Baptiste Gasnier [4]

[1] Centre de Morphologie Mathématique (CMM) – MINES ParisTech - École nationale supérieure des mines de Paris – 35 rue Saint-Honoré 77305 Fontainebleau cedex, France
[2] CEA Le Ripault – CEA Le Ripault – France
[3] Centre de morphologie Mathématiique – MINES ParisTech - École nationale supérieure des mines de Paris – France
[4] Centre de Morphologie Mathématique – MINES ParisTech - École nationale supérieure des mines de Paris – France

The influence of a population of randomly-oriented cracks on the macroscopic thermal and linear-elastic response of a hexagonal polycrystal is addressed using a self-consistent method. The present approach does not use Eshelby's general solution for a crack oriented arbitrarily in an anisotropic medium, as it is not known explicitely. Instead, the coupling between the crystals and the cracks is taken into account through the isotropic effective medium, assuming the same typical size ℓ for the crystals's mean dimension and for the cracks's length. In the absence of cracks, the present method coincides with the self-consistent estimate of Berryman (2005) for pure polycrystals, although the two approaches are based on different ideas. If, however, cracks are present but the medium lacks crystal anisotropy, the method derived here yields predictions that are in disagreement with the estimates of Budiansky and O'Conell (1976), Benveniste (1987) or the bounds of Ponte Castañeda and Willis (1995) for randomly-oriented cracks embedded in a homogeneous matrix.

To assess the accuracy of the present approach, the self-consistent predictions are compared to Fourier-based numerical computations for a simple Voronoï microstructure-model with superimposed cracks. In this model, the orientations and positions of the cracks and of their neighbouring crystals are uncorrelated. In the abscence of anisotropy, the self-consistent approach yields excellent estimates with respect to numerical full-field predictions, up to a crack-density parameter of η.

Keywords: Cracked polycrystals, Homogenization, Thermoelasticity, Self, consistent estimates, Percolation

*Speaker

Non-linear spectral homogenization solvers: How and why they work?

Jan Zeman *† [1], Tom De Geus [2], Jaroslav Vondřejc [3], Ron Peerlings [4], Marc Geers [4]

[1] Czech Technical University in Prague (CTU) – Zikova 1903/4, 166 36 Prague 6, Czech Republic
[2] Ecole Polytechnique Federale de Lausanne (EPFL) – Rte de la Sorge, CH-1015 Lausanne, Switzerland
[3] Technische Universität Braunschweig (TUB) – Mühlenpfordtstrasse 23, D-38106 Braunschweig, Germany
[4] Eindhoven University of Technology (TU/e) – PO-box 513 5600 MB Eindhoven, Netherlands

Applications of spectral solvers in computational homogenization arose from the seminal work of Moulinec and Suquet in 1994. The original formulation – referred to as the standard scheme in what follows – builds on an approximate solution of an integral equation of the Lippman-Schwinger type with an iterative-collocation procedure. This format makes the algorithm memory-efficient and easy to implement, but only conditionally convergent. Moreover, the convergence is governed by choice of an auxiliary boundary value problem, whose Green function forms the kernel of the integral equation. This intricate dependence between algorithm and the governing equation renders extensions to non-linear problems challenging.

We show that the standard scheme admits an equivalent variational characterization, which allows formulating spectral solvers in the language of finite element methods and developing more efficient, robust, and versatile algorithms. In particular, we start with a suitable weak form, proceed to the Galerkin discretization and the numerical quadrature, up to the solution of nodal equilibrium equations by an iterative Newton-Krylov solver. No auxiliary linear problem is thus needed. We present these developments for non-linear small-strain elasticity first, for the sake of clarity, and, consequently, outline applications to finite-strain/inelastic problems.

Keywords: homogenization, spectral methods, Moulinec, Suquet scheme, finite element methods, computational inelasticity

*Speaker
†Corresponding author: Jan.Zeman@cvut.cz

S20: Advanced modelling techniques: stochastics in materials mechanics

Scalable numerical homogenization scheme for random polycrystalline materials

Regis Cottereau *† [1], Thiago Milanetto Schlittler [1], Moindze Soilahoudine [1]

[1] MSSMat - CentraleSupélec, CNRS – CNRS : UMR8579, CentraleSupélec – France

Coupling methods, in general, allow the study of multi-scale systems, taking into account the different physical processes at each scale. These methods can be classified in several different types, depending on the desired application. Methods like the VMS and the HMM, and similar others, are used when the macro-scale's model parameters are not known, but depend on the micro-scale over the whole domain. They can be classified as embedding methods, with the VMS enriching the macro-scale with the micro-scale model over element patches, and the HMM altering the quadrature evaluation of the weak formulation. If, on the other hand, the macro-scale quantity of interest depends on the micro-scale only over a part of the former's domain, more local methods are used. Examples include the non-overlapping domain decomposition methods. They are derived from domain decomposition techniques developed to solve numerically PDEs over large-scale computer clusters, and they are used when the coupling is done over an interface between the models.
For overlapping domains, still in the context of a limited domain coupling, methods based on volume couplings can be used, such as the Arlequin framework and the bridging domain method. They keep the same weak formulation as the other methods but differ from the interface methods by defining a volume coupling over the overlapping domains. These methods differ mainly on the choice of this coupling term. In both cases, the coupling matrix is built using an intermediary mesh, constructed by meshing the geometrical intersections between the elements of the macro and micro domain meshes. Finally, methods such as Nitsche method have points in common with both the interface and volume couplings. There is a volume overlap between the models, but the formulation defines the coupling over an interface between the overlapping domains only.

Generally speaking, the coupling step is not parallelized for methods following the formulations above. In many cases, this is justified because the mediator space is smaller when compared to the models associated with it. However, as a consequence, even when the parallel implementations associated to each of the numerical models scale well, the serial coupling step breaks this scalability of the algorithm as a whole. Previous works using the coupling algorithms and parallelism focused on simulating several couplings between a single global model and many local models, with each coupling being associated to one processor. Here, we use a different approach, and present a version of the Arlequin framework with a parallelized and scalable coupling step. As an example of this implementation, we study the homogenization of a polycrystalline material model. The scalability in that case becomes essential because repeated microstructures have to be computed.
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Keywords: stochastic homogenization, polycristallyne material, Arlequin coupling

*Speaker
†Corresponding author: regis.cottereau@centralesupelec.fr

Representative Volume Element Size for Viscoplastic Properties in Polycrystalline Copper

Justin Dirrenberger *† [1], Shaobo Yang [1], Eric Monteiro [1], Nicolas Ranc [1]

[1] Procedes et Ingenierie en Mécanique et Matériaux [Paris] (PIMM) – Arts et Métiers ParisTech, Conservatoire National des Arts et Métiers (CNAM), CNRS : UMR8006, Conservatoire National des Arts et Métiers [CNAM] – 151 boulevard de l'hôpital, 75013 Paris, France

Microstructural heterogeneities play a critical role on the macroscopic physical properties of materials. One common way to account for this underlying complexity is resorting to homogenization techniques. Many approaches, including analytical and computational, are available for determining the homogenized properties of random media. Most of them necessitate the existence of a representative volume element (RVE). Assuming ergodicity for the heterogeneous media considered, Kanit et al. (2003) proposed a method based on a statistical analysis for computing the minimal RVE size for a given physical property Z and precision in the estimate of effective properties. This method is applied and extended here to the case of viscoplasticity within Copper polycrystalline aggregates. As a matter of fact, the assumption of equivalence between the micro- and macro-viscoplastic strain rate sensitivity is classically made for polycrystalline aggregates, i.e. the strain rate sensitivity at the scale of the polycrystal is expected to be some average of the sensitivities at the scale of the slip systems. In this work, we intend to investigate the veracity of this assumption depending on sample size and representativity. Microstructural stochastic modelling using Neper (Quey et al., 2011) is performed based on Voronoi tessellations. Computational homogenization for mechanical properties is performed through finite elements based on a crystal plasticity framework, over multiple realizations of the stochastic microstructural model, using periodic boundary conditions. The generated data undergoes statistical treatment for determining RVE sizes in the case of viscoplasticity.

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Keywords: representative volume element, crystal plasticity, viscoplasticity, Copper, finite element analysis

*Speaker
†Corresponding author: Justin.dirrenberger@ensam.eu

Multiscale analysis of lightweight structures with uncertain material microstructure

Jörg Hohe * [1], Carla Beckmann [1], Peter Tempel [1], Sascha Fliegener [1]

[1] Fraunhofer-Institut für Werkstoffmechanik (IWM) – Wöhlerstr. 11 79108 Freiburg, Germany

In lightweight construction, composite materials such as fibre reinforced plastics, particle reinforced materials or cellular solids such as solid foams are important materials. Many of these materials feature microstructural uncertainties caused by local fibre misalignments, variations in the local fibre volume fraction or distributed small defects. The microstructure of particle and short fibre composites as well as solid foams per-se features geometric uncertainties. The geometric uncertainties on the microstructural level lead to scatter and uncertainties in the effective material properties and subsequently in the structural response.
The present study is concerned with a numerical prediction of uncertainties in the response of lightweight structures made from composite and cellular materials with microstructural uncertainties. Starting from the microstructural uncertainty, a probabilistic homogenization scheme is proposed to determine the effective material properties together with their probability distributions and correlations. These properties are used as the input for a structural analysis on the macroscopic level.

In this two-step procedure, the effective material properties of the composite and their uncertainty are computed. For this purpose, a probabilistic homogenization procedure is established, based on the analysis of the mechanical response of small scale "testing volume elements". The testing volume elements are defined either by a repeated random generation of small-scale computational models for the microstructure or – alternatively – are defined as subsets of a large-scale, statistically representative volume element. Alternatively, a direct determination of the microstructure of a real material by computed tomography of neighbouring subsets can be employed for generation of a set of testing volume elements. The individual testing volume elements are not representative by themselves, however, the entire set of testing volume elements is representative for the microstructure of the material in a statistical manner. Therefore, the set of effective material properties computed by a homogenization analysis of all testing volume elements is statistically representative for the material response. The resulting probability distributions for the material properties and the corresponding inter-correlations and spatial correlations are employed as input parameters for a random field generation to describe the uncertain material response in a numerical analysis of macroscopic structures.
As examples for the proposed scheme, the material response of discontinuously fibre reinforced materials with variability in the local fibre content, length and orientation and solid foams are considered. In a case study, a single edge clamped sandwich beam with metal foam core is analysed. In this example, the material uncertainty is found to cause only minor scatter in the deformation of the beam, however, significant uncertainties are observed in a strength analysis.

Keywords: Composites, Microstructure, Uncertainties, Multiscale analysis

*Speaker

Stochastic 3D microstructure modeling for the prediction of permeability and conductivity of three-phase microstructures on the example of solid oxide-fuel cells

Matthias Neumann * [1], François Willot [2], Volker Schmidt [1]

[1] Institute of Stochastics, Ulm University – Helmholtzstraße 18, D-89069 Ulm, Germany
[2] Center for Mathematical Morphology – MINES ParisTech - École nationale supérieure des mines de Paris – 35 rue Saint-Honoré, F-77305 Fontainebleau, France

We compare a graph-based (Neumann et al., 2016) and a pluri-Gaussian (Abdallah et al., 2016) microstructure model that have been introduced to model three-phase microstructures occurring e.g. in solid oxide fuel cell (SOFC) electrodes. Both models are parametric and are based on tools from stochastic geometry. However, their construction and the morphological characteristics used for model fitting differ notably. In the graph-based approach a certain class of random geometric graphs is used to model the backbones of the three phases. Model parameters are optimized according to mean geodesic tortuosity, the length of the triple-phase boundary and constrictivity. The latter measures bottleneck effects which affect both, electrical conductivity (Stenzel et al., 2017) and permeability. In the pluri-Gaussian model, the three phases are represented by means of two underlying independent random sets that are modeled to fit their covariance function and specific surface area. This approach allows us to validate the assumption that the microstructure can be represented by the aid of two independent random sets. Moreover, parameter estimation for the pluri-Gaussian model requires only 2D image data without any optimization procedure (Masson et al. 2015). In the present study, we fitted both microstructure models to the 3D image data discussed in (Neumann et al. 2016), which shows a representative cutout of an SOFC anode obtained by FIB-SEM tomography. The two models are compared in terms of morphological characteristics (like mean geodesic tortuosity and constrictivity) and in terms of effective permeability and conductivity. The Stokes flow in the porous phase and transport properties in the solid phase are computed numerically for realizations of the two models as well as for the 3D image data using Fourier methods. The local and effective physical responses of the model realizations are compared to that obtained from 3D image data. Finally, we assess the accuracy of the two methods to predict permeability, electronic and ionic conductivity of the anode.

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*Speaker

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Keywords: 3D microstructure model, Stochastic geometry, Effective transport properties, Solid oxide fuel cell

Quantifying uncertainties in contact mechanics of rough surfaces using the Multilevel Monte Carlo method

Valentine Rey * [1,2], Sebastian Krumscheid [3], Fabio Nobile [3]

[1] Ecole Polytechnique Fédérale de Lausanne (EPFL) – Swiss Federal Institute of Technology EPFL-FSTI IEL-LTS2, Station 11 Lausanne 1015 - Switzerland, Switzerland
[2] Institut de Recherche en Génie Civil et Mécanique (GeM) – Université de Nantes, Ecole Centrale de Nantes, Centre National de la Recherche Scientifique : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[3] Calcul Scientifique et Quantification de l'Incertitude, Ecole Polytechnique Fédérale de Lausanne (CSQI EPFL) – Bât. MA Station 8 CH-1015 Lausanne, Switzerland

Understanding the mechanical response to contacts between interfaces is a major scientific challenge for many engineering applications. However, it is a difficult question because of the multiscale nature of the contact interfaces (surfaces are not perfectly flat but are made of multiple asperities that exist at all length scales).
To account for this contact geometry, the rough surfaces are usually modeled as semi-affine fractal surfaces [1]. Despite the fact that some surface properties can be measured, the knowledge on the roughness is not complete so that surfaces are considered to be random and are usually characterized only through their statistical properties. Moreover, since numerical computations are done on a finite size surfacewith periodic boundary conditions (to model semi-infinite surfaces), an error due to homogenization is introduced. As a consequence, in addition of providing the mean value of a quantity of interest, the quantification of uncertainties, discretization error and periodicity error is required.

Since the contact problem is already computationally challenging (non linear problem and large number of degrees of freedom to represent the roughness), the classic Monte Carlo method is often prohibitive. In this work, we investigate the benefits of the multilevel Monte Carlo techniques [2] applied to random rough contact mechanics problems with a key strategy to carefully balance statistical errors and discretization errors. Numerical assessments are presented for the estimation of the contact area and the number of contact clusters in the case of frictionless non adhesive normal contact between one semi-infinite flat linear elastic solid and one semi-infinite rigid rough surface. We compare multilevel Monte Carlo to standard Monte Carlo to highlight the great computational gain offered by the multilevel approach, which enables considering large parametrical studies and then improve our understanding of contact mechanics.

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Keywords: contact, rough surfaces, multilevel Monte Carlo method

*Speaker

Structural response under stochastic impact loading

Renata Troian * [1], Leila Khalij [2], Didier Lemosse [3], Manel Dallali [1]

[1] Laboratoire de Mécanique de Normandie (LMN) – INSA Rouen – France
[2] Laboratoire de Mécanique de Normandie (LMN) – Institut National des Sciences Appliquées [INSA] - Rouen – EA 3828 BP08 Avenue de l'université - 76801 - Saint Etienne du Rouvray Cedex, France
[3] Laboratoire de Mécanique de Normandie (LMN) – Institut National des Sciences Appliquées [INSA] - Rouen : EA3828 – BP08 Avenue de l'université - 76801 - Saint Etienne du Rouvray Cedex, France

The problem of the vulnerability of structures facing explosions came to the front line of the scientific scene in the last decades. It is a subject of actual interest for many researchers around the world, but works on structural reliability under a stochastic impact loading remain rare.
Uncertainty of the environmental conditions and material properties have to be taken into account. The corresponding numerical models are very complex and depend on numerous parameters. Consequently, such models are cursed with issues which limit their use for real applications. Most of the existing approaches are based on a deterministic point of view, and are not able to represent the extreme sensitivity of a model towards uncertain parameters. That is why the uncertainty analysis is needed.

The proposed research is devoted to the analysis of a structural behavior under an uncertain impact loading. Elasto-plastic Bernoulli beam model is used as structural model for the case simplicity, while the different formulation for impact itself are studied to simulate the wide range of possible types of impact.

Model sensitivity is studied first. The influence of input parameters on structural behavior, that are the impact force, duration and position, as well as beam material are then considered.
The obtained insights can provide the guidelines for modeling the structure under the explosive loading taking into account the uncertainties.

Keywords: impact, soft, rigid, stochastic loading, beam

*Speaker

Dynamic fragmentation of rings : Experimental and Numerical Approach

Joris Vermunt [1], Don-Pierre Zappa [1], Gilles Damamme [1], Helmut Klocker *† [2]

[1] CEA-Gramat – DAM – BP 80200 46500 Gramat, France
[2] Laboratoire Georges Friedel, UMR 5307 (emse) – Ecole Nationale Supérieure des Mines de St-Etienne, France – 158 cours Fauriel 42023 Saint Etienne, France

During World War II, fragmentation studies of expanding cylinders, to predict the debris distribution for conventional warheads became imperative. In 1943, Mott and Linfoot [1] extended Lienau's [2] purely mathematical line break-up model to develop the initial theory of dynamic plate fragmentation. Soon after, Mott made a conceptual breakthrough by deciding to consider the cylinder as a stack of steel rings. With this brilliant hypothesis and the introduction of several probability distributions of initial defects, he was able to predict fragment mass scattering [3-5]. Right from the beginning, Mott considered stress relaxation waves. Mott waves are one of the keystones needed to predict bomb debris size because unloaded parts of warheads are prevented from further crack nucleation. Unfortunately, Mott needed to simplify crack propagation through thickness as instantaneous, given the computational limits of the 1940s. Grady, the very first to deal with non-instantaneous crack propagation [6], was able to predict the mean mass of the fragments but not their mass distribution.
In present work, first Mott's wave propagation has been revisited taking in to account the failure energy. In a second step, the distribution of initial defects is determined by material observations and finite element analysis of strain localization. Finally, in the last step, the new Mott's wave propagation and nucleation model are used to predict the fragment distribution of expanding rings. This work leads to better understanding of Mott's wave propagation, defect nucleation related to strain localization and finally the overall fragmentation process.

