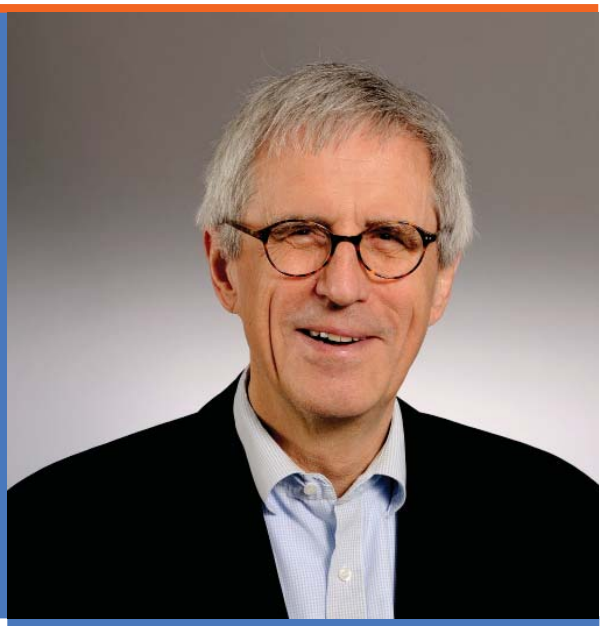
New Horizons in Materials Mechanics

Symposium

June 5th - 7th, 2013
in celebration of the 70th birthday of

Prof., Dr.Tech. Viggo Tvergaard



The Viggo Tvergaard Symposium: New Horizons in Materials Mechanics

The Viggo Tvergaard Symposium: New Horizons in Materials Mechanics is a tribute to a world leading scientist on the occasion of his 70th birthday. Throughout his career Viggo has made important scientific contributions to the field of solid mechanics. His central interests have been plasticity, materials mechanics, fracture mechanics, and structural stability and his research has revolved around these subjects and their intersections. In the 44 years of Viggo's academic career until now, he has been a highly active scientist and he has developed international relations and collaborations with the strongest researchers around the world, many of whom are gathered at this symposium.

Viggo has been a central teacher and advisor at the Technical University of Denmark. He has undertaken teaching on all levels from basic Strength of Materials courses to advanced courses on Plasticity, Fracture Mechanics and General Continuum Mechanics. Viggo has been advisor for numerous PhD student's, of which many hold influential positions in Danish industries.

The scientific accomplishments of Viggo have been recognized by the community on many occasions, and we shall not try to list them, but only mention that Viggo's recent election for president of IUTAM serves as recognition that Viggo is not only a gifted scientist and educator, but also a person who will have the great impact on our research field for years to come.

It is our pleasure and privilege to organize this symposium and we look forward to three rewarding days of presentations and scientific discussions, as well as future collaboration and interaction with Viggo.

Gerda Helene Fogt, Brian N. Legarth, Lars P. Mikkelsen and Christian F. Niordson

Scientific Committee:

Alan Needleman, University of North Texas.
John W. Hutchinson, Harvard University.
Norman A. Fleck, University of Cambridge.
Robert McMeeking, University of California, Santa Barbara.
Christian F. Niordson, Technical University of Denmark.

Local Organizing Committee:

Gerda Helene Fogt.
Brian N. Legarth.
Lars P. Mikkelsen.
Christian F. Niordson.

Sponsors:

Myhrwolds Fond.
Otto Mønsteds Fond.
Thomas B. Thriges Fond.

Programme

Wednesday, June 5, 2013

(Chair morning: Brian Nyvang Legarth)
(Chair afternoon: Henrik Myhre Jensen)

7:30-8:30	Registration + breakfast
8:30-8:45	***Welcome.*** Christian F. Niordson
8:45-9:15	***Mechanics and simulation of ductile fracture.*** John W. Hutchinson
9:15-9:45	***Ductile vs brittle fracture behaviors and deformation mechanisms in nanostructured materials.*** Huajian Gao
9:45-10:15	***Correlating toughness and ductile fracture surface roughness.*** Alan Needleman
10:15-10:45	Coffee break
10:45-11:15	***Strategies for tough solids.*** Norman A. Fleck
11:15-12:00	***On coalescence-controlled ductile fracture - Discussion session.*** Amine A. Benzerga
12:00-13:30	Lunch
13:30-14:00	***Challenges in the modelling of the behaviour of aluminium alloys for structural applications.*** Odd Sture Hopperstad
14:00-14:30	***Polyhedral finite elements in computational solid mechanics.*** Mark Rashid
14:30-15:00	***Effects of Lode angle on yielding and fracture of materials.*** Ahmed Benallal
15:00-15:15	Questions and discussion
15:15-15:45	Coffee break
15:45-16:15	***On the strong influence of imperfections upon the quick deviation of a crack loaded in mode I+III from its original plane.*** Jean-Baptiste Leblond
16:15-16:45	***The cohesive band model: a cohesive surface formulation with stress triaxiality.*** René de Borst
16:45-17:00	Questions and discussion
19:00	Dinner

Programme

Thursday, June 6, 2013

(Chair morning: William Curtin)
(Chair afternoon: Ole Sigmund)

7:30-8:30 Breakfast

8:45-9:15 ***Crushing of open-cell foams.***
Stelios Kyriakides

9:15-9:45 ***A coupled framework for climb-assisted glide in Discrete Dislocation Plasticity.***
Vikram Deshpande

9:45-10:15 ***From cavity to hurst exponent***.
Erik van der Giessen

10:15-10:45 Coffee break

10:45-11:15 ***Some properties of acoustic metamaterials***.
John R. Willis

11:15-12:00 ***Multiscale materials modeling: success stories and current challenges - Discussion session.***
Javier Llorca

12:00-13:15 Lunch

13:15-13:45 ***Mechanics of hydrogels.***
Zhigang Suo

13:45-14:15 ***Gel mechanics: A thermo-mechanically coupled theory for fluid permeation in elastomeric materials.***
Lallit Anand

14:15-14:30 Questions and discussion

14:30-15:00 Coffee break

15:00-15:30 ***Pressure due to confinement of a bio-membrane undergoing thermal fluctuations.***
Ben Freund

15:30-15:45 Questions and discussion

16:00-18:00 ***Boat excursion***

19:00 Dinner

Programme

Friday, June 7, 2013

(Chair morning: Bob Svendsen)
(Chair afternoon: Michael Thouless)

7:30-8:30 Breakfast

8:45-9:15 ***A gradient crystal plasticity theory at finite strain and its application to three-dimensional simulation of micro-pillar compression***.
Mitsutoshi Kuroda

9:15-9:45 ***Length scales in crystal plasticity: the dislocation mean free path length.***
Jeffrey Kysar

9:45-10:15 ***Size and rate dependent ductility of thin metallic films***.
Thomas Pardoen

10:15-10:45 Coffee break

10:45-11:15 ***A phenomenological model for microstructural evolution during plastic flow***.
John Bassani

11:15-12:00 ***On the critical role of the mechanics of interfaces - Discussion session.***
Marc Geers

12:00-13:30 Lunch

13:30-14:00 ***An analytical model of reactive diffusion for transient electronics.***
Yonggang Huang

14:00-14:30 ***Surface instabilities of neo-Hookean solids and ruga mechanics.***
Kyung-Suk Kim

14:30-14:45 Questions and discussion

14:45-15:15 Coffee break