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Keywords: Mott's wave, Fragmentation, Failure energy, Dynamic, Ductile material

*Speaker
†Corresponding author: helmut.klocker@mines-stetienne.fr

S21: Advanced modelling techniques: phase field and diffuse-interface approaches

Migrating grain boundaries in a combined crystal plasticity and phase field approach

Anna Ask * [1], Samuel Forest [1], Benoît Appolaire [2], Kais Ammar [1], Oguz Umut Salman [3]

[1] MINES ParisTech, PSL Research University, MAT – Centre des matériaux, CNRS UMR 7633 – MINES ParisTech - École nationale supérieure des mines de Paris – BP 87 91003 Evry, France
[2] Institut Jean Lamour (IJL) – Université de Lorraine, Centre National de la Recherche Scientifique - CNRS : UMR7198 – Institut Jean Lamour, 2 allée André Guinier, Campus Artem, 54000 NANCY, France
[3] Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – université Paris 13, Université Sorbonne Paris Cité, Institut Galilée, Centre National de la Recherche Scientifique : UPR3407 – Institut Galilée, Université Paris 13, 99 avenue Jean-baptiste Clément, F-93430 Villetaneuse, France

Macroscopic material properties of metals can be tuned by thermomechanical processing which significantly alters the microstructure at the grain scale. The underlying dynamics of these phenomena span different length and time scales which present significant challenges when formulating simulation models. On the grain scale, crystal plasticity models provide the most complete tools to model microstructure evolution induced by viscoplastic deformation, including heterogeneous lattice reorientation and evolution of stored dislocation densities. These models do not however contain a priori evolution laws for migrating grain boundaries. In the vast majority of coupled models dealing with recrystallization after or during plastic deformation, the crystal plasticity model is used in conjunction with some criterion for the generation of new nuclei together with a model, such as level-set or phase field approaches, for migrating grain boundaries. To date, no overall unified field framework exists to model concurrent viscoplastic deformation and recrystallization and grain growth in metal polycrystals.
In this work a Cosserat crystal plasticity model is enhanced with an order parameter to account for diffuse, mobile grain boundaries in analogy with a phase field model. The model is established based on energy principles and solved as a monolithic system of partial differential equations by means of the finite element method. The Cosserat directors are taken to represent the lattice orientation of the grains. In order to introduce an evolution law for reorientation during grain boundary migration, the skew-symmetric part of the Cosserat deformation tensor is associated with a dissipative stress according to the formalism developed by Gurtin (1996). The formulation in terms of the Cosserat deformation provides a natural way to couple reorientation due to deformation and reorientation due to grain boundary migration. In the absence of displacements and for a particular choice of free energy function the model can be considered a generalization to three dimensions of the Kobayashi–Warren–Carter (KWC) orientation phase field model (2000, 2003).

The proposed 3D anisotropic constitutive framework couples the changing orientation at a material point due to migrating grain boundaries (which is essential to the KWC model) to the lattice reorientation due to displacements and plastic slip. Due to the coupling of the Cosserat directors and the elastic reorientation, the bulk rotation of the grains which is inherent to the KWC model (and considered an artefact here although it can nevertheless be desirable in certain cases) can be controlled and even suppressed.
The model contains two contributions of dislocations to the energy stored in the material during viscoplastic deformation: stored energy due to so-called geometrically necessary dislocations related here to the lattice curvature tensor, and stored energy due to statistically stored dislocations. The latter is an important driving force for grain boundary migration. Numerical examples of grain boundary migration due to gradients in statistically stored dislocations demonstrate that the model is capable of predicting grain boundary motion from regions of low dislocation density into regions of high dislocation density as well as the static recovery taking place in the wake of the sweeping grain boundary.

*Speaker

Keywords: Phase field methods, Cosserat crystal plasticity, Recrystalllization

Surface tension in a diffuse interface approach presented at the example of sintering

Efim Borukhovich * [1]

[1] Department of Materials Science and Engineering (KTH) – Department of Materials Science and Engineering KTH SE-100 44, Stockholm, Sweden

Diffuse interface formulations are often the method of choice in full field modelling since they provide a possibility to treat morphology of arbitrary complexity without the need of involved interface treatment algorithms. In general, they are based on a continuous differentiable shape function that is evolved in time by integration of a partial differential equation (PDE) describing the modelled morphology evolution. Even though the diffuse interface's length scale, i.e. the interface width, is often of purely modelling nature the models are built such that the variables of interest are interface width independent. Some of these are the interface movement velocity resulting from a specified driving force, or the interface energy integrated over the interface. However, since this does not hold true for all variables a careful investigation for every variable of interest is crucial. The current contribution provides a formulation of surface tension in the context of diffuse interface approaches in that spirit. In multiphase descriptions, especially with liquid phase present, coupled PDE systems of Navier-Stokes equations with a phase field PDE are common. The phase field describes the morphology and its evolution while the Navier-Stokes momentum equation yields the velocity field resulting from external forces and pressure gradients. This setup is perfectly appropriate for modelling of processes where the influence of the surface tension on the pressure and convection of material in the system is to be studied. An alternative calculation of curvature via the phase field variable will be suggested leading to a Laplace pressure contribution in the Navier-Stokes momentum equation. The resulting PDE system is benchmarked against an analytic solution. Concluding, the applicability of the framework is demonstrated on simulation of irregularly shaped powder particles sintering.

Keywords: phase field, curvature, surface tension, Laplace pressure, Navier, Stokes

*Speaker

Inverse Ripening of Precipitates

Reza Darvishi Kamachali * [1]

[1] Max-Planck-Institut für Eisenforschung (MPIE) – Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Fine dispersion of small precipitates can significantly contribute to the strengthening of a metallic alloy without reducing its toughness. The size and distribution of the precipitates, however, are subjected to change due to ripening that results in destabilization of the microstructure. Extensive studies have been devoted to investigate precipitation growth and ripening under interfacial, chemical and mechanical driving forces and the combinations of them. In this work, we have extended the actual model of growth and ripening by introducing a cross-coupling of chemical and mechanical states of the system [1]. 3D phase-field simulations of precipitation growth and ripening have been conducted [2]. It is found that the 'chemomechanical' coupling results in an inverse ripening of the precipitates in which the smaller precipitates grow at the expense of larger ones (See Figure 1 in the supplementary materials). This is accompanied with spatial rearrangement of the precipitates due to strong elastic interaction. A theory of growth and ripening under chemomechanical coupling has been developed.

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Keywords: Precipitation, Ripening, Chemomechanical coupling, Phase, field simulation

*Speaker

Influence of elastic interactions on the precipitate arrangement in single-crystal superalloys

Matthieu Degeiter * [1], Yann Le Bouar [2], Benoît Appolaire [3], Mikael Perrut [1], Alphonse Finel [2]

[1] ONERA - The French Aerospace Lab (Chatillon) – ONERA – F-92322 Chatillon, France
[2] Laboratoire d'étude des microstructures (LEM - ONERA - CNRS) – ONERA, Centre National de la Recherche Scientifique : UMR104 – F-92322 Chatillon, France
[3] Institut Jean Lamour (IJL) – Université de Lorraine, Centre National de la Recherche Scientifique : UMR7198 – Institut Jean Lamour, Parc de Saurupt, Rond-point Marguerite de Lorraine, CS 50840, 54011 NANCY cedex, France

In multiphase alloys, internal elastic fields often arise as a result of a coherently adjusted misfit between the lattices of coexisting phases. Given their long-range and usually anisotropic nature, the interaction of these fields is known to significantly alter the kinetics of diffusion-controlled phase transformation, as well as influence the shapes and arrangement of the misfitting precipitates. The microstructure of single-crystal nickel-base superalloys, obtained by precipitation of the L1-ordered γ' phase in the FCC γ matrix, is a perfect example where such evolutions occur. Besides modifying the interface thermochemical equilibrium, elasticity causes the precipitate shapes to grow from spheroids to cuboids, which affects in turn the landscape of their long-range interactions. Ensuing from the anisotropy of the strain energy and the diffusion of alloying species during coarsening, γ' precipitates tend to align along the elastically soft directions of the matrix. This reconfiguration process leads to the formation of a long-range spatially-correlated microstructure, in which the nearly periodic alignments of cuboids are separated by narrow channels of matrix.
However, the resulting modulated structures display many defects in the precipitate alignments, which are observed both experimentally and numerically. At high volume fractions, forks and dislocations in the modulations systematically disrupt the periodicity of the precipitate arrangement. At lower volume fractions, arrays of precipitates respectively aligned along [100] and [010] tend to be adjacent, thus forming "$Gamma$-shaped" alignments to which we will refer as chevrons or herringbone patterns. Despite a significant number of studies devoted to the formation of the γ/γ' microstructure, the understanding of the reconfiguration process is still partial. Specifically, the origin and evolution of these alignment defects are still unclear.

We first adress the question of the origin of the defects in the precipitate alignments of the γ/γ' microstructure. By means of semi-analytical and phase-field calculations, we carry out stability analyses of the periodic arrangement of elastically interacting precipitates. Although this ideal microstructure was expected to be stable, the calculations proved the periodic arrangement of cubic γ' precipitates to be unstable against specific infinitesimal perturbations. These instabilities are likely to be responsible for the spontaneous formation of the alignment defects.
Secondly, the influence of the γ' volume fraction and of elastic parameters on the stability of this ideal microstructure is evaluated. Their contributions, either further stabilizing or destabilizing the periodic arrangement, will be discussed with regards to the formation of the alignment defects.

Keywords: Phase transformation, Elasticity, Stability analysis, Phase field, Superalloys, Coarsening

*Speaker

A Sharp Interface Phase Field Method

Alphonse Finel * [1], Yann Le Bouar [1], Benoît Dabas [1]

[1] Laboratoire d'Étude des Microstructures (LEM) – CNRS : UMR104, ONERA – Chatillon, France

Phase Field methods (PFM) are extensively used for modeling microstructures. The reason for this success is that, using simple symmetry arguments and the conserved/non-conserved character of the fields needed to describe the situation of interest, it is easy to extend free energy functionals and kinetic equations to complex situations where different phenomena are coupled. However, as the fields are supposed to be continuous, the numerical grid spacing must be much smaller than the smallest internal length scale, i.e. the interfaces widths. This "diffuse interface" constraint limits drastically the overall accessible linear dimensions.
We propose a new PFM formulation, in which interfaces widths may be as small as the grid spacing, without any pinning when the interfaces move, allowing to multiply the linear dimensions by an order of magnitude. Also, to couple this "sharp interface" PFM to elastic fields, we propose a new elastic solver that efficiently treats strong elastic heterogeneities.
The effectiveness of this new formulation will be illustrated through its application to different situations (cracks, voids, phase transitions).

Keywords: phase field methods, microstructures, phase transitions, elastic equilibrium

*Speaker

Phase field modeling of deformation twinning in β-metastable titanium alloys

Juba Hamma *† [1], Benoît Appolaire [2], Yann Le Bouar [1], Alphonse Finel [1]

[1] Laboratoire d'Étude des Microstructures (LEM) – ONERA, Centre National de la Recherche Scientifique - CNRS : UMR104 – Laboratoire d'Étude des Microstructures, 29 Avenue de la Division Leclerc, 92322 CHATILLON, France
[2] Institut Jean Lamour (IJL) – Université de Lorraine, Centre National de la Recherche Scientifique - CNRS : UMR7198 – Institut Jean Lamour, 2 allée André Guinier, Campus Artem, 54000 NANCY, France

Recently, new β-metastable titanium alloys, so-called "TRIP/TWIP titanium alloys" (TRIP for TRansformation Induced Plasticity and TWIP for TWinning Induced Plasticity), have been developed to exhibit improved mechanical properties. Among them, we notice their high strength (up to 1200 MPa in Ultimate Tensile Strength) and their ductility of about 45% at fracture, accompanied by an unprecedented strain hardening for titanium alloys at ambient temperature. These mechanical properties are attributed to some very complex microstructures engendered by the mechanical destabilization of the initial bcc phase in the course of the deformation. Indeed, the microstructure features numerous twins following the peculiar $\{332\}$ twinning mode of the bcc phase (β), specific to β-titanium alloys, as well as orthorhombic (α") and simple hexagonal (ω) phases ensued from concomitant displacive transformations. Moreover, experimental observations revealed the possible activation of secondary deformation mechanisms, meaning the formation of secondary twins and/or α" inside primary twins of the bcc phase β.

In view of having a better understanding of the formation of the complex microstructures described above, we propose a numerical model using the phase field method. This method provides a thermodynamically consistent framework to couple the mechanisms at the origin of the microstructure evolution. As a first step of modeling the evolution of the β-metastable titanium alloys microstructure upon deformation, the phase field model hereby presented is focused on the $\{332\}$ twinning mode of the bcc phase β.

Phase field models proposed so far for deformation twinning exhibit several essential flaws preventing them to be applied in our case. First, some of them are formulated using the small strain approximation of the elastic energy contribution. Considering the large shear strains contributions introduced in the eigenstrain associated with twinning ($\gamma = 0.17$ in the case of the $\{332\}$ twins), the use of the infinitesimal strain theory cannot be justified, in particular because the accommodation mechanisms resulting from the crystalline rotations are not correctly taken into account. Second, the proposed models are all restricted to primary twinning by construction, meaning that the free energy landscape is built in such a way that it cannot allow the formation of secondary twinning.

In this work, we propose a novel phase-field model free of the above mentioned deficiencies. Indeed, the model relies on (i) a finite strain formalism; and (ii) a reaction pathway of the free energy landscape as proposed originally by C. Denoual and A. Vattré (JMPS, 2016) in the case of martensitic transformations, for accounting for the possible activation of secondary mechanisms. We will show with simple calculations the capabilities of the present model to describe the $\{332\}$ twin growth. A comparison with a model formulated in a small strain formalism will also be presented to show the influence of the geometrical non-linearities introduced in the finites strain framework.

*Speaker
†Corresponding author: juba.hamma@onera.fr

Keywords: titanium alloys, phase field, deformation twinning, reaction pathway

Modeling of L´uders band formation using the phase field approach

Nikhil Kulkarni *† [1], Christoph Herrmann‡ [2], Daniel Schneider§ [1], Britta Nestler¶ [1]

[1] Institute of Applied Materials (IAM-CMS), Karlsruhe Institute of Technology (KIT) – Kaiserstrasse 12, 76131 Karlsruhe Germany, Germany

[2] Institute of Materials and Processes (IMP), Karlsruhe University of Applied Science – Moltkestrasse 30, D-76133 Karlsruhe, Germany, Germany

Materials exhibiting yield point phenomenon show a characteristic drop in their stress-strain curve under tensile load. It is observed that, plastic strains appear locally and propogate in band shape through the specimen, these bands are known as Lüders bands. Eventhough this was described more than 150 years ago, the yield point phenomenon is not yet fully understood. Based on the publication done by Schwab and Ruff [1], the yield point phenomenon is explained based on three major points: 1) true upper yield point, 2) typical strain hardening behaviour and 3) the triaxiality of the stress state that develops at the Lüders front. In the present investigation, a multiphase system considering of purely elastic and plastic phases are taken into account for the formation of Lüders bands [2] [3]. In this process, when a tensile load is applied on the specimen, the transformation of a elastic phase into plastic phase happens once the true upper yield point is reached. On comparing the results obtained by Schwab and Ruff [1], the behaviour of the stress-strain curve is satisfied. The motivation of formation of Lüders bands using the phase field method is to overcome the high gradients of stress and strain formed at the sharp interface between the plastic and elastic phase in case of sharp interface models. Overall this study describes the yield point phenomenon correctly using phase field model.

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Keywords: phasefield model, mechanical jump conditions, plasticity model, L´uders band formation

*Speaker

†Corresponding author: nikhil.kulkarni@kit.edu

‡Corresponding author: christoph.herrmann2@hs-karlsruhe.de

§Corresponding author: daniel.schneider@kit.edu

¶Corresponding author: britta.nestler@kit.edu

Phase Field of Modeling of Pore Annihilation in Nickel-base Superalloys During Hot Isostatic Pressing

Yann Le Bouar * [1], Antoine Ruffini [1], Benoit Dabas [1], Alphonse Finel [1]

[1] Laboratoire d'étude des microstructures (LEM - ONERA - CNRS) – ONERA, Centre National de la Recherche Scientifique : UMR104 – F-92322 Chatillon, France

High-pressure turbine blades are critical components of aircraft engines. They are cast as single-crystals of nickel-base superalloys. A negative side effect is the formation of casting micropores initiating fatigue failure during service. The pores can be removed by hot isostatic pressing (HIP) performed at temperature close to solidus. However, pore annihilation in single-crystals at high temperature is a complex multiscale physical process, which is still poorly understood [1]. In this work, we present the results of two phase-field models developed to analyze important driving forces in this process.
First, a three-dimensional phase-field model of dislocations is developed with a discretization scheme that explicitly captures the face-centered cubic geometry. Within this framework, continuous fields are discretized in a way that allows considering strongly heterogeneous materials and sharp interfaces (free surfaces, stiffer precipitates, pores...) without generating numerical artifacts [2]. The model reproduces dislocation glide, junction formation and a particular attention is devoted to the dislocation core behaviors. The model is then applied to analyze the evolution of dislocations in the vicinity of a pore in HIP conditions. We show that the anisotropy of the elastic tensor significantly impacts the microstructure evolution and that the dislocations evolve in such a way as to align their edge component with the center of the pore.

Second, a phase field model is developed to analyze the climb of edge dislocations in the vicinity of the pore. The model includes vacancy diffusion, dislocation climb as well as surface tension of the pore. The model is implemented in Fourier space, and three-dimensional simulations are performed to analyze the kinetics of the pore annihilation. Finally, the results are compared to experiments performed in the CMSX-4 nickel-base superalloy at 1288◦C.

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Keywords: phase field, dislocation, pore, superalloys

*Speaker

Acicular microstructures in metallic alloys : phase-field coupling between diffusion, elasticity and plasticity

Hocine Lebbad * [1], Benoît Appolaire [1,2], Yann Le Bouar [1], Alphonse Finel [1]

[1] Laboratoire d'étude des microstructures (LEM - ONERA - CNRS) – ONERA, Centre National de la Recherche Scientifique : UMR104 – F-92322 Chatillon, France
[2] Université de Lorraine – Institut Jean Lamour, UMR 7198 CNRS - Université de Lorraine, Parc de Saurupt - CS 50840, 54011, Nancy Cedex, France – France

Metallic alloys developed for structural applications are multiphase materials. The mechanical properties of these alloys strongly depend on the spatial arrangement of the phase domaines, called microstructure. Thermal and thermo-mechanical treatments are usually performed to control and optimise the microstructure for a given application. The present work is devoted to Widmanst´atten microstructures that are known to have a negative impact on resistance to fatigue. These microstructures, consisting in acicular precipitates growing in colonies, are observed in many metallic alloys (Ti alloys, brass, steels ...). Their formation, and in particular the precipitate growth at constant velocity (in isothermal conditions), is singular for a diffusion-controlled phase transformation. Despite several analysis, the mechanisms responsible for this growth mode are not fully understood. By analogy with the dendritic growth during solidification, it has often been stated that the anisotropy of the interface energy is of prime importance, in spite of unrealistic amplitudes needed to simulate any platelike growth. Recently, using a phase field approach and 2D simulations, Cottura et al. [1] have shown that the anisotropy of the elastic energy caused by the change of crystalline structure during the phase transformation is a key ingredient to explain the acicular shape of plates and their growth kinetics.

Along this line, the present work brings new insights on the Widmanst´atten growth process. First, a phase-field model coupling both chemical and elastic effects is developed to analyze the growth of needles and plates in three dimensions. In agreement with observations performed in several alloys [2], our calculations predict a lengthening at constant velocity and a thickening proportional to $\sqrt{(t)}$. The growing tip is then analyzed in two and three dimensions. Using model cases, we show that the shape and size of the tip are not sensitive to the supersaturation and are the result of the competition between interfacial and elastic energies. This implies that the criterion based on the maximum growth velocity, mentioned in the literature to predict the radius of curvature of the tip, is irrelevant and a new criterion based on elasticity is proposed.
Second, the phase-field model is extended to include the plastic relaxation that is expected to occur when high transformation-induced stresses are generated in the microstructure. We have considered two different relaxation modes, either by including the effect of misfit dislocations or the plastic strain generated by a plastic activity in the matrix. We show on specific examples that these relaxation modes significantly impact the growth kinetics and the size of the tip, and a quantitative comparison with Widmanst´atten structures in Ti alloys is performed.

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*Speaker

Keywords: Widmanst´atten, phase field, elastic anisotropy, phase transformation, plasticity

Nucleation and transmission of co-zone {10-12} deformation twins in Mg: A phase field simulation study

Hong Liu * [1], Fengxiang Lin [2], Nele Moelans [3]

[1] Hong Liu – Belgium
[2] Fengxiang Lin – Belgium
[3] Nele Moelans – Belgium

A phase-field simulation model is constructed and implemented to study the nucleation, growth and transmission of twins in polycrystalline Mg samples. It is found that the twin nucleation sites are determined by both the grain orientation and the stress concentrated at grain boundaries. Considering only the effect of grain orientation, the interaction energy between the pre-existing stress field and the to-be-nucleated twins is constant within the same grain and it is most favourable for twins to form in the grain that has the most negative interaction energy. Within this grain, the energetically most favourable nucleation site is determined by the stress concentrated near grain boundaries. In three sandwich distributed grains, two factors, the applied strain and the stress concentrated at the tip of the pre-existing twin decisive for twin transmission from the grain in the middle to the grains on the two sides. In the region near the tip of the pre-existing twin, the contribution of the concentrated stress on the twin transmission is larger than that of the applied strain. When the grains on the left-/right-hand sides rotate more than 42◦ counter-clockwisely relative to the grain in the middle, the twin cannot transmit because the driving force becomes insufficient. The calculation results of both the resolved shear stress of twins and the interaction energy distributed in the grains are effective approaches to predict the twin nucleation. These two methods are roughly equivalent mathematically, but the interaction energy results are able to also consider effects of higher order terms of the strain tensor.

Keywords: Mg, Deformation twinning, Twin nucleation, Twin transmission, Phase, field simulation

*Speaker

On stress and driving force calculation within multiphase-field models: applications to martensitic phase transformations

Daniel Schneider * [1,2], Ephraim Schoof [2], Felix Schwab [1], Christoph Herrmann [2], Michael Selzer [1,2], Britta Nestler [1,2]

[1] Institute of Applied Materials (IAM-CMS), Karlsruhe Institute of Technology (KIT) – Kaiserstrasse 12, 76131 Karlsruhe Germany, Germany
[2] Karlsruhe University of Applied Sciences, Karlsruhe University of Applied Sciences – Moltkestr. 30 D-76133 Karlsruhe, Germany

Numerical simulations based on phase-field methods are indispensable in order to investigate certain interesting and important phenomena in the evolution of microstructures.
Microscopic phase transitions are highly affected by mechanical driving forces and therefore the accurate calculation of the stresses in the transition region is essential.
We present methods for stress calculations within the phase-field framework for infinitesimal and for finite deformations, which satisfy the mechanical jump conditions corresponding to sharp interfaces, although the sharp interface is represented as a volumetric region using the phase-field approach.
The models allow to calculate phase inherent stresses and deformations even in regions where many phases coexist.
Since the phase inherent variables are known, appropriate methods can be used for the calculation of the internal variables in the bulk regions.
We demonstrate that the models reflect the mechanical configurational forces for phase transition and is applied to the martensitic phase transformation process.

Keywords: phase, field, miltiphase, field, mechanical configurational forces, mechanical jump conditions, martensitic phase transformation

*Speaker

Elasto-plastic multiphase-field modeling of martensitic phase transformation in an EBSD-based dual-phase microstructure

Ephraim Schoof * [1], Christoph Herrmann [1], Daniel Schneider [2], Michael Selzer [3], Britta Nestler [2]

[1] Institute of Materials and Processes (IMP) Karlsruhe University of Applied Science – Germany
[2] Institute of Applied Materials (IAM-CMS), Karlsruhe Institute of Technology (KIT) – Kaiserstrasse 12, 76131 Karlsruhe Germany, Germany
[3] Institute of Applied Materials (IAM-CMS), Karlsruhe Institute of Technology (KIT – Germany

Automotive industry, like other industrial sectors, demands dual-phase steel due to the attractive combination of high strength and good formability. The high strength is achieved by the displacive phase transformation of austenite which yields martensite during quenching. The resulting microstructure and their mechanical properties are significantly characterized by the applied process parameters. Hence, a better understanding of their effects are fundamental to design a material of desired properties. The phase-field method has emerged as a powerful tool in order to simulate grain boundary motion phenomena. In case of martensitic phase transformation, a special challenge lies in considering the effect of grain boundaries in polycrystals as the growth is hindered by them. To account for this, we present a multiphase-field model based on the model of Nestler et al. [1]. Each grain contains its own set of order parameters consisting of an austenitic phase and a defined arbitrary number of martensitic variants. The mechanical part is solved according to our recently published work [2], which is capable of fulfilling the mechanical jump conditions at the interface and uses configurational forces as mechanical driving forces for phase transformations [3, 4]. We present simulations of martensitic phase transformation in an EBSD-based dual-phase microstructure. The austenitic grains transform into martensite depending on their orientation and the chosen process parameters while the ferritic grains remain inert. We discuss the nucleation and propagation behavior of the martensitic variants and the resulting stress and plastic strain distribution in the dual-phase microstructure.

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Keywords: Multiphase field, Martensitic phase transformation, Mechanics of metallic materials

*Speaker

Curing simulations on the basis of a phase-field model

Felix Schwab *† [1], Ephraim Schoof [2], Schneider Daniel [1,2], Michael Selzer [1,2], Colin Denniston [3], Britta Nestler [1,2]

[1] Institute of Applied Materials (IAM-CMS), Karlsruhe Institute of Technology (KIT) – Straße am Forum 7, 76131 Karlsruhe, Germany
[2] Institute of Materials and Processes (IMP) Karlsruhe University of Applied Science – Moltkestr. 30, 76133 Karlsruhe, Germany
[3] Department of Applied Mathematics, University of Western Ontario (UWO) – 1151 Richmond Street, London, ON, N6A 3K7, Canada

Abstract. The extended use of fibre-reinforced polymers (FRP) throughout industries needs computational models and methods to accompany this development. Especially the difference in material properties and the influence of fibre placement have an effect in production and application.
One of the crucial steps is the moulding process, in which the FRP structure is shaped. In the setting of thermoset-based FRPs, the polymer experiences volume shrinkage due to the curing reaction. This and high temperatures in the mould lead to eigenstresses in fibres and matrix.

To comprehend these processes, on top of a phase-field model [1] we employ a thermodynamically consistent thermo-chemo-mechanical model for curing thermoset-based FRPs. Fibre-matrix interfaces are treated accordingly to the balance equations at singular surfaces [2,3,4] to maintain a quantitative behaviour. The exothermic model for the curing process is based on reaction kinetics. For evaluation a set of FRP-based volume elements are used. We apply a phase-field based crack model [5] to investigate the influence of eigenstresses on micro-crack formation during the production process.

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Keywords: phase, field, fibre, reinforced polymers, curing simulation, eigenstresses, micro, cracks

*Speaker
†Corresponding author: felix.schwab@kit.edu

Open issues in phase field approaches to brittle fracture

Michael Strobl * [1], Thomas Seelig [2]

[1] Institute of Mechanics, Karlsruhe Institute of Technology (IfM, KIT) – Kaiserstraße 12 76131 Karlsruhe, Germany
[2] Institute of Mechanics, Karlsruhe Institute of Technology (IfM, KIT) – Germany

Phase field approaches to fracture have steadily gained popularity to compute complex crack patterns in statics and dynamics, including initiation of cracks and determination of unknown crack paths. The smooth approximation of cracks without explicit description of the crack surface by introducing an internal length parameter and gradual degradation of material stiffness are key features of the method, which is said to result in mesh independent solutions. This contribution is concerned with open issues in phase field approaches to brittle fracture. The underlying conceptually simple techniques like isotropic stiffness degradation by a scalar-valued phase field and the corresponding isotropic phase field evolution severely restrict the scope of application. Hence, basic concepts from continuum damage mechanics like tension-compression splits have been adapted and are widely established. But, with the exception of a few special cases, common splits like the volumetric-deviatoric split of strain or the spectral decomposition violate the specific conditions at cracks like traction free crack surfaces. Instead, fracturing of brittle solids is a highly anisotropic process. Therefore, at least some additional constitutive assumptions have to be taken into account for the damage description in phase field models to obtain physically reasonable results. However, the incorporation of phenomenologically motivated approaches is to some extent incompatible within the underlying variational framework of the phase field method. Another important issue is a suitable choice of the internal length parameter. On the one hand, it is introduced as a regularization parameter in describing the surface energy density. It has to be chosen small enough to accurately approximate the crack. On the other hand, it can be interpreted as a material parameter, which determines the tensile strength in conjunction with the (e.g. polynomial) stiffness degradation function. In many situations, these points of view are in conflict. In the case of crack initiation, the internal length parameter plays a crucial role and has to fulfill additional requirements. Moreover, in the absence of severe initial stress concentrations gradual degradation of stiffness leads to large damaged areas prior to crack initiation. One of our main focus is the simulation of *indentation fracture* by using the phase field approach. In this specific task, which constitutes a non-standard problem of fracture mechanics, the proper treatment of every aforementioned of the issues is essential. Numerical results are discussed for various modifications and the method's capabilities are illustrated by comparison with other numerical techniques and experimental results.

Keywords: phase field, indentation fracture, constitutive assumptions, anisotropy

*Speaker

Modelling inheritance of plastic deformation during migration of phase boundaries using a phase field method

Kais Ammar *† [1], Samuel Forest [1], Benoît Appolaire [2]

[1] MINES ParisTech, PSL Research University, MAT - Centre des matériaux – MINES ParisTech, PSL Research University – France
[2] Laboratoire d'Etude des Microstructures, CNRS/ONERA – ONERA – France

Recent advances in phase field modelling include the description of elastoviscoplastic material behaviour of the phases combined with diffusion and phase transformation. The corresponding models can be classified into two main groups of theories, referred to as interpolation and homogenisation models in the present work. It is shown that both approaches strongly differ concerning the question of inheritance of plastic deformation after the passing of a phase transformation front. Inheritance of plastic deformation is to be distinguished from the inheritance of the microstructure hardening and the corresponding dislocation structures. That is why the analysis is performed in the absence of hardening in the constitutive model. Finite element simulations of the growth of elastic misfitting precipitates embedded in a rate-independent elastoplastic matrix material reveal that the interpolation model allows for total inheritance of plastic deformation in contrast to the homogenisation model. The residual stress field and the growth kinetics are shown to be impacted by this essential property of the models. The results suggest that new models should be designed that allow for partial and controlled inheritance.

Keywords: Phase field, Plasticity, Inheritance, Homogenization method, Finite element method

*Speaker
†Corresponding author: kais.ammar@mines-paristech.fr

S22: Reduced order and data-driven material models

Composite surface characterization and classification through datamining.

Clara Argerich Martin * [1], Angel Leon Collado [1], Ruben Ibanez Pinillo [2], Anaïs Barasinski [1], Emmanuelle Abisset-Chavanne [2], Francisco Chinesta [3]

[1] GeM – École Centrale de Nantes – France
[2] ESI Group – École Centrale de Nantes, Ecole Centrale de Nantes – France
[3] ESI Group – École Nationale Supérieure d'Arts et Métiers (ENSAM) – France

Composite processing implies the deformation of surfaces, where the characterization of the last leads to different kind of descriptors. Most often geometrical description is considered from the use of roughness parameters for example, although efficient forming seems requiring physically based descriptors. Indeed many studies had been carried out to statistically analyze the aspects of a surface from the mathematical point of view. However, none had addressed the physical induced properties of the surface.
The main object of this work is to provide a reliable method for characterizing surfaces in order to accurately estimate "a priori" their physical behavior, and more precisely the deformation under a thermo-mechanical loading of a pre-impregnated surface, modeled as an homogeneous non-Newtonian fluid in a first approach. This operation is a key stage in the Automated Tape Placement (ATP) process for thermoplastic composites, which involves an in-situ consolidation between polymer layers due to the simultaneous application of temperature and pressure on the surface of the composite, if the process is well exploited.
The first step here is to build a wide surfaces database by the measurement of various composite surfaces with a scanning microscope. From this, different descriptors of the surface are investigated, both at macro and micro scales. Then using a computational model, the consolidation step, dealing with the crushing of the surface is carried out, and the time evolution of the degree of intimate contact is evaluated. At this point the surface behavior is known and a deep study with data-mining, more specifically regression algorithms and neural networks, is carried out in order to estimate the surface response beforehand. Thanks to data-mining techniques, not only the behavior can successfully be predicted a priori, but also the parameters that play a role into the physical process that the material undergoes can be identified. We prove that the curvature is a reliable parameter that explains the physical processes taking part in the consolidation step during ATP process, which involves squeeze flow, thermal diffusion, and intimate contact evolution among others. We also prove the feasibility of using regression trees and neural networks to predict the behavior of composites, and thus reducing the number of simulations.

Keywords: Datamining, surface characterization, composite processing

*Speaker

Model & system learners, optimal process constructors and kinetic theory-based goal-oriented design: a new paradigm in materials and processes informatics.

Francisco Chinesta * [1]

[1] Institut de Calcul Intensif (ICI) – Ecole Centrale de Nantes – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France

Usual design procedures link in a causal way processes, structures, properties and performances, however, in reality, in order to generate innovation and stimulate discovering, materials and processes design should proceed in the opposite way: form performances to properties, structure and processes.
In our recent works we focused on model and system learners, able to extract the subjacent and assumed unknown model, from the only knowledge of the systems dynamics, i.e. of its state and the evolution of it.

To overcome issues related to nonlinear behaviors, the just described rationale was inserted within a kinetic theory framework making use of both the master and Fokker-Planck equations.
The last equations allow addressing nonlinear dynamical systems while keeping the linearity of the equation governing the evolution of the probability distribution function defined in the space of the state coordinates. Thus, other than evaluate all the possible states for a given dynamical system, e.g. its steady state (when it exist), its attractors, ... while circumventing its inherent curse of dimensionality by employing advanced dimensionality reduction techniques, the kinetic framework makes also possible to proceed in the inverse sense: given the target, obtaining the dynamics, and from both, the state and its dynamics, extracting the model using model learning.

Keywords: Optimal design, Data, driven, Kinetic theory

*Speaker

Application of a machine learning approach for the correction of experimental measured residual stresses based on the incremental hole drilling technique

Sergey Chupakhin [1], Sören Keller [1], Nikolai Kashaev [1], Norbert Huber [1], Benjamin Klusemann [*†] [1,2]

[1] Institute of Materials Research, Materials Mechanics, Department Joining and Assessment, Helmholtz-Zentrum Geesthacht – Max-Planck-Str. 1, 21502 Geesthacht, Germany
[2] Institute of Product and Process Innovation, Leuphana University of Lüneburg – Volgershall 1, 21339 Lüneburg, Germany

Laser shock peening (LSP) is an innovative surface treatment technique that is applied to modify the local properties to improve the overall fatigue performance of metallic structures. The peening locally generates deep compressive stresses, which retard or even suppress crack initiation and growth. Arranging the shots in an optimal design, a significant improved fatigue behavior can be observed. The compressive stresses are a result of the introduced high pressure waves caused by the expanding plasma trapped on the material surface. These shock waves lead to high strain rates within the material. One particular difficulty is the experimental determination of non-uniform residual stresses. Here, we apply the hole drilling method, which is a widely-known technique for determination of non-uniform residual stresses in thin metallic structures by measuring strain relaxations at the material surface caused through the stress redistribution during drilling the hole. Hole drilling is based on the Integral method, relying on finite element calculated calibration data, which assumes linear elastic material behavior. That restricts the measurement of residual stresses approaching the yield strength of the material. There is lack of study regarding to the stress fields correction with high gradients typically observed in laser shock peening. For this purpose, we propose a data-driven correction method which is capable of covering a wide range of stress profiles in different materials. For this purpose, the hole drilling process involving plasticity was simulated in ABAQUS and the Integral method was applied to the relaxation strain data to obtain the stress field. The simulation procedure has to be repeated hundred times to cover the relevant range of materials behavior and the majority of LSP-shaped stress profiles. The proposed approach employs artificial neural network (ANN) as an arbitrary function approximation mechanism for solving inverse problems. The ANN has been trained on a large number of patterns, extracted from simulations, in order to identify the relationship between predefined profiles in the model and plastically affected simulated stress profiles, obtained through the Integral method. The network provides accurate stress corrections and demonstrates simultaneously high generalization feasibility [1]. Results of a successful application of the proposed approach will be presented and results will be compared to determined residual stress profiles from process simulations of LSP.

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Keywords: machine learning, laser shock peening, hole drilling, artificial neural network

*Speaker
†Corresponding author: benjamin.klusemann@leuphana.de

Data-driven computational mechanics based on manifold learning for elastic and plastic behaviors

Ruben Ibanez [1], Emmanuelle Abisset-Chavanne *† [1], Aguado Jose Vicente [1], Domenico Borzacchiello [1], Elias Cueto [2], Francisco Chinesta [3]

[1] Institut de calcul intensif (ICI) – Ecole Centrale de Nantes, École Centrale de Nantes – France
[2] Aragón Institute of Engineering Research (I3A) [Zaragoza] – I3A, Edificio I+D+i C/ Mariano Esquillor s/n, CP 50018, Zaragoza, Spain
[3] Institut de Calcul Intensif (ICI) – Ecole Centrale de Nantes – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France

In classical mechanics, numerical simulations are based on two types of equations. The first one of axiomatic character is related to balance laws such as momentum, mass or energy conservation. The second one consists of models extracted from collected data, experimental or synthetic. In order to bypass the use of these models that introduce irremediably errors in the simulations, a proposition is to directly link collected data to computers and balance laws.
For that purpose, we take advantage of the machine learning techniques, developed for data mining, and in particular manifold learning approaches that allow to extract the relevant information from large experimental datasets. The idea is to obtain from the experimental tests results, namely the stress-strain couples and all the needed relevant parameters, low dimensional manifolds and to use them instead of the classical constitutive laws. In this work, we will propose an overview of the applications of the proposed approach for different material behaviors, from the simple elastic Hooke's law to more complex plasticity including hardening.
Moreover, as the accuracy of the techniques relies on the completeness of the data available, we will propose a methodology that, from a non-homogeneous experimental test, allows to collect as many data as possible.

Keywords: Data, driven, constitutive law, elasticity, plasticity

*Speaker
†Corresponding author: emmanuelle.abisset-chavanne@ec-nantes.fr

The use of compressive sensing in computational mechanics.

Ruben Ibanez Pinillo *† [1,2], Emmanuelle Abisset-Chavanne [2,3], Elias Cueto [4,5], Pierre Guillormini [6], Amine Ammar [7,8], Antonio Huerta [9], Francisco Chinesta‡ [6,10]

[1] ESI Group – École Centrale de Nantes, Ecole Centrale de Nantes – France
[2] Institut Calcul Intensive – École Centrale de Nantes – France
[3] Institut de Recherche en Génie Civil et Mécanique (GeM) – Ecole Centrale de Nantes – 1, rue de la Noé, France
[4] Aragón Institute of Engineering Research (I3A) [Zaragoza] – I3A, Edificio I+D+i C/ Mariano Esquillor s/n, CP 50018, Zaragoza, Spain
[5] Universidad de Zaragoza – Spain
[6] ENSAM ParisTech – ENSAM ParisTech – France
[7] Arts et Métiers ParisTech - Angers – ParisTech – 2 Bd du Ronceray, 49035 Angers, France
[8] ENSAM Angers – ENSAM Angers – France
[9] Universitat Politècnica de Catalunya [Barcelona] (UPC) – Universitat Politècnica de Catalunya C. Jordi Girona, 31. 08034 Barcelona, Spain
[10] Institut de Calcul Intensif (ICI) – Ecole Centrale de Nantes – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France

Computational mechanics is taking an enormous importance in industry nowadays. On one hand, numerical simulations can be seen as a tool that allows the industry to perform less experiments, reducing costs. On the other hand, the physical processes that are intented to be simulated are becoming more complex, requiring more computational effort to achieve the desired precision. For instance, problems exhibiting localization requires extremely fine mesh resolutions. Also, stability and accuracy constraints lead to prohibitive time steps for realistic dynamic applications. Indeed, these issues compromise real time applications.
Model order reduction techniques could be an appealing technique to alleviate time constraints. Indeed, POD-like methods, where a set of snapshoots are used to construct a reduced basis, are proved to be effective when there are few modes carrying most part of the information. Another appealling alternative is the use of PGD-like methods, where a specific tensorial separated representation is seeked. By means of the last technique, parametrique solutions are obtained in a very efficient way, just like the possibility of uncoupling spatial dimensions i.e. in-plane-out-of-plane separated representation.
In the present work, the use of compressive sensing techniques into the computational mechanics field is analyzed. Compressive sensing techniques are widely used in image reconstruction, where a lot of data stocakge is saved due to the fact that only the information at certain pixels is required. The key ingredient behind such techniques is a proper base change where a high percentage of coefficients in the new base are zero i.e. the representation of the information in the new base is sparse. Combining the sparsity together with the minimization of a functional that seeks for sparsity allow to find, among the infinity of solutions related to an underdetermined system of equations, the sparsest one. Several applications of the compressive sensing are tested, opening an alternative route with respect to traditional numerical methods.

Keywords: Compressive Sensing, Data, Driven

*Speaker
†Corresponding author: ruben.ibanez-pinillo@eleves.ec-nantes.fr
‡Corresponding author: Francisco.Chinesta@ec-nantes.fr

Fast and Memory Efficient Two-Scale Simulations of Components by Combining Model-Reduction Methods with the Composite Voxel Technique

Matthias Kabel * [1]

[1] Fraunhofer ITWM – Fraunhofer-Platz 1 D-67663 Kaiserslautern, Germany

For the simulation of industrial components made of composite materials, model order reduction (MOR) methods are commonly applied. These methods can be split into an "offline" and "online" phase. In the "offline" phase an effective material law for the macro-scale is derived by micro-scale simulations. In the "online" phase only ordinary differential equations for the reduced variables need to be solved to obtain the stress response of the composite material at each integration point of the component simulation.
Since the microstructure is different at each integration point the necessary precalculations in the "offline" phase depend linearly on the number elements in the mesh of the component. If plastic effects are to be taken into account for the component simulation, the computational effort for the "online" phase of the pRBMOR method of Fritzen and Leuschner [1] also scales cubically with the resolution of the micro-scale.

In this talk we will discuss the combination of the composite voxel technique of Kabel et al. [2] with the NTFA-TSO of Michel and Suquet [3] as well as the pRBMOR of Fritzen and Leuschner [1] to accelerate two-scale simulations of components with elasto-viscoplastic deformations.

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Keywords: Model order reduction, FFT based homogenization, Composite voxel

*Speaker

Application of a non-intrusive and parametric reduced order model of crash simulation in several design processes.

Yves Le Guennec * [1], Jean-Patrick Brunet [1], Fatima Daïm [2], Yves Tourbier [3]

[1] IRT SystemX – IRT SystemX, IRT SystemX – France
[2] ESI-Group – ESI-Group, ESI GROUP – France
[3] RENAULT – Renault – France

Industrials have an intensive use of numerical simulations in order to avoid physical testing and to speed up the design stages of their products. The numerical testing is indeed quicker to set-up, less expensive, and supply more informations about the system under study. Moreover it is much closer to the physical tests as the computation power increases. Despite the rise of this power, time consuming simulations remain challenging to be used in design process, especially in an optimization study. Crash simulations belong to this category. These rapid dynamic computations are used by RENAULT during the sizing of the vehicle body in white in order to ensure that it meets standards set up to reach safety in case of accidents. Here, the optimization study tries to minimize the mass of the vehicle (and thus its energy consumption) by modifying the thickness of some parts (from 20 to 100 variables). Industrials as RENAULT currently perform optimization studies based on numerical designs of experiments. The number of computations requires by this technique is from 3 to 10 times the number of variables. This is too much in order to be intensively used in a design process.
In order to decrease the time-to-market and to explore alternative technical solution, we explore the potential of using a parametrized reduced order model in the optimization studies. The parametrized reduced model gives an estimation of the high-fidelity result for a set of parameters without using the solver by analysing the results of existing computations. The developped reduced order model is called Re-CUR. It is partly based on a CUR approach, and on a regression analysis . The regression statistical model built uses the data of a few calculations made with the solver. Classical tools used in regression and data analysis such as clustering, or linear programming will be used in this construction. The similarity with existing machine learning techniques is very interesting to note.
It has been observed that it drastically reduces the number of required simulations compared to a classic optimization study. In this talk, the construction of the reduced order model will be quickly outlined. Then, the effects of this reduced model on the number of simulations required for optimization of a full car model will be studied. Lastly, we will investigate the potentialities on other design processes offered by this reduced model such as sensitivity analysis or gradient computation.

Keywords: reduced order model, crash simulation, regression analysis, linear programming

*Speaker

A Latin-PGD approach for high cycle fatigue computations

Udo Nackenhorst * [1], Mainak Bhattacharyya [1], Amelie Fau [1], David Neron [2], Pierre Ladeveze [2]

[1] Leibniz Universität Hannover (University of Hannover) – Appelstr. 9A 30167 Hannover, Germany
[2] Laboratoire de Mécanique et Technologie (LMT) – École normale supérieure - Cachan, Centre National de la Recherche Scientifique : UMR8535 – Bât. Léonard de Vinci 61 Av du président Wilson 94235 CACHAN CEDEX, France

Classical approaches on modeling of fatigue lifetime are based on semi-empirical approaches, i.e. S-N curves investigated in laboratory experiments. Concepts of linear damage accumulation like Palmgreen-Miner rule or Paris-law are widespread in engineering applications. Nonetheless, physically based approaches, which enable for complex three-axial loading, frequency and amplitude dependency etc. based on continuums damage mechanics theories are still missing. Here, the challenge remains the numerical treatment of large number of load cycles. First attempts in that direction have been introduced by cycle jumping approaches for example, c.p. Lesne and Savalle (1989), Oskay and Fish (2004).
In this presentation, a new Latin-PGD approach will be introduced for efficient fatigue damage simulation with high and very high number of cycles. Large Time Inkrement (Latin) methods have been established by Ladeveze (1999) and its efficiency has been demonstrated for a number of inelastic material behavior in the past. With the introduction of damage a new complexity arises because the linear part of the state equations, i.e. the equilibrium conditions, get time dependent (non-linear). A new operator split technique is introduced to tackle that issue within the overall algorithmic treatment. A second ingredient for efficient computation of large number of load cycles is based on a two-scale treatment of the Latin method in time, c.p. Cognard and Ladevèze (1993). In common with a PGD-approximation of the response functions, this enables for a very efficient computation of large number of fatigue damage load cycles based on sophisticated continuums damage mechanics approaches.

The efficiency of the proposed approach will be demonstrated on a number of numerical examples with increasing complexity.

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Keywords: cyclic fatigue, model reduction, Latin, Proper Generalized Decomposition

*Speaker

On the combination of stochastic modeling, image analysis and numerical simulation for virtual materials testing

Matthias Neumann [1], Volker Schmidt * [1], Lorenz Holzer [2]

[1] Institute of Stochastics, Ulm University – Helmholtzstraße 18, D-89069 Ulm, Germany
[2] Institute of Computational Physics, Zurich University of Applied Sciences – Wildbachstrasse 21, CH-8400 Winterthur, Switzerland

Analysis and modeling of big data is changing industries, businesses and research. One of the reasons that has contributed to this success is that large amounts of data are available nowadays. In the area of microstructures, however, acquisition of (3D tomographic image) data is difficult and time-consuming. On the other hand, large amounts of data representing the geometry of virtual, but realistic 3D microstructures can be generated using stochastic microstructure modeling. Combining the output of stochastic microstructure modeling with image analysis and numerical simulations, microstructure-property relationships can be determined. We call this approach virtual materials testing. It can be used to quantify relationships between descriptors of microstructures and the corresponding functional properties such as e.g. properties of heat transfer, effective permeability and conductivity or mechanical properties (Kulosa et al., 2017; Roland et al., 2015; Stenzel et al., 2016) In this talk we discuss the results of a case study, where we predict effective conductivity given by well-defined microstructure characteristics, which can be computed by the aid of image analysis. For this purpose, we consider the following microstructure characteristics: connected-phase volume fraction ϵ, mean geodesic tortuosity
tau and constrictivity β of the conducting phase. In (Stenzel et al., 2016) the quantitative relationship between these microstructure characteristics and effective conductivity has been investigated based on 43 virtual microstructures, where the following formula
σeff $= \sigma 0\ \epsilon$ˆ1.15 βˆ0.37
tauˆ-4.39 (1)

was derived by parametric regression analysis. Here $\sigma 0$ denotes the intrinsic conductivity of the material. In a recent study we analyzed a total of 8119 microstructures generated by two different stochastic 3D microstructure models (Stenzel et al., 2017). This is - to the best of our knowledge - by far the largest set of microstructures that has ever been analyzed. Non-parametric prediction tools from statistical learning like artificial neural networks and random forests are used to validate the prediction formula given in (1) by more than 8000 virtual microstructures and show that it is possible to predict effective conductivity more accurately using methods from statistical learning. The proposed concept leads to a better understanding of microstructure-property relationships and thus, it has the potential to generate recommendations for new, more efficient microstructures.

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*Speaker

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Keywords: Virtual materials testing, Big data, Effective conductivity, Stochastic microstructure modeling, Image Analysis

POD based model reduction for SFEM based computational homogenization

Dmytro Pivovarov *† [1], Paul Steinmann [1], Kai Willner [1]

[1] LTM, Friedrich-Alexander University Erlangen-Nürnberg – Germany

The computationally most expensive part of stochastic FEM based homogenization is the inversion of the stochastic stiffness matrix. The reduction of computational costs was addressed for stochastic PDEs by many authors, but most approaches are based on Karhunen-Loeve expansion (KLE) or stochastic spectral decomposition of the stochastic differential operator. In the current work we examine the application of the POD based model reduction without decomposition of the differential operator. POD modes are evaluated using the snapshots of the nonlinear stochastic problem. Thus simultaneous reduction in stochastic and physical dimensions is performed. Method's convergence, accuracy and reduction of computational costs are discussed. Finally the proposed method is applied to the computational homogenization of heterogeneous materials with aleatoric uncertainty in the geometry of the microstructure.

Keywords: Stochastic FEM, POD, Computational homogenization, Random geometry

*Speaker
†Corresponding author: dmytro.pivovarov@fau.de

Stamping Hybrid Twin

Giacomo Quaranta * [1], Simon Guévelou [2], Emmanuelle Abisset-Chavanne [1], Mustapha Ziane [2], Yann Debray [2], Domenico Borzacchiello [1], Jean-Louis Duval [2], Francisco Chinesta [3]

[1] ESI Group Chair, ICI Institute at Ecole Centrale de Nantes – École Centrale de Nantes – France
[2] ESI-Group – ESI-Group, ESI GROUP – France
[3] ESI Group Chair, PIMM Institute at ENSAM ParisTech – ENSAM ParisTech – France

In the previous (third) industrial revolution, "digital twins" (emulating a physical system from the accurate solution of the mathematical model expected describing it) were major protagonists, making accurate designs possible. Numerical simulation is nowadays present in most of scientific fields and engineering domains, making possible the virtual evaluation of systems responses, alleviating the number of experiences on the real system that the numerical model represents. However, usually virtual models (digital twins) are static, that is, they are used in the design of complex systems and their components, but they are not expected to accommodate or assimilate data so as to define dynamic data-driven application systems. The characteristic time of standard simulation strategies is not compatible with the real-time constraints compulsory for control purposes and significant deviations between the predicted and observed responses are noticed, limiting the use of digital twins in many applications requiring online adaptation.
Thus, nowadays, it is generally accepted the urgent need of more reliable modeling approaches as well as the dynamic assimilation of collected data on running simulations, for defining efficient Dynamic Data-Driven Application Systems —DDDAS—.

The present work focuses in the Hybrid-Twin concept where data-driven modeling are employed to fill the gap between the parametric deterministic solution computed by using the non-intrusive PGD constructor (and whose parameters will be determined by assimilating data) and the measured fields. As soon as the data-driven model allows making accurate predictions, control strategies can be safely applied. At the scale of (complex) systems (the machine, the factory or the networks and grids), 3D partial differential equations representing models of parts and processes, are replaced by 0D and 1D systems, elaborated from simplified models or phenomenological rules acquired from data-analytics. The parametric solutions of such kind of models (e.g. using modeling tools as Modelica and Scilab), and their improvement / correction via enhancement or reconfiguration by using data-driven modeling is of major interest in the case of autonomous cars, driver-twins, factory 4, internet of things – IoT-, smart grids (electric or water grids), transport, pedestrian and population dynamics.
In particular in the present work the Hybrid-Twin concept will be used on a on a stamping chain process consisting of two machines in series in order to solve the complex mathematical models under real-time constraints, assimilate data and adaptthe model online to evolving environment.

Keywords: model reduction, data, driven, hybrid, twin, stamping

*Speaker

Non-parametric identification of material state database from full-field measurements

Julien Réthoré * [1], Adrien Leygue [1], Michel Coret [1], Erwan Verron [1], Laurent Stainier [1]

[1] Institut de Recherche en Génie Civil et Mécanique (GeM) – Université de Nantes, Ecole Centrale de Nantes, Centre National de la Recherche Scientifique : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France

Recently, unprecedented attention has been devoted to data-driven approaches. This is due to the development of both experimental techniques enabling the acquisition of rich data fields and data based prediction algorithms. An experimental database should span a domain of the stress/strain space as large as possible for reliable data based predictions. Further, in the case of non-linear dissipative material behaviours additional state and internal variables are required to define the material state unequivocally. For these reasons, classical homogeneous experiments may be a limitation by themselves. In this contribution, it is proposed to analyse complex heterogeneous displacement fields obtained by digital image correlation so that, not only total strain fields can be estimated but also stress and anelastic strain fields. Using such a strategy the subspace of the stress/strain space explored during one single experiment can be much larger than using hundreds of classical homogeneous experiments. One of the key features of the method is its non-parametric nature that allows for estimating material states with no assumption on the constitutive relations. The ability of the proposed methodology to extract rich admissible material state database from heterogeneous experiments will be illustrated through several examples including: anisotropic elasticity, heterogeneous isotropic elasticity and elasto-plasticity.

Keywords: experiments, full, field measurement, databse

*Speaker

A data-driven approach for orientation kinematics of suspended rigid fibres

Adrien Scheuer * [1,2], Emmanuelle Abisset-Chavanne [1], Francisco Chinesta [1], Roland Keunings [2]

[1] ESI-Chair Group & ICI, Ecole Centrale de Nantes – École Centrale de Nantes – France
[2] ICTEAM, Université catholique de Louvain – Belgium

Properties of reinforced polymers strongly depend on the microstructure state, that is the orientation state of the fibres suspended in the polymeric matrix, induced by the forming process. Most models used to describe the orientation behaviour of rod-like particles suspended in a viscous fluid flows are built upon Jeffery's pioneering work, which describes the evolution of a single particle immersed in a Newtonian fluid at the miscroscopic scale. Coarser macroscopic models aimed at describing the orientation state of a population of particles through orientation tensors were then introduced by Advani and Tucker. Such models however involve closure approximations in their derivations, that can impact the accuracy of the prediction. In this work, we show how to run data-driven macroscopic simulations of orientation development in dilute suspensions of rigid fibres, circumventing the use of closure approximations. In particular, this approach provides reliable predictions for flows in confined geometries, that is in gaps narrower than the fibre's length, for which state-of-the-art closures proved to be inadequate.

Keywords: Fibre suspensions, Jeffery's equation, Data, driven simulation

*Speaker

Model Order Reduction of Nonlinear Homogenization Problems by a Hashin-Shtrikman Type Finite Element Method

Stephan Wulfinghoff * [1], Fabiola Cavaliere [1], Stefanie Reese [1]

[1] Institute of Applied Mechanics [Aachen] – Mies-van-der-Rohe-Str. 1D-52074 Aachen, Germany

This talk presents a computational nonlinear homogenization approach, the starting point of which is a model order reduction method based on data-clustering. To this end, the micromechanical data from numerical experiments (snapshots) is analyzed in order to identify characteristic microstructural deformation patterns. These describe how the macroscopic strain typically localizes within the microstructure. The outcome of the procedure is a subdivision of the microstructure into a set of clusters of material points. Within each cluster the strain is then approximated as being constant.
The mechanical problem is formulated in terms of a three-field Hashin-Shtrikman type variational formulation which is based on the introduction of a linear-elastic reference medium. After discretization, most of the global unknowns can be eliminated via static condensation leaving the piecewise constant cluster strains as the primary unknowns. The resulting homogenization scheme includes, as special cases, the finite element method as well as Hashin-Shtrikman and Talbot-Willis type homogenization approaches with phase-wise constant trial fields (as well as related bounds). The limit case 'finite element method' allows to transfer knowledge from finite element technology and thus provides new strategies for the choice of the stiffness of the reference material. The method is applied to several nonlinear microstructures with different inclusion volume fractions and varying degree of anisotropy.
The results are shown to be in good agreement with full-field FE-simulations. Furthermore, the method is used to compute a refined upper bound of the Talbot-Willis type (compared to phase-wise constant trial fields), which converges to the finite element solution with increasingly refined discretization.

Keywords: homogenization, model order reduction, finite element technology, variational formulation, Hashin, Shtrikman

*Speaker

Wavelet Based Reduced Order Model for Computational Homogenisation

Rody Van Tuijl * [1], Cale Harnish [2], Karel Matouš [2], Joris Remmers [1], Marc Geers [1]

[1] Department of Mechanical Engineering (Eindhoven University of Technology) – P.O. Box 513, 5600 MB, Eindhoven, Netherlands
[2] Department of Aerospace and Mechanical Engineering (University of Notre Dame) – 367 Fitzpatrick Hall of Engineering, Notre Dame, IN 46556, United States

The Computational Homogenisation framework provides an accurate tool to analyse material behaviour propagating across the scales [1]. A repetitive evaluation of the micro-structural model for each macroscopic material point is required to resolve the macro-scale problem. Micro-structures with non-linear path-dependent material behaviour often rely on stored parameters to track the material state. Both the required computation time and the required memory to resolve each micro-structural problem limit the maximum problem size that can be considered.
A Reduced Order Model (ROM) [2] of the micro-structure is constructed to decrease the computational costs of solving the system of equations. Using a limited number of physical modes instead of the original discretisation, the kinematics are characterised with fewer degrees of freedom. However, non-linearly path-dependent models still require the full stress-field to be resolved.

To overcome the computational costs associated with the evaluation of the non-linear terms, the field can be approximated by selecting and weighting sample points. This calls for an adaptive sampling scheme to determine a subset of points dedicated to the load-case at hand. Wavelet bases have proven to be an efficient tool to reduce the computational overhead in solving partial differential equations [3]. In this contribution, a novel method combining an interpolating wavelet basis and a reduced basis is presented that adequately handles the non-linearities and path-dependency in the micro-structural model. The focus in this abstract lies on the implementation and the accuracy of the method as well as the reduction in required memory and computation time.

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Keywords: Reduced Order Modelling, Reduced Basis, Wavelet, Adaptive, Computational Homogenisation, Microstructural modelling

*Speaker

EuroMech Award

Multi-scale modelling of the chloride diffusivity of hydrated cement pastes

Mohamad Achour * [1], François Bignonnet† [1], Jean-François Barthelemy‡ [2], Emmanuel Roziere§ [1], Ouali Amiri¶ [1]

[1] Institut de Recherche en Génie Civil et Mécanique (GeM) – Ecole Centrale de Nantes, Université de Nantes, CNRS : UMR6183 – 1, rue de la Noë BP92101 44321 Nantes cedex 3, France
[2] Centre d'études et d'expertise sur les risques, l'environnement, la mobilité et l'aménagement (CEREMA) – CEREMA – 25, avenue François Mitterrand - CS 92 80369674 Bron Cedex, France

The microstructure of cement-based materials has a major influence on the mechanical and physical properties of concrete such as elastic properties, diffusivity and permeability. Consequently it is necessary to study the pore structure in order to understand the transport properties and durability of cementitious materials. Based on a multi-scale representation of the microstructure, a model is proposed in this study to predict the diffusion coefficient of chloride ions in the cement paste as well as the stiffness of the cement paste. The heterogeneity of cement paste manifests itself at several length scales. The complexity of the cement paste microstructure is handled in a simplified way thanks to a hierarchy of Eshelby-based homogenization schemes, namely the self-consistent and the Mori-Tanaka schemes. The model focuses on the estimation of the effective chloride diffusion of CEMI-based cement pastes as a function of the water/cement ratio.
The microstructure of the cement paste is modelled at three scales. The largest scale is the paste scale, which is made up of composite inclusions (an anhydrous core surrounded by two layers called respectively an inner and outer hydration products) and large capillary pores ($>$ 100nm). At an intermediate scale, the inner hydration products are considered as a porous poly-cristal, which comprises high density C-S-H gel and nano-sized crystal hydrates. The outer hydration products is a mixture of small capillary pores (_˜3-100nm), low density C-S-H gel and micro-sized crystal hydrates. At the finest scale, the low and high density CSH gels are described as disordered assemblages of solid C-S-H bricks and gel pores.

The model was developed for a range of water /cement ratio between 0.3 and 0.6. It is clearly shown that the electrical double layer (EDL) effect on the chloride diffusivity properties in the pore space must be taken into account for the gels pores, but not for the capillary pores, for which the diffusivity properties in the bulk solution must be considered. A comparison with experimental results indicates that the proposed model allows to predict the chloride diffusivity of cement paste as a function of the water/cement ratio.
Further, this representation of the microstructure also allows to model the evolution of the mechanical properties w.r.t. the water/cement ratio as the effective Young's modulus, with a good agreement with experimental data at long term.

Keywords: Microstructure, Cement paste, Diffusivity, Homogenization, Hydration, Multi, scale modelling

*Speaker
†Corresponding author: francois.bignonnet@univ-nantes.fr
‡Corresponding author: jean-francois.barthelemy@cerema.fr
§Corresponding author: emmanuel.roziere@ec-nantes.fr
¶Corresponding author: ouali.amiri@univ-nantes.fr

Cohesive zone calibration using GTN material model

Rasmus Andersen *† [1,2], Christian Felter [2], Kim Lau Nielsen [1,2]

[1] Technical University of Denmark, Department of Mechanical Engineering (DTU Mechanical Engineering) – Nils Koppels Allé, Bld. 404, Denmark
[2] Section of Solid Mechanics, Department of Mechanical Engineering, DTU – Denmark

Thin-walled structures, consisting of plates with in-plane dimensions much larger than the plate thickness, are widely used - from ship hulls and airplane fuselages to shipping containers with goods and products. Their application is many, but common is their vulnerability to overloading events that can trigger crack initiation, and subsequent growth, leading to structural collapse. For the analysis of potential structural collapse, engineers typically rely on cohesive zone elements embedded in a finite element model to ensure a computationally efficient approach to deal with the large-scale plate tearing involved. However, this way of predicting crack growth is phenomenological and the calibration of the crack surface traction-separation relation that governs material failure has to be conducted carefully to ensure accurate model predictions. This can pose a significant challenge as existing traction-separation relations do not mimic the underlying mechanics that govern the crack propagation, but rather relies on cracks to initiate at a predefine peak traction while subsequent crack growth occurs when a specified cohesive energy has been reached in the element. In contrast, engineers can turn to micromechanics-based approaches such as the Gurson-Tvergaard-Needleman (GTN) material model. This model homogenizes the porous material, assuming small voids to be present in the material in the undeformed state and as the material is loaded, the voids grow larger and eventually interact to cause coalescence and the formation of micro-cracks. Unfortunately, the GTN material model has its own drawbacks; it is inherently mesh dependent when adopted in a finite element framework and thus, a very fine mesh must be deployed in the fracture process zone to capture the crack propagation. In fact, the mesh size has to scale with the dominant void spacing and this raises the computational effort to an unrealistic level if real life structures are to be modeled. To bridge the gap between the two modeling strategies, the present study employs the GTN model in a full 3D analysis to simulate ductile crack initiation and growth to steady-state on a large-scale pre-cracked plate subjected to mode I loading. The outcome is the traction levels and the dissipation of energy in the fracture process zone; parameters that can be directly fed back into existing cohesive traction-separation relations in a commercial finite element software. Thus, the study is an attempt to allow the GTN model provide the calibrated data for the cohesive zone model.

Keywords: Plate tearing, Cohesive zones, Work of fracture

*Speaker
†Corresponding author: rgra@mek.dtu.dk

Model experiments on void growth and coalescence: effect of crystallographic orientation, strain hardening capability and strain localization

Pierre-Olivier Barrioz * [1], Jérémy Hure [1], Benoît Tanguy [1]

[1] CEA – Commissariat à l'Énergie Atomique et aux Énergies Alternatives (CEA) - Saclay, Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA) - Saclay – France

Void growth to coalescence is the classical mechanism involved in ductile fracture of structural alloys, thus are the key features to better understand fracture toughness of these materials. Growth regime is characterized by a diffuse plastic flow around voids, while coalescence corresponds to localized plastic flow between adjacent voids. Analytical models, numerical simulations and experimental data have clearly shown that both regimes strongly depend on the mechanical behavior of the material around the voids, where yield stress, strain-hardening modulus and anisotropy are key parameters. Anisotropy is particularly important for voids smaller than the grain size, thus at the crystal scale. Irradiation by high-energy particles, e.g. encountered in nuclear power plants, leads to the creation of crystalline defects such as dislocations, dislocation loops, nano-voids and precipitates in metallic materials. Consequently, an evolution of the mechanical properties is observed, such as hardening, loss of strain hardening capability, as well as modification of deformation mechanisms with increasing strain localization at the grain scale. Therefore, irradiation is used in this study as a tool to modify the mechanical properties of materials, and to assess experimentally their influence on void growth and coalescence. In addition, it gives experimental data relevant for irradiated materials used in nuclear power plants. Experiments are performed on coarse grain 304L austenitic stainless steel at the reference state, or irradiated with 2MeV protons penetrating up to few tens of a micron. Thinning down the samples up to thicknesses of about 20 microns allows to get a polycrystalline material with mostly one grain along the thickness, either at the reference state or fully irradiated. Drilling intragranular cylindrical voids (with diameters ranging from 5 to 15 microns) using Focused Ion Beam (FIB) allows finally to get a model experiment to study void growth and coalescence at the single crystal scale, with different behaviors of the material around the voids (reference state vs. irradiated). In-situ SEM (Scanning Electron microscope) tensile tests were performed, and void growth and coalescence are observed as a function of plastic strain. High resolution Digital Image Correlation were performed in order to get full-field deformation measurements, including strain localization phenomena, by using a speckle pattern (of typical size 150nm) generated by the remodeling of a deposited gold layer. Experimental observations quantity the influence of crystallographic orientation and strain-hardening modulus, and are satisfactorily compared to finite element simulations. Indications about the influence of strain localization at the grain scale on void growth to coalescence are also provided.

Keywords: Ductile fracture, void growth, coalescence

*Speaker

An experimental analysis of the effect of precipitate strengthening on the mechanical response of Al-Cu alloys by means of micropillar compression

Bárbara Bellón *† [1], Alejandro Rodríguez-Veiga [1], Ilchat Sabirov [1], Javier Llorca [2,1]

[1] Institute IMDEA Materials – Tecnogetafe 28906 Getafe Madrid, Spain
[2] Polytechnic University of Madrid (UPM) – 28040 – Madrid, Spain

An Al - 4 wt. % Cu (1.7 at. %) alloy was prepared using high- purity metals by induction casting in an induction furnace (VSG 002 DS, PVA TePla). Samples were machined from the central region of the ingot and subjected to a solution heat treatment during 22 h at 540°C, followed by natural aging at ambient temperature as well as artificial aging at 180°C for different times (6, 18, 30, 72, 120 and 168 hours). The precipitate structure was carefully characterized by means of transmission electron microscopy (FEI Talos) and the structure, size, aspect ratio, spatial distribution of the precipitates was measured in the naturally aged condition as well as in underaged, peak-aged and overaged samples. Micropillars were machined from grains in different orientations using a dual-beam FEG-FIB microscope (FEI Helios 600i) in samples with different precipitate structure and the critical resolved stress was determined by means of micropillar compression tests carried out in a nanoindenter (Hysitron TI950). The effect of the micropillar diameter was ascertained for each precipitate distribution by means of mechanical tests in micropillars with different diameters (in the range 3 to 10 μm). Micropillars with the minimum diameter to obtain size-independent values of critical resolved stress were then used to determine the strengthening provided by the different precipitate structures (either Guinier-Preston zones, q'' or q' precipitates) in samples oriented for single, double and multiple slip. In addition, the deformation mechanism were analysed by means of in situ micropillar compression tests within the scanning electron microscope as well as from the analysis by transmission electron microscopy of foils extracted from the deformed micropillars. The results of the mechanical tests (in terms of the critical resolver shear stress and of the deformation mechanisms) were compared with those obtained from classical Orowan models of precipitate strengthening as well as with the predictions provided by multiscale approaches based on either atomistics or discrete dislocation dynamics.

Keywords: Micropillar compression, Aluminium alloys, Precipitation, Critical resolved shear stress

*Speaker
†Corresponding author: barbara.bellon@imdea.org

Dislocation-phase boundary interaction – a Peierls-Nabarro Finite Element approach

Franz Bormann *† [1], Ron Peerlings [1], Marc Geers [1]

[1] Mechanics of Materials, Department of Mechanical Engineering [Eindhoven] (TU/e) – PO-box 513 5600 MB Eindhoven, Netherlands

Abstract

Interface decohesion due to dislocation activity in polycrystalline microstructures is a complex process that is not fully understood yet. To obtain a better insight in the underlying mechanisms we perform a numerical study of a simplified two-phase continuum microstructure. The model comprises a soft Phase A that is enclosed by a harder Phase B. Embedded in both subdomains lies a single glide plane which is continuous across the phase boundaries. Centred within Phase A we assume an edge dislocation source emitting dislocation dipoles under sufficiently high stress. On the remote boundary a shear stress is introduced that triggers dislocation nucleation and acts as a driving force for the dislocations. As a result of the phase contrast dislocations are obstructed at the phase boundary and pile up. Once the applied shear stress exceeds a certain threshold, i) a dislocation is transmitted into phase B or ii) a crack nucleates at the phase boundary. Other mechanisms such as dislocation reflection into phase A or dislocation nucleation at the phase boundary are not considered.

To investigate the dislocation-phase boundary interaction in such a two-phase microstructure a phase-specific and non-singular dislocation description is required. Hereto, we adopt the Peierls-Nabarro model [1] in a 2D plane strain finite element framework. Each phase is split into two linear elastic regions connected by the glide plane. Along the glide plane we employ a phase specific energy based interface model based on the Peierls-Nabarro model. It entails a periodic, and thus nonconvex, potential in terms of the disregistry between both regions to capture the effect of lattice periodicity. To capture crack nucleation at the phase boundary, an exponential cohesive zone law is introduced. As a result, the total free energy, which is comprised of the elastic strain energy plus the defect energy of the glide plane and of the phase boundary, is highly nonconvex. To solve this nonconvex energy minimisation problem in a numerically stable and computationally efficient manner we adopt the Truncated Newton method, along the lines proposed by Nash [2].

The proposed model provides a natural interplay between dislocations, external boundary conditions and phase boundary. Hence, the material and size dependent resistance against dislocation transmission is automatically included. The material dependency does not only relate to the long-range image stresses as derived by Head in 1953. It also arises from the change in glide plane properties across the phase boundary and the resulting change in resistance against glide. The origin of the size dependency lies within dislocation dipole self-stresses that are directly controlled by the size of Grain A. The numerical solutions obtained allow us to study the interplay between dislocations and interface decohesion as a function of material properties of bulk, glide plane and interface, as well as the current internal dislocation configuration.

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*Speaker

†Corresponding author: F.Bormann@tue.nl

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Keywords: Micromechanics, Dislocations, Peierls Nabarro model, FEM, Phase boundaries, Damage, Multi phase materials

Numerical solution of strain-gradient elasticity based on an immersed boundary B-spline framework

David Codony * [1], Onofre Marco [1], Sonia Fernández-Méndez [1], Irene Arias† [1]

[1] Universitat Politècnica de Catalunya [Barcelona] (UPC) – C. Jordi Girona, 31. 08034 Barcelona, Spain

Classical continuum theories are sufficient to model physical phenomena at the macro-scale. However, at the micron- and sub-micron scales, generalized continua theories are required in order to take into account size or length-scale effects. In the case of elasticity, such scales can be represented using the "strain-gradient elasticity" theory developed by Mindlin, where the elastic energy density depends on the strain, but also on its spatial gradient.
When this problem is formulated in terms of displacements, the governing partial differential equation is of fourth order. To numerically solve it, high-order ($C1$) continuity is required for the approximation of the solution, and therefore the usual Finite Element Method (FEM) is not suitable. Several alternatives can be found in the literature, such as Hermitian FEM, Mixed FEM or Meshfree Methods. These methods are relatively expensive: Hermitian and Mixed FEM circumvent the high-order continuity requirement at the expense of increasing the number of degrees of freedom of the problem, whereas Meshfree Methods use $C\infty$smooth basis functions which are difficult to evaluate and integrate, and which lead to frequent overlapping due to their global nature.

In this contribution, we propose a new method to efficiently solve the strain-gradient elasticity problem on arbitrary domain shapes, based on an Immersed Boundary B-spline approach. B-spline interpolation is based on smooth piece-wise polynomial basis functions, which maintain the number of degrees of freedom, avoid excessive overlapping and can be computed and integrated very efficiently. However, the B-spline basis is globally defined on a Cartesian-like grid, which hinders its use on arbitrary domain shapes. To overcome this, we consider the Immersed Boundary (IB) concept, where the domain is embedded into the fixed Cartesian mesh supporting the B-spline basis. A characteristic feature of IB approaches is that boundary conditions must be weakly enforced, since the mesh does not conform to the domain boundary. To this end, we consider the Nitsche's method, which is the consistent version of the classical penalty method. It permits also deriving an alternative setup of the boundary value problem with different boundary conditions, avoiding the additional constraints on non-smooth regions of the domain boundary arising in the classical Mindlin's theory.
We present the theoretical formulation of our strain-gradient elasticity approach based on the Nitsche's method, as well as the corresponding numerical scheme. We also derive the expression of the lower bounds for the penalty parameters that this method involves. Finally, we show some examples of numerical solutions on arbitrary domain shapes.

Keywords: Strain gradient elasticity, Bspline method, Immersed boundary method, Nitsche's method

*Speaker
†Corresponding author: irene.arias@upc.edu

Tiling concept in the RVE size determination: a step beyond Periodic Unit Cell in modelling heterogeneous materials

Martin Doškář * [1], Jan Zeman [1], Daniela Jarušková [1], Jan Novák [1]

[1] Czech Technical University in Prague (CTU) – Zikova 1903/4, 166 36 Prague 6, Czech Republic

The Representative Volume Element (RVE) and its size play an essential role in numerical homogenization and multi-scale analyses. Because the original Hill's definition of an RVE as a microstructural sample whose macroscopic response is insensitive to the adopted type of homogeneous boundary conditions is attainable only in the limit sense, an acceptable discrepancy threshold in the apparent properties must be introduced in order to define a practical, finite-size RVE. The RVE size is governed by the interplay of three factors: a geometrical composition of the investigated microstructure, a physical phenomena under investigation, and a contrast in thermo-mechanical properties of individual microstructural components. Consequently, recommendations on the RVE size are typically highly specific, keeping the methodology of the RVE size determination an open topic. The majority of current approaches rely on generating ensembles of gradually larger and larger realizations of an investigated microstructure and controlling statistics of the ensemble apparent properties. Such an approach features two bottlenecks: (i) the involved process of generating statistically similar microstructural samples, (ii) repetitive solutions to Boundary Value Problems (BVP) pertinent to the numerical homogenization.
We present a methodology for the RVE size determination that addressed the both bottlenecks, building on the representation of microstructural geometry by means of the abstract tiling concept. Our approach generalizes the concept of Statistically Equivalent Periodic Unit Cell (SEPUC). Instead to a single cell, geometrical characteristics of an investigated microstructure are attributed to a handful of domains with pre-defined mutual compatibility, which we describe adopting the formalism of Wang tiles. The approach decouples the generation of microstructural samples into the off-line and the on-line phase. In the computationally intensive off-line phase, the microstructure is compressed within a set of domains—tiles–using similar methods developed for designing a SEPUC. However, unlike SEPUC, tiles do not represent the investigated microstructure individually; only when the tiles are assembled into a tiling, placing side-by-side only the tiles compatible at the congruent edges, the assembled system resembles the investigated microstructure in terms of spatial statistics. In the on-line phase, random but statistically consistent microstructural realizations are reconstructed almost instantly with a simple stochastic assembly algorithm, making it particularly appealing for the outlined RVE size determination where multiple microstructural samples are required.

Additional advantage of the tiling concept stems from the inherent partitioning of the reconstructed microstructural samples, allowing us to relate the theoretical RVE to an infinite tiling and consider any finite-size tiling as a subdomain of the theoretical RVE. As a result, we can employ methods of statistical sampling to infer bounds on the homogenized properties and define the RVE size criterion. Finally, the repeating occurrence of individual tiles in the reconstructed samples allows for accelerated solution of the pertinent BVPs. Each tile is considered as a macro-element and factorized only once, at the beginning of the RVE size analysis. In the spirit of the Schur complement method, BVP of a microstructure realization then corresponds to a coarse grid problem composed of the macro-elements, resulting in significantly less unknowns.
We illustrate the methodology with the identification of the RVE size of three two-dimensional microstructural models: a microstructure with mono-disperse elliptic inclusions, foam, and sandstone.

*Speaker

Keywords: RVE size, microstructure reconstruction, Wang tiling

A volume-based aspiration method to estimate in-vivo soft tissues stiffness: evaluation of the device with silicone samples

Seyed Ali Elahi * [1], Nathanael Connesson† [1], Yohan Payan [1]

[1] Techniques de lÍngénierie Médicale et de la Complexité - Informatique, Mathématiques et Applications [Grenoble] (TIMC-IMAG) – Centre National de la Recherche Scientifique : UMR5525, Université Grenoble Alpes – Domaine de la Merci - 38706 La Tronche, France

Computer Assisted Medical Interventions (CAMI) involving soft tissues require devices that model such tissues in order to estimate the way they are going to be deformed and/or resected by the surgical gesture. The corresponding biomechanical patient-specific models require an estimation of the constitutive behavior of the soft tissues. Since the mechanical behavior of living tissues varies between *in-vivo* and *ex-vivo* conditions, it is important for the CAMI devices to offer an *in-vivo* estimation with non-traumatic measurements that should undergo sterile conditions. For this purpose, among all the methods proposed in the literature, aspiration/suction is the most widely used technique due to its simplicity and robustness.
For such a technique, a device with a hole is put in contact with the soft tissue while a negative pressure aspires part of this tissue. Knowing the relationship between the negative pressure and the aspired tissue height, an inverse problem is then solved to identify the material mechanical properties. In the literature, the apex height is usually measured with a camera and a mirror or a prism, which induces design difficulties, in particular in regards on the required sterilization process for *in-vivo* measurements. This paper introduces a new method that replaces the optical apex height measurement with a measurement of the aspired tissue volume. The method is referred to as "rate-based method". The camera, mirror and all electronic parts are not required, which makes our device the simplest, lightest and cheapest one could achieve. In particular, this simplification enables the system to meet the severe sterilizations constraints that can be present for some surgeries. Indeed, the proposed device is only composed of a cylindrical plastic chamber (with a hole at its basis), some connection tubes, a syringe pump, a manometer and an aspiration chamber. The idea is to aspirate the tissue inside the chamber using the syringe pump, while measuring the negative pressure and the corresponding removed volume. Such a volume is due to both the aspired tissue volume inside the chamber and the volume changes in the device (air expansion and elasticity of the connections, tubes, syringe, *etc.*). An off-line calibration process is defined to differentiate the volume changes due to tissue aspiration from the volume changes due to the compressibility of the device (tubes, connections, syringe).

Our device was evaluated with the estimation of the constitutive behavior of two bulk cylindrical silicone samples, one being slightly softer than the other one. For each silicone, thin flat samples were extracted to characterize their constitutive behavior using a classical traction experiment (MTS Criterion machine, Model 41) and an equibiaxial extension (bulge test). Such experiments respectively provide Young modulus of 16.82kPa and 24.87kPa for silicones #1 and #2.
The aspiration tests on each silicone sample were repeated nine times to check the reproducibility of the results. The inverse method to estimate the constitutive behavior assumed a hyper-elastic Gent model with material constants computed using an updated FE simulation. The results validate the ability of our method to discriminate the two silicones with equivalent Young moduli estimated to 18.35kPa and 26.52kPa for silicones #1 and #2.

*Speaker
†Corresponding author: nathanael.connesson@gmail.com

Keywords: Aspiration Method, In, vivo Measurement, Soft Tissues Characterization, Experimental Mechanics, Inverse Characterization

Micromechanical modeling of cleavage fracture on a pearlitic-ferritic steel

Jinshan He * [1], Junhe Lian† [1], Sebastian Münstermann [1]

[1] Department of Ferrous Metallurgy, RWTH Aachen University (IEHK, RWTH Aachen University) – Department of Ferrous Metallurgy, RWTH Aachen University, 52072 Aachen, Germany, Germany

Pearlitic-ferritic steels have wide applications in engineering structures such as nuclear pressure vessels, offshore facilities, etc., where a low ambient temperature is very likely to be met. At low temperatures, most steels with bcc crystal structure often experience unstable cleavage fracture failure at multiple sonic speeds with few prior plastic deformations, leading subsequently to catastrophic consequences [1]. Therefore, the safety assessment for cleavage fracture is of great importance for structure design and material selection. In our previous study [2], a general and reliable macroscopic model was proposed for the accurate prediction of cleavage fracture under different stress states and non-proportional loading condition. The model introduces a general strain-based description of microcrack initiation with stress-state dependency to the classical Orowan cleavage fracture model. The extension enhances the model applicability from the conventional steels, where stress-controlled crack propagation is the dominant cleavage fracture process, to the modern steels, in which the strain-controlled microcrack initiation is also critical for the cleavage fracture due to the high purity of these steels. Resulting from the statistical distribution of cleavage fracture, it utilizes the Weibull distribution to describe the strain scatter of microcrack initiation. The model reaches good predictive capability compared to other existing cleavage fracture models; however, due to its phenomenological character it also involves many material parameters that need to be calibrated by different experiments under low temperatures. This limits the easy use of the model and more importantly, it disconnects the material microstructure information from the cleavage fracture behavior description. Thus, a multiscale modeling approach is employed in this study to link the microstructural features with the phenomenologically determined material parameters in the macroscopic cleavage fracture model. In order to describe the microstructural features of the pearlitic-ferritic steel, numbers of simplified three dimension 200 μm x 200 μm representative volume element (RVE) models containing more than 100 grains are generated with statistical microstructure information, such as phase fraction and grain size distribution. To describe the plasticity behavior of ferrite and pearlite phase, two different approaches are implemented in this study. A phenomenological crystal plasticity (CP) constitutive law is employed for the ferrite grains and tensile tests of a pure ferritic steel containing similar ferrite microstructure information are applied to calibrating the CP parameters for ferrite. Owing to the complicated lamellae structure in pearlite colonies, mechanism-descriptive model is difficult to be implemented in finite element modelling for pearlite. Instead, its plasticity behavior is assumed homogeneous and isotropic described by the Mises yield criterion and an isotropic hardening law. The RVEs are subsequently loaded with different boundary conditions to achieve various stress states. In the study, the plane strain and equibiaxial tension conditions are applied as typical stress states for the RVE. Coupled with appropriate crack criterion of the perlite, the cleavage microcrack initiation strains for the macroscopic cleavage fracture model are successfully predicted by the micromechanical simulations. For better comparison, the microcrack initiation strains predicted by the micromechanical simulation and calibrated by the experiments are applied to two virtual experiments with the characteristic stress states. In addition, the phase fraction influence on cleavage fracture is also investigated with this approach.

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*Speaker

†Corresponding author: junhe.lian@iehk.rwth-aachen.de

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*Corresponding author
E-mail address: junhe.lian@iehk.rwth-aachen.de (Dr. Junhe Lian)

Keywords: Micromechanical modeling, cleavage fracture, Crystal plasticity

The effect of randomness at the micro-scale on failure of discontinuous composites

Joël Henry *† [1], James Finley [1], Soraia Pimenta [1]

[1] Department of Mechanical Engineering [Imperial College London] – South Kensington Campus London SW7 2AZ, United Kingdom, United Kingdom

Composite materials have several intrinsic sources of randomness at the micro-scale, related to the geometry of the microstructure, and to the micromechanical properties of the fibres, matrix, and interfaces. It has been widely accepted that these sources of randomness create weak regions in composites which eventually trigger their failure; for instance, longitudinal tensile failure of continuous-fibre composites is governed by the variability of fibre strength and triggered by the presence of weak-fibre clusters. However, there is a striking lack of studies that quantify how large and how weak these regions need to be, in order to significantly influence the failure of composites.
As composite microstructures become more complex, new sources of randomness are added to this problem; for instance, the location of fibre-ends in discontinuous composites and the intermingling of fibre-types in hybrid composites are in general random variables which may influence the failure of these materials. Consequently, this work aims to identify and quantify the sources of randomness which affect the final failure of hybrid and non-hybrid discontinuous composites. To do so, we use our recently-developed virtual testing framework for aligned discontinuous composites with one or more fibre types.

This modelling framework uses a shear-lag model to predict matrix failure, and Weibull statistics to predict fibre failure. Moreover, the model simulates a virtual specimen with individual fibres and matrix represented explicitly, thus allowing us to realise spatial distributions of fibre-types, fibre strengths, fibre-end locations, matrix strength, fibre diameters, etc. This model also uses a non-linear fracture mechanics criterion to identify the location, size and shape of the critical weak region triggering failure of the entire specimen. This allowed us to run Monte-Carlo simulations of specimens to determine the average characteristics of these weak regions.

The results obtained show how failure of aligned discontinuous composites is affected by the randomness of (i) fibre strength, (ii) the distance between the ends of neighbouring fibres, and (iii) intermingling of different fibre types (for hybrid composites). Our results show that, for aligned discontinuous composites with long fibres, variability in the fibre-strength is a critical factor for failure of the composite, as failure is initiated in 4-fibres clusters which are 20% weaker than the average in the composite. On the contrary, failure of composites with short fibres is governed not by fibre-strength, but by the variability in the distance between fibre-ends, as the composite tends to fail in clusters of 9 fibres in which the fibre-ends are 18% closer to each other than average. Finally, it is also concluded that failure of hybrid composites is triggered by small clusters of the low-elongation fibre-type, and that a random allocation of fibre-types within a specimen leads to a strength reduction of over 26% compared to a specimen with perfect intermingling of fibre-types.
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Keywords: discontinuous composites, hybrid composites, virtual testing, failure, variability

*Speaker
†Corresponding author: joel.henry13@imperial.ac.uk

Modeling deformation twinning in the framework of gradient crystal plasticity with focus on Mg single crystal

Edgar Husser * [1], Swantje Bargmann [2]

[1] Hamburg University of Technology, Institute of Continuum Mechanics and Material Mechanics (TUHH) – Eißendorfer Str. 42, 21073 Hamburg, Germany
[2] Chair of Solid Mechanics, University of Wuppertal – Germany

Magnesium (Mg) alloys have attracted considerable attention in the early past due to its high capability for a variety of industrial lightweight applications. Still, the technological potential of Mg-based alloys has not been fully utilized. For that reason, there is a great interest in understanding the mechanical behavior of the primary metal. The complex deformation behavior is strongly influence by deformation twinning. In Mg, tensile twinning represents an essential mode of deformation which must be exploited for targeted improvement of ductility in Mg alloys. In this respect, it is essential to understand the associated twin formation mechanisms which can be categorized in three stages: twin nucleation, propagation (lateral elongation), and growth (transverse thickening). On the basis of a well-established gradient crystal plasticity framework, deformation-induced twinning is consistently incorporated in terms of dissipative-like processes including the associated lattice reorientation. A nucleation criterion is proposed which considers the natural competition between slip and twinning in a continuum sense. The morphological characteristics of twinning in terms of twin band formation and growth are modeled by a non-local approach. As an exemplary case study, microcompression of Mg single crystal favored oriented for activation of {1 0 -1 2}-tensile twins is investigated. Numerical results are quantitatively compared against experimental data.

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Keywords: twinning, strain gradient, Magnesium

*Speaker

Constitutive modeling of strain-induced crystallization based on the analytical network averaging concept

Vu Ngoc Khiêm * [1], Mikhail Itskov [2]

[1] Department of Continuum Mechanics, RWTH Aachen University (KM RWTH) – Kackertstr.9 52072 Aachen, Germany
[2] Department of Continuum Mechanics, RWTH Aachen University (KM RWTH) – Kackertstr. 9, 52072 Aachen, Germany

The high regularity of the side group orientations in polymer chains allows natural rubbers to crystallize when undergoing deformation. Strain-induced crystallites are supposed to play an important role in the elastomer reinforcement and enhance the resistance to crack growth in natural rubbers. To date, the microsphere concept has been extensively used in constitutive modeling of strain-induced crystallization. However, large errors in the stress-strain relation of microsphere models due to the numerical integration over the unit sphere have been reported recently (see e.g. Khiêm and Itskov, 2016). In this contribution, we present a physically-motivated full network model for strain-induced crystallization in natural rubbers on the basis of the generalized analytical network-averaging concept (Khiêm and Itskov, 2016). The theory assumes the existence of a distribution function of polymer subnetworks in the rubber matrix. Under deformation, the spatial alignment of subnetworks in the stretching direction introduces the stress hardening into the model. By this means, the averaged deformation fields and the evolution of crystallinity can be both computed analytically. The proposed model includes very few physically motivated material constants and is compared with experimental data of strain-induced crystallization in natural rubbers. Good agreement is obtained with respect to all measurable experimental values.

Khiêm, V. N., and Itskov, M., 2016. Analytical network-averaging of the tube model: Rubber elasticity, *Journal of the Mechanics and Physics of Solids* **95**, 254–269.

Keywords: Natural rubber, Analytical network averaging, Phase transition, Crystallization kinetics

*Speaker

Light-guided Topographical Switching of Azobenzene-functionalized Liquid Crystal Polymers

Ling Liu * [1], Patrick Onck [1]

[1] Micromechanics of Materials, Zernike Institute for Advanced Materials, University of Groningen – 9747 AG Groningen, Netherlands

Liquid crystal (LC) polymers co-polymerized with ultra-violet (UV) sensitive azobenzenes can respond to light through an anisotropic conformational change [Liu & Onck, PRL, 2017, 057801].
This deformation can be employed to generate light-triggered surface texture modulations on liquid crystal polymeric films, in order to create controllable friction and wetting properties [Liu, et.al., PNAS, 2015, 3880].
In this presentation, an overview of a recent computational analysis and study of this peculiar light responsive system is given.
Taking advantage of the self-assembling nature of liquid crystals, various surface textural modifications can be achieved by patterning the LC molecular orientation.
Diverse topographical changes were generated under diffuse light exposure, featuring an alternating undulatory profile, a randomly corrugated modulation or a serpentine "fingerprint" texture, due to distinct pre-designed molecular distributions inside the films.
In addition to on-off switching, a rotating polarized UV light input source can give rise to travelling-wave-like surface deformations, which can be applied to generate fluid propulsion or cargo transportation.

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Liu, L. & Onck, P. R. Enhanced Deformation of Azobenzene-Modified Liquid Crystal Polymers under Dual Wavelength Exposure: A Photophysical Model. Physical Review Letters 119, (2017).

Keywords: liquid crystal polymers, light, sensitive materials, functional surfaces, topographical switching

*Speaker

Computational micromechanics and homogenization of anisotropic polyurethane foams

Mohammad Marvi Mashhadi * [1,2], Claudio Lopes [1], Javier Llorca [2,1]

[1] IMDEA Materiales – C/ Eric Kandel, 2, Tecnogetafe, 28906 Getafe, Madrid, Spain
[2] Department of Materials Science, Polytechnic University of Madrid/Universidad – Politecnica de Madrid, E. T. S. de Ingenieros de Caminos. 28040 - Madrid, Spain, Spain

This work reveals an accurate modelling and simulation strategy for PU foams taking into account the anisotropy of its microstructure. Towards this end, the mechanical behaviour of closed-cell PU foams with different degrees of anisotropy has been modelled through computational homogenization using finite element simulation of a representative volume element (RVE). Laguerre tessellation was used to create the 3D geometry of PU foam, including cell edges and cell walls, according to the cell aspect ratio that represents the anisotropy of microstructure. Micromechanical characterization revealed the microstructure features of foams such as cell size distribution, cell anisotropy, cell wall thickness and strut shape. These features have been carefully implemented in the generated RVEs. The mechanical properties of the bulk PU, constituting the cell walls and cell edges, were obtained by means of in-situ nanoindentation. The predicted values for the homogenized foam stiffness and strength are in good agreement with experimental measurements. The higher mechanical performance of foams along the direction of cell elongation is well captured by the models. A deeper study on deformed RVEs showed that the struts present a higher potential to carry the loads before buckling when they are preferentially aligned with the loading direction.

Keywords: Experimental micromechanics, anisotropic polyurethane foam, computational homogenization

*Speaker

Quantification of shear flexoelectricity in ferroelectrics

Alice Mocci * [1], Amir Abdollahi [1], Irene Arias† [1]

[1] Universitat Politècnica de Catalunya [Barcelona] (UPC) – C. Jordi Girona, 31. 08034 Barcelona, Spain

It is well known that electric polarization can be generated by deforming a special class of materials called piezoelectrics. A relatively recent discovery is that electric polarization can also be generated by bending any dielectric material, irrespective of its symmetry. This effect is called flexoelectricity and it is an electromechanical coupling between polarization and strain gradient. It is known that besides bending, strain gradients can also be generated by applying torsion. However, the flexoelectric effect under torsion is still to be investigated and it may provide a means to quantify the poorly characterized shear component of the flexoelectric tensor. In this work, we develop a general formulation based on torsion mechanics to quantify the shear flexoelectric response in different crystal symmetry groups, particularly focusing on ferroelectric materials which exhibit strong flexoelectric effects. We show that only a non-uniform and non-circular beam is able to generate a non-zero electric polarization in ferroelectrics due to shear flexoelectricity. However, the deformation of a non-circular beam under torsion is highly complex and the general torsion formulation is not appropriate in this case for quantifying shear flexoelectricity. To tackle this complexity, we resort to a self-consistent model of flexoelectricity $[1, 2]$ able to simulate the coupled electro-mechanical deformation of a three-dimensional non-circular beam under torsion. We use a maximum entropy mesh-free method with basis functions exhibiting C^{∞} smoothness, to address the high-order nature of the flexoelectric equations. Simulation results suggest a relationship between the actual and analytical polarization fields. Finally, and based on this relationship, we develop a formulation to quantify the shear flexoelectric coefficient in ferroelelctrics.

Keywords: Ferroelectrics, Shear flexoelectricity, Coupled problems.

*Speaker
†Corresponding author: irene.arias@upc.edu

Atomistic-continuum coupling of random alloys

Shankha Nag * [1], William Curtin [1]

[1] Laboratory for Multiscale Mechanics Modeling, École polytechnique fédérale de Lausanne (LAMMM, EPFL) – CH-1015 Lausanne, Switzerland

Random alloys are multicomponent systems where the atomic type on each lattice site is uncorrelated. Such systems have statistical fluctuations in local atomic configurations and properties, which prevents accurate application of standard atomistic/continuum coupling methods. In this study, two methods for atomistic/continuum coupling that mitigate errors are proposed, studied, and validated. In one method, a fully-relaxed atomistic sample, with atoms displaced from the perfect lattice sites, is carved out of a larger random sample. The outer atoms of the atomistic sample then (i) define nodal positions from which an outer continuum model is constructed and (ii) serve as so-called pad atoms that move with the continuum nodes and transmit forces onto the atoms in the inner atomistic domain. This method ensures no spurious stresses at zero loading, and only small spurious stresses arise under loading. A second method replaces the pad atoms and two layers of real atoms with "average" atoms that, in principle, match the average bulk lattice and elastic constants of the random alloy. This method effectively separates the random/homogeneous boundary from the atomistic/continuum boundary, avoiding the serious errors that arise when the two boundaries are at the same position. This method creates small spurious stresses under zero load, due to small mismatches in the actual properties of the "average" atoms as compared to the real atoms, and small additional spurious stresses under applied load. The two methods are examined for three different solid solution alloys (dilute Al-5%Mg, Ni-15%Al, and medium entropy FeNiCr, all described by EAM interatomic potentials). Spurious errors for both methods and across all three materials are small ($\approx$ 10MPa) up to applied strains of 10–3, beyond which non-linear effects enter. These methods enable the accurate study of mechanics boundary value problems in random alloys for problems where it is essential to capture atomistic phenomena in some localized region of the sample.

Keywords: random alloys, atomistic/continuum coupling

*Speaker

Experimental characterization of the local mechanical property gradients in thermo-oxidized polymers and polymer matrix composites

Marina Pecora * [1], Olga Smerdova [2], Marco Gigliotti [2]

[1] Institut Pprime (PPRIME) – CNRS : UPR3346, Université de Poitiers, ENSMA, Université de Poitiers, ENSMA – ISAE-ENSMA - Teleport 2 1 Avenue Clement Ader - BP 40109 F86961 FUTUROSCOPE CHASSENEUIL Cedex, France
[2] Institut Pprime (PPRIME) – CNRS : UPR3346, Université de Poitiers, ENSMA – ISAE-ENSMA - Teleport 2 1 Avenue Clement Ader - BP 40109 F86961 FUTUROSCOPE CHASSENEUIL Cedex, France

The growing use of polymer-matrix composites in aircraft structures leads to the need of understanding the degradation phenomena occurring due to their exposure at elevated temperatures. For "warm" temperatures, the main degradation phenomena are related to thermo-oxidation of the polymer matrix that promotes the formation of a dark brittle oxidized layer on the sample surface. Depending on the aging conditions and the type of polymer material, the oxidized layers can reach a thickness of several hundreds of microns. A convenient way to study the gradients of mechanical properties induced by thermal oxidation is the instrumented indentation test at the relevant scale [1]. However, the classical indentation procedure [2] used in previous studies is not able to capture the viscous nature of the polymer behaviour. In this work, the local mechanical behaviour of thermally aged polymers and polymer composites has been investigated through the use of a cyclic indentation loading method. By this method, it is possible to emphasize several aspects of the time-dependent material behaviour. The aging of PR520 epoxy bulk resin and carbon fiber based composite samples has been characterized by Ultra-Micro Indentation by a force-controlled Fischerscope H100C equipment. The material was aged at 150◦C, in air at atmospheric pressure up to 1000 hours and under pure oxygen environment at a pressure of 2 bar, to accelerate the oxidative aging.
Firstly, the oxidized layer of aged bulk polymer samples have been characterized at different distances from the external surface. From load-displacement curves, a change in the mechanical response of the polymer due to aging can be observed. In particular, the mean displacement (ratcheting) is lower close to the surface, and similar to that of the virgin material at the sample core. The Elastic Indentation modulus (EIT) calculated at each cycle, is higher at the surface. The irreversible work of indentation, characterizing a part of the time-dependent behaviour, is rather similar for aged and virgin polymers except the first cycle.

The cyclic indentation method is then applied to the surface and along the thickness of aged polymer composite samples. In the case of virgin samples, the Elastic Indentation Modulus of in-situ resin is slightly higher (less than 1%) than that of the bulk material. For tests carried out on the surface of aged samples the difference is of about 20%.

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Keywords: Ultra, Micro Indentation, Polymers, Polymer, matrix composites, Thermal ageing

*Speaker

Impact of machine stiffness and heat treatments on crack propagation instabilities in an Al-Mg-Si alloy

Tom Petit * [1,2], Claire Ritter [1], Jacques Besson [2], Thilo Morgeneyer [2]

[1] CEA Saclay (CEA) – Commissariat à l'énergie atomique et aux énergies alternatives – 91191 Gif-sur-Yvette cedex, France
[2] Centre des Matériaux (MAT) – CNRS : UMR7633, MINES ParisTech - École nationale supérieure des mines de Paris – Centre des matériaux P. M. Fourt RN 447 - BP 87 91003 EVRY CEDEX, France

This study investigates rapid but limited crack propagation associated with a sudden decrease in load sometimes observed during fracture toughness tests. This phenomenon is often referred to as "pop-in". Tests are performed on an age hardened aluminum alloy subjected to various heat treatments to obtain various metallurgical states. Longer aging is shown to lead to pop-ins. The effect of specimen geometry and mechanical loading on pop-in behavior is studied by varying the test machine stiffness using an innovative setup to vary the system compliance. The final objective is to model this phenomenon using finite-element analysis.
Limited rapid crack extension and arrest (so called pop-in) is reported in fracture toughness tests on various materials: low alloyed steel, welded joints, aluminum. It is often associated with a sudden decrease in load. This phenomenon is little studied in the literature and only few authors provide explanations. In steels, pop-in is often linked with the presence of a local brittle zone (LBZ). In welded joints, pop-in significance has been reported to depend on the loading mode. For aluminum alloys, pop-in is reported to be either related to dynamic strain aging or to microstructural features such as clusters of coarse precipitates. In that case, clusters act as weak spots with a local low toughness although the overall behavior remains ductile.

In order to provide more insights in pop-in phenomenon and its potential link with microstructural features, this study focuses on the behavior of an aluminum alloy with the objective to develop modeling tools. These aim at providing a practical assessment procedure which is of pop-in significance in structural integrity assessment. The 6xxx aluminum alloy series (Al–Mg–Si) ranks among the most versatile of the age hardened aluminum alloys. A 6061 alloy in the reference metallurgical heat-treated state -T6-, with optimal structural hardening (nanoprecipitation of Mg2Si) and good mechanical properties was used. Various heat treatments were performed on six material blocks (136x76x87 mm3) to investigate different metallurgical states. Investigations were based on fracture toughness tests and on microstructural characterizations.

Tensile and compact tensile specimens were machined from blocks which were subjected to homogenization, hot forging, solution annealing (4 h at 530 or 550 ∘C), water quenching and isothermal ageing (4 or 8 or 12 or 16 h at 175 ∘C) heat treatments. Tensile and fracture toughness tests (monotonic and with partial unloading) have been performed. The observed mechanical behavior was correlated to metallurgical characterizations in two dimensions (scanning electron microscopy, EBSD, profilometer) and three dimensions (tomography, synchrotron laminography, atom-probe tomography).

The results show an influence of the increase of solution annealing temperature only on tensile properties (increase of yield and tensile strength) and an influence of ageing time on both tensile and fracture toughness properties. Increasing the ageing time reinforces the yield and tensile strength. For 4 and 8 hours of ageing time the material investigated does not show pop-in occurrence whereas pop-in is observed on 50% of specimens after 12 hours and on 100% after 16 hours.

3D scans were made via synchrotron laminography (ESRF, France) on flat specimens extracted from a CT

*Speaker

specimen, containing a stopped crack. Reconstructions show very rough crack surface and the heterogeneous presence of large clusters of porosity at the crack tip.
An innovative assembly has been designed in order to vary machine compliance during a toughness test. It is shown that the appearance of pop-in is related to the competition between crack growth toughness and the double system stiffness (contributions of machine and specimen). An instability criterion has been investigated by an energy approach.

Keywords: ductile fracture, aluminum, instability, fracture toughness, crack propagation, fracture mechanisms, J integral

Influence of viscosity and plasticity on the chemical reaction front propagation in solids

Svetlana Petrenko * [1,2], Eric Charkaluk [1], Alexander Freidin [2,3]

[1] Laboratoire de Mécanique des Solides – Ecole Polytechnique Université Paris Saclay – UMR 7649, CNRS, Ecole Polytechnique, Palaiseau, France
[2] Institute for Problems in Mechanical Engineering of Russian Academy of Sciencies – Bolshoy Pr., 61, V.O., St. Petersburg, 199178, Russia
[3] St. Petersburg Polytechnic University – Polytechnicheskaya Str., 29, St. Petersburg, 195251, Russia

Establishing relationships between chemical transformations and the stress-strain state became particularly urgent in recent decades due to the increasing use of micro- and nano-sized structural elements in microsystems technology and due to stricter requirements for predicting the lifetime of structural elements under conditions of joint thermomechanical and chemical effects.

Stress-controlled chemical reactions are also elements of technological processes. This makes to be necessary the development of theoretical basis for example for the control of the silicon oxide size and geometry of silicon micro and nano structures used in microelectronics.

Usually stress-controlled processes are accompanied by significant changes in volume. This expansion leads to internal stresses which in turn affect the kinetic of the oxidizing process. The influence of external and internal stresses on the reaction front kinetics was examinated by many researches and some models have been developed. To take into account stress effects, these models proposed stress dependent chemical reaction parameters: surface reaction rate, oxidation diffusivity, oxide viscosity and etc., but the dependencies of parameters on stresses were introduced heuristically.

Our approach to studying the influence of stresses and strains on the kinetics of a propagating chemical reaction front is based on the expression of the chemical affinity tensor $[1, 2]$ and formulation of the kinetic equation on a form of the reaction front dependence on the normal component of the affinity tensor. This allow us to incorporate stresses into the model in a natural manner. In previous studies this approach was used for the problems on spherical $[3]$ reaction fronts in which the solid constituents were linear elastic.

In this work we focus of the effects of linear and non-linear viscosity and plasticity of the reaction products. We consider a linear elastic sphere subjected to a homogeneous external all-round loading. The chemical reaction starts at the outer surface of the sphere, the propagation front is spherical and the reaction sustained by the diffusion of the gas through the transformed material. We consider three cases for different transformed material: linear visco-elastic, non-linear visco-elastic and elasto-plastic. We find stresses in each case taking into account the kinetic equation that determines the reaction front velocity on the normal component of the chemical affinity tensor that in turn depends on stresses and strains at the reaction front. We compare all three cases and the solution for the elastic reaction product with each other and we study in details how viscosity and plasticity affect the velocity of the reaction front propagation.

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*Speaker

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Keywords: Mechanochemistry, Thermomechanics, Chemical affinity tensor

Molecular dynamics simulation of stress distribution in 2D systems

Robert Pezer [1], Ivan Trapić [*†] [2], Jurica Sorić [2]

[1] University of Zagreb Faculty of Metallurgy (UniZgSiMet) – Aleja narodnih heroja 3 HR 44103 Sisak, Croatia
[2] University of Zagreb Faculty of Mechanical Engineering and Naval Architecture (UniZgFSB) – Ivana Lučića 5 10002 Zagreb, Croatia

The need to produce down to atomistic scale accurate representations of mechanical deformation processes has been ever more and more important to power up new solutions to tackle modern technology challenges. Standard elastic theories within continuum mechanics approach provide a well-established framework to do practical engineering simulations at the macro scale with wide range of applications. One of the most promising techniques to scale resolution down to the nanolevel is molecular dynamics simulations (MDS). In this work stress distribution around circular opening has been analyzed in the atomistic model of single layer 2D atomistic system, with atom interactions described by realistic interaction potential. Calculations were conducted on the problem of stress distribution around the elliptic hole in 2D sheet subject to uniaxial loading. Results for atomistic stress, calculated as spatial average by using Hardy formulation. One of the goals in this research is development of the efficient switching adaptive mechanism for local continuum to atomistic simulation transition. Quantitative measure for local switching suitable for fast calculation in multiscale simulation is proposed. As an example we provide calculation results in graphene where we have plenty of benchmark data. We point out routes to the development of the fully physically driven strategy for continuum to atomistic coupling where computationally expensive MDS is triggered upon local conditions identification. MDS is run up to the fracture of graphene with investigation of the structural changes in relation to the various conditions like temperature and loading rate.

Keywords: molecular dynamics (MD), stress distribution, materials length scales

*Speaker
†Corresponding author: ivan.trapic@fsb.hr

On the compressibility of rubber: experiments and theoretical considerations

Robert Plachy *† [1], Stefan Scheiner [1], Krzysztof Luczynski [2], Armin Holzner [2], Christian Hellmich [1]

[1] Vienna University of Technology (TU Wien) – Austria
[2] Semperit Technische Produkte GmbH – Austria

Accurate computational simulation of the flow behavior of (unvulcanized) rubber is believed to significantly improve the efficiency in the manufacturing of extrusion dies. However, despite considerable ongoing and previous efforts, this task remains an open challenge. Evidently, one of the reasons for this unsatisfactory situation is insufficient consideration of, or knowledge on, the mechanical compressibility of the extrudate material. Aiming for shedding light on the compressibility of (unvulcanized) rubber, three different types of specimens, namely one natural rubber and two EPDM (ethylene-propylene-diene-monomer) rubber compounds, were tested under hydrostatic loading in a capillary rheometer with closed extrusion canal, and the resulting hydrostatic pressures and volume changes were recorded. In order to consider possible dependencies on loading speed, maximum pressure and overall loading time, those factors were varied in the course of the testing campaign. The volume changes then entered various relevant strain measures (Green-Lagrange strains, Hencky strains, linearized strains), while the pressures were mathematically transformed into energetically conjugate stress measures (second Piola-Kirchhoff stress, Kirchhoff stress, Cauchy stress). Insertion of these measures into the dissipation inequality resulting from the two fundamental laws of thermodynamics, revealed that the investigated materials behave purely elastically under hydrostatic pressure, albeit in a non-linear fashion. It could also be shown that, irrespective of the format chosen for elasticity theory, the elastic bulk modulus relates to the hydrostatic pressure via a power function – with the bulk modulus gradient decreasing with increasing hydrostatic pressure (although an asymptote could not be found). Further variation of testing parameters also revealed a dependence of the bulk modulus from changes of temperature, with the former decreasing when the latter is rising. Statistical evaluation of the corresponding power law coefficients allowed for derivation of upper and lower bounds of the bulk modulus as functions of the hydrostatic pressure (and of the temperature). In the future, the new constitutive relations revealed in this work, describing the compressibility behavior of (unvulcanized) rubber allow, on the one hand, for improving the accuracy of rubber extrusion simulations, and, on the other hand, for optimized material characterization in terms of the number of required tests per material.

Keywords: unvulcanized rubber, pressure and temperature dependent compressibility, statistical confidence intervals, sample identification

*Speaker
†Corresponding author: robert.plachy@tuwien.ac.at

Seal Ring Toughness Characterization: A modified Four-Point Bending Method for Crack Front Monitoring

Idir Raid *† [1], Rafael Estevez [2], Sébastien Gallois-Garreignot [1], Vincent Coutellier [1]

[1] STMicroelectronics – STMicroelectronics (FRANCE) – STMicroelectronics, 850 rue Jean Monnet, 38926 Crolles Cedex, France, France

[2] SIMaP – Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, F-38000 Grenoble, France. – Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMAP, 38000 Grenoble, France, France

A Seal Ring (SR), or commonly referred at as crack-stop (CS), is a key structure contributing to a chip's mechanical reliability. In few words, it consists on a copper structure surrounding a chip, protecting it from any exterior chemical and physical aggressions. However, the quantification of its toughness remains problematic and often relies on an empirical optimization. That is why this poster aims to present a developed experimental method to characterize such a structure's toughness when it comes to prevent a crack growth.
To do so, four-point bending (FPB) tests were used as experimental approaches to initiate and propagate a crack in the interconnect levels of interest. The method was used on four different chips with different SR structures, *i.e.* different Back-End of Line (BEoL) stacks and materials. Each sample is composed of a matrix of several dies (each kind of die is evaluated separately) of different size. Once the experimental method set up following [1], force vs. displacement curves had to be interpreted as important force drops were noticed. The point was to correlate such drops to SRs locations on the tested samples. At first, the strategy was to perform scanning acoustic microscopy (SAM) on several samples in order to match the number of force drops to the SRs that the crack grew through. However, this method could give partial information about the last force drop only. Thus, a modified FPB set up was used in order to monitor the crack growth in real time by replacing the silicon counter-place by a glass one.

The experimental set appeared to be steady and robust in that about 100% of the tested samples show that delamination occurred in the interconnect levels no matter the considered stack. This has been validated by Focused Ion Beam & Scanning Electron Microscopy (FIB-SEM) analyses. Additionally, SAM observations highlight the presence of several fringes indicating an incremental crack growth, as suspected, following the several force drops observed in the Force-Displacement curve. After the tests, the crack front was also observed close to the Seal Ring structures, even if some variability has been found on this item.

Furthermore, the Through Glass Inspection (TGI) allowed to correlate force drops to the crack front positions and thus to confirm the fact that after a certain crack length, the front grew from a SR to another. Indeed, due to the copper properties, crack propagation is stopped, or at least, slowed in proximity of copper structure inducing specific force vs. displacement signature. Similar behaviour has been observed by [2-3-4].

This work investigates the behaviour of crack stop structure during a FPB test. Experimental observations are provided to highlight the mechanisms induced during a crack propagation towards such structure. The crack path and kinetic are discussed in order to provide deeper understanding of the phenomena enabling further optimization of crack stops.

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*Speaker
†Corresponding author: idir.raid@st.com

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Keywords: Four, Point Bending, Through Glass Inspection, Crack, Stop, Crack Growth Monitoring

Influence of UV aging on the mechanical properties of polycarbonate

Sonya Redjala *† [1,2], Nourredine Aït Hocine‡ [3], Michel Gratton [4], Nathalie Poirot [5], Rabeh Ferhoum [2], Said Azem [6]

[1] Laboratoire de Mécanique et Rhéologie, INSA Centre Val de Loire (LMR, INSA CVL) – Institut National des Sciences Appliquées (INSA) - Centre Val de Loire : INSA- CVL – 3 rue de la Chocolaterie, BP 3410, 41034 Blois, France, France
[2] Le Laboratoire Élaboration et Caractérisation des Matériaux et Modélisation, Université Mouloud MAMMERI de Tizi-Ouzou (LEC2M, UMMTO) – BP 17, Tizi-Ouzou 15000, Algérie, Algeria
[3] INSA Centre Val de Loire, Laboratoire de Mécanique et Rhéologie (LMR, INSA CVL) – INSA - Institut National des Sciences Appliquées – 3 rue de la Chocolaterie, CS 23410 – 41034 Blois cedex, France
[4] INSA Centre Val de Loire, Laboratoire de Mécanique et Rhéologie (LMR, INSA CVL) – INSA - Institut National des Sciences Appliquées – 3 rue de la Chocolaterie, BP 3410, 41034 Blois, France, France
[5] Groupe de Recherche en Matériaux, Microélectronique, Acoustique et Nanotechnologies; Université de Tours - CNRS - INSA (GREMAN, IUT de Blois) – INSA Centre Val de Loire – 15 rue de la chocolaterie, 41000 Blois, France, France
[6] Laboratoire Elaboration et Caractérisation des Matériaux et Modélisation, Université Mouloud MAMMERI de Tizi-Ouzou (LEC2M, UMMTO) – BP 17, Tizi-Ouzou 15000, Algérie, Algeria

Polycarbonate (PC) is a promising polymer with high transparency in the range of the visible spectrum and is used in various fields, for example medical, electronic, automotive. Its low weight, chemical inertia, high impact resistance and relatively low cost are of major importance.
In recent decades, some materials such as metals and ceramics have been replaced by polymers because of their superior advantages. However, some characteristics of the polymers are highly modified under the effect of ultraviolet (UV) radiation and temperature. The changes induced in the material by such aging depend on the exposure time, the wavelength of the UV radiation and the temperature level. The UV energy is sufficient to break the chemical bonds leading to a cleavage of the molecular chains. This causes changes in the mechanical, thermal, optical and morphological properties of the material.

The present work is focused on the study of the effects of aging under ultraviolet (UV) radiation and under different temperature values on the physical-chemical and mechanical properties of a PC. Thus, various investigations, such as FTIR and XRD analyses, SEM and optical microscopy observations, micro-hardness measurements and monotonic and cyclic tensile tests, were carried out on the PC in the initial state and after aging.
Results have shown the impact of aging on the properties of the PC studied. In fact, the MEB highlighted changes in the superficial morphology of the material by the presence of cracks and material de-bonding in the form of debris. The FTIR spectra reveal an attenuation of the peaks like the hydroxyl (OH) groups located at 3520 cm-1. The XRD lines shift towards a larger angle, reaching a maximum of 3○. In addition, Vickers micro-hardness measurements show that aging affects the surface and the core of the material, which results in different mechanical behaviours under monotonic and cyclic tensile tests. This study pointed out effects of aging on the macroscopic properties of the PC studied, in relationship with its microstructural changes.

Keywords: Polycarbonate, UV aging, temperature aging, physical, chemical properties, mechanical properties.

*Speaker
†Corresponding author: radjalasonya@gmail.com
‡Corresponding author: nourredine.aithocine@insa-cvl.fr

Discrete Dislocation Dynamics Simulation of Dislocation/Precipitate Interaction in Al-Cu alloys

Rodrigo Santos * [1], Laurent Capolungo [2], Javier Segurado [3,4], Javier Llorca [4,5]

[1] IMDEA Materials Institute – Spain
[2] Materials Science and Technology Division, Los Alamos National Laboratory (LANL) – Los Alamos, NM 87544, USA, United States
[3] Department of Materials Science, Polytechnic University of Madrid, Madrid – Spain
[4] IMDEA Materials Institute – Getafe, Madrid, Spain, Spain
[5] Department of Materials Science. Polytechnic University of Madrid. Madrid, Spain – Spain

Precipitation hardening is the most effective strengthening mechanism in many metallic alloys. The precipitates act as obstacles to dislocation glide in the slip planes, which have to overcome the precipitates by the formation of an Orowan loop. The increase in the critical resolved shear stress for dislocation motion has been traditionally analyzed by means of the Orowan model, which assumes a constant line tension model for the dislocation to compute the critical resolved shear stress necessary to overcome a periodic array of spherical precipitates. Later developments included the effect of the interaction stresses between dislocation segments but their predictions cannot provide accurate quantitative estimations of the hardening because many important parameters that influence the dislocation/precipitate interaction are not accounted for. They include the actual size, shape and crystallographic orientation of the precipitates, the anisotropy, the image stresses arising from the modulus mismatch between the alloy and the precipitate as well as the complex stress field around the precipitates due to the misfit and stress-free transformation strains.

This paper presents a comprehensive multiscale modelling strategy based on DDD to study precipitation strengthening. The methodology is applied to Al-Cu alloys but it is general and can be extended to any other metallic alloy. The details of the Theta' (Al2Cu) precipitates (size, shape and orientation) as well as the stress-free transformation strains around the precipitate were obtained in a previous investigation by the coupling of ab initio and atomistic simulations with computational thermodynamics and phase-field models [1] and were in good agreement with the experimental data. In addition, the elastic constants and the dislocation mobility laws were obtained from ab initio and atomistic simulations, respectively, and this information was used to determine the actual mechanisms of dislocation/precipitate interaction in this system by means of discrete dislocation dynamics (DDD) simulations in which all the relevant physical processes were accounted for. The DDD simulation is based in the Discrete Continuous model coupled with the fast Fourier transform method [2] to obtain the mechanical fields and solve the boundary value problem in the simulation box. In particular, the influence of the precipitate shape, orientation, modulus mismatch and stress-free transformation strain on the dislocation/precipitate interaction mechanisms was analyzed in Al-Cu alloys strengthened with Theta' precipitates and their influence on the critical resolver shear stress was determined and compared with the predictions of the classical models for dislocation/precipitate interaction.

Keywords: Dislocation dynamics, precipitate strengthening, multiscale modeling

*Speaker

A Multi-Scale Method for Non-Linear Mechanical Behavior of Nano-Structures Based on Coarse-Grained Model

Seyedeh Melika Vokhshoorikoohi *† [1], Amir Khoei [2], Mohsen Jahanshahi [1]

[1] School of Engineering, Sharif University of Technology, International Campus – Amirkabir Sq. Kish Island Postal Code: 79417-76655, Iran

[2] Center of Excellence in Structural and Earthquake Engineering, Department of Civil Engineering, Sharif University of Technology, P.O. Box. 11365-9313, Tehran, Iran. – Iran

The ever-increasing growth of Nanotechnology has elevated the necessity for the development of new numerical and computational methods that are better capable of evaluating systems at this scale. The existing techniques, such as Molecular Dynamics Methods, in spite of being fully capable of evaluating nanostructures, lack the ability to simulate large systems of practical size and time scales. Therefore, in order to be able to provide a realistic simulation of a large model, simulation of which is limited by the computational cost of the current molecular dynamics methods at hand, Coarse-Graining technique has recently become a very effective and beneficial method which refers to development of simplified models of molecular systems with reduced number of degrees of freedom which is achieved by reducing the number of interaction sites, resulting in a model that is computationally less expensive than the original atomistic model. Up until recently, the coarse-grained models have only been used to simulate large biomolecules such as proteins, lipids, DNA, and polymers since they consist of massive and complex structures which make them impossible to be modeled by previous molecular methods available. However, in this research, we have focused on applying the Iterative Boltzmann Inversion Coarse-Graining Technique to FCC metal crystal structures in order to be able to simulate larger models of practical size, modeling of which would be time and energy consuming by the molecular dynamics methods available. In this particular technique, the goal is to determine a Coarse-Grained potential in such a way that the target radial distribution function of the reference all-atom system, which structurally characterizes the atomistic system, is reproduced. The interatomic potentials developed by the inversion of the radial distribution function of the systems have shown promising and adequate capability in simulating systems which are reasonably representative of the reference all-atom models. The mechanical behavior of the atomistic system is well reproduced by the coarse-grained system and it is proven to be a good representative of the reference all-atom model in the thermodynamic state in which it was derived. Due to a few drawbacks of the IBI method such as failing to produce state-independent potentials, we also investigated the influence of the Multi-State Iterative Boltzmann Inversion Technique on reducing state dependency. In general, the aim of Multi-State IBI, as an extension to the standard IBI method, is to derive a potential that can be used over various thermodynamic states. In this research, the investigation for the positive outcome of using MS IBI for deriving CG potential has shown to be successful and the resulted potential manifests satisfying applicability to a range of thermodynamic states as well as producing an acceptable representation of the mechanical behavior of the original all-atom system.

Keywords: Multi Scaling, Nanostructures, Coarse Graining, Iterative Boltzmann Inversion, FCC Crystals

*Speaker

†Corresponding author: melika_bm85@yahoo.com

A coupled-field model of silicon anode charging in lithium-ion batteries

Marek Werner * [1], Kerstin Weinberg† [1]

[1] Universität Siegen – Fakultät IV, Dept. Maschinenbau, Institut für Mechanik und Regelungstechnik, Paul-Bonatz-Str. 9-11 57076 Siegen, Germany

Lithium-ion batteries are known to have the highest gravimetric energy density of all rechargeable storage media and so they are of interest for several applications, e.g., electric vehicles, mobile devices and cordless machines. A lithium-ion battery's construction consists of two electrodes, a separator in between and an electrolytic solution which allows for transport of charge in form of lithium ions. Typically, multicomponent compositions like LiCoO 2 or LiFePO 4 are used as cathode material and single substances like silicon or graphite are developed as anode material. In the latest battery developments anodes of silicon are used, a material, which has after oxygen the second highest abundance within the earths' crust. However, by now the high volumetric change of silicon during intercalation - sometimes a factor of four has been reported - leads to pulverization and capacity fade of the anode. To account for the intercalation induced volumetric swelling and phase segregation, the mechanical, thermal, chemical, electrical and diffusion field equations have to be coupled which leads to a complex description based on fourth order partial differential equations. Our numerical solution of the arising multi-physics problem is based on an isogeometric concept. The NURBS based ansatz has been used already for similar types of problems and has proven to be reliable and efficient, especially for binary systems. Using a NURBS based description also for the geometry, we study several examples for single silicon particles like a topology optimized pillar or a round particle as well as intercalation through a flat planar film and an initially curved surface. To avoid transition from amorphous to crystalline silicon ordering, mainly structures below a few microns edge length are considered. Also the adaption of the right physical parameters like the elastic modulus for nano-scaled materials is vital and the deviations from macro-scale deduced values are still under debate. Most of the values are reported for a temperature of 298 K (STP), so we will restrict our consideration to an isothermal framework. Different mechanical boundary conditions will be adapted by a one sided adhesive junction of silicon with nickel, where the latter underlies no volumetric change during lithiation.

Keywords: Multi, physics, Diffusion problems, Finite deformations, lithium battery

*Speaker

†Corresponding author: kerstin.weinberg@uni-siegen.de

A physically-based methodology for the deterministic prediction of microstucturally-sensitive fatigue crack growth

David Wilson * [1], Fionn Dunne† [1]

[1] Department of Materials, Imperial College London – United Kingdom

The stage of crack growth during which a strong microstructural sensitivity exists may comprise a quite substantial fraction of fatigue life. The path of the crack growth is often tortuous being influenced by local grain-level anisotropic elasticity and slip, as well as by morphological, crystallographic and grain boundary features (and many others); mixed trans- and inter-granular growth modes are often observed. The rate of growth is also significantly influenced by these features. A stored energy based measure of the local driving force for crack growth has previously been introduced which can predict the onset of crack growth. Here, a physically-based methodology is presented to calculate both the growth rate and direction in the context of a fatigue loading simulation with explicit representation of the growing crack. The methodology thus provides a prediction of the full crack growth history. The methodology has been validated against a number of experimental cases to evaluate the accuracy of the model, and further provide insight into the behaviour of the crack under the influence of the features described above. Particular focus is given to the behaviour of the crack around grain boundaries to assess the relationship between the angle of a grain boundary and its resistance to fatigue crack growth. This model thus complements experimental methods and allows a more comprehensive understanding of the fatigue resistance of different textures and morphologies.

Keywords: Fatigue, Fracture, Microstructural Sensitivity, Crack Growth, XFEM

*Speaker
†Corresponding author: fionn.dunne@imperial.ac.uk

List of participants

A

Abisset-Chavanne Emmanuelle
Achour Mohamad
Alipour Atefeh
Amani Yasin
Amiot Fabien
Ammar Kais
Andersen Rasmus
Argerich Martin Clara
Arias Irene
Ask Anna

B

Bain Cédric
Balit Yanis
Balutch Thomas
Barick Mohamed Cheikh
Barnwal Vivek Kumar
Barrioz Pierre-Olivier
Bellón Bárbara
Ben Elhaj Salah Sami
Benallal Ahmed
Benzerga Amine
Bertram Albrecht
Bésuelle Pierre
Bianchini Marta
Bigoni Davide
Böhlke Thomas
Bormann Franz
Boussattine Zaid
Boyat Xavier
Brassart Laurence
Brenner Renald
Brewick Patrick
Bronstein Emil
Brusselle Nadege
Bruzy Nicolas
Burlayenko Vyacheslav

C

Cartraud Patrice
Chang Xuyang
Chastand Victor
Chemani Halima
Cheng Long
Chester Shawn
Chevalier Jérémy
Choleridis Antonios
Chudoba Thomas
Ciambella Jacopo
Codony David
Comi Claudia
Connesson Nathanael
Cornelius Thomas
Cottereau Régis
Croonenborghs Maïté
Croquelois Benjamin
Csati Zoltan
Cundiff Kenneth

D

Dalemat Marie
Dallali Manel
Danas Kostas
Darvishi Kamachali Reza
Davin Tanguy
De Araujo Carlos Jose
Degeiter Matthieu
Delannay Laurent
Dendievel Rémy
Dépinoy Sylvain
Dereure Corentin
Deshpande Vikram
Desrues Jacques
Diaz Lopez Olga
Dirrenberger Justin
Doskar Martin
Doumalin Pascal
Dunne Fionn
Durif Alan
Dzepina Branislav
Dæhli Lars Edvard

E

Elahi Seyed Ali

F

Fang Xufei
Faran Eilon
Favata Antonino
Findeisen Claudio
Finel Alphonse
Fletcher Lloyd
Forest Samuel
Foti Federico
Fourt Erwan
Freidin Alexander

G

Galich Pavel
Gasser T.christian
Geers Marc
Ghasemi Milad
Gigliotti Marco
Gizzi Alessio
Godard Pierre
Gonzalez Carlos
Gornet Laurent
Goshkoderia Artemii
Goudenhooft Camille
Guedes Rui
Guglielmi Paula
Guillet Alain
Guin Jean-Pierre
Gunkelmann Nina
Gurrutxaga-Lerma Benat

H

Habraken Anne Marie
Hadji Lazreg
Hamma Juba
Harte Allan
Hary Benjamin
He Jinshan
Henry Joël
Heuzé Thomas
Hillgärtner Markus
Hodapp Max
Hohe Jörg

Hopperstad Odd Sture
Huchet François
Hund Jonas
Huneau Bertrand
Hure Jérémy
Husser Edgar
Hütter Markus

I

Ibáñez Pinillo Rubén
Idrissi Hosni
Irani Nilgoon
Ismail Karim
Itskov Mikhail
Ivan Trapic

J

Jaddi Sahar
Janarthanam Hemanth
Jaumier Thibaud
Johnston Robert
Jordana Fabienne

K

Kabel Matthias
Kassem Wassim
Khiêm Vu Ngoc
Klocker Helmut
Klusemann Benjamin
Kodjo Kossi-Mensah
Kouznetsova Varvara
Kroon Martin
Kuebel Christian
Kulkarni Nikhil

L

Labusch Matthias
Lacoste Grégory
Laschet Gottfried
Le Benoît
Le Bouar Yann
Le Guennec Yves
Lebbad Hocine
Legoll Frederic
Lemke Veronica
Lesage Thibault
Leygue Adrien
Li Yang
Lin Fengxiang
Liu Hong
Liu Ling
Liu Guixian
Llorca Javier
Lopez-Pamies Oscar
Lührs Lukas
Luo Wei

M

Maclachlan Duncan
Magliulo Marco
Mahajan Dhiraj Kumar
Mahnken Rolf
Maire Eric
Marckmann Gilles
Mareau Charles
Marom Yulia
Martin Anthony
Martin Christophe L.
Marvi Mashhadi Mohammad
Massart Thierry
Maurizi Enrici Tommaso
Menzel Andreas
Mertens Anne
Mezi Dihya
Michel Coret
Michel Bruno
Miotti Bettanini Alvise
Mishra Sushil
Mocci Alice
Moelans Nele
Moës Nicolas
Molinari Jean-François
Mompiou Frédéric
Morelle Xavier
Morgeneyer Thilo
Morozov Aleksandr

N

Nackenhorst Udo
Nag Shankha
Naya Fernando
Neumann Matthias
Nguejio Josiane
Nguyen Ngoc-Son
Nielsen Kim Lau
Norazrina Mat Jali
Nozay Cynthia

O

Onck Patrick
Onimus Fabien
Ovalle Cristian

P

Pappas Georgios
Pardoen Thomas
Parry Guillaume
Pecora Marina
Peerlings Ron
Peng Xianglong
Persenot Théo
Petit Tom
Petrenko Svetlana
Petrowiste Steven
Pierron Fabrice
Pinho Silvestre
Pivdiablyk Ivanna
Pivovarov Dmytro
Plachy Robert
Platzer Auriane
Poh Leonghien
Poinot Delphine
Poluektov Mikhail
Portelette Luc
Prasad G. Durga
Purushottam Raj Purohit Ravi Raj Purohit

Q

Quaranta Giacomo

R

Raabe Dierk
Radi Kaoutar
Raid Idir
Rajendran Mohan Kumar
Raphael Ilan
Rappel Hussein
Reali Luca
Redjala Sonya
Reese Stefanie
Remmers Joris
Renaud Adrien
Renversade Loïc
Réquilé Samuel
Réthoré Julien
Rey Valentine
Reyne Baptiste
Rezaei Shahed
Richert Claudia
Robard Pierre
Rokos Ondrej
Romain Quey
Romera Jesus Maria
Rousselier Gilles
Rouxel Tanguy
Rozycki Patrick
Rudykh Stephan

S

Sumith S.
Saintier Nicolas
Saliya Kanssoune
Sandfeld Stefan
Santos Guillermo
Santos Rodrigo
Scheiner Stefan
Scherer Jean-Michel
Scheuer Adrien
Schmidt Volker
Schnabel Jan Eike
Schneider Daniel
Schoof Ephraim
Schwab Felix
Schwaiger Ruth
Seghir Rian
Serveaux Jérémy
Sharma Luv
Shilo Doron
Shveykin Alexey
Simar Aude
Solyaev Yury
Sridhar Ashwin
Stainier Laurent
Strobl Michael
Sudmanns Markus
Svendsen Bob

T

Tanguy Döme
Tanguy Benoit
Thilly Ludovic
Tiirats Tauno
Toups Elisabeth
Triki Ennouri
Tromas Christophe
Trumel Hervé
Tutcuoglu Abbas

U

V

Van Dommelen Hans
Van Tuijl Rody
Vandoren Bram
Varun Raj Ramachandran
Vayssette Bastien
Verron Erwan
Verschueren Jonas
Vettorel Matteo
Villani Aurelien
Vokhshoorikoohi Seyedeh Melika
Volegov Pavel

W

Wang Jingya
Waseem Abdullah
Wendler Frank
Werner Marek
Westbeek Steyn
Wilkinson David
Wilmers Jana
Wilson David
Wu Zhicheng
Wulfinghoff Stephan

Y

Yang Hua

Z

Zeman Jan
Zergoug Mourad
Zghal Jihed
Zhang Zhen
Zhao Lv
Zhou Jianqiang
Zoubida Khelifa
Zu Qun


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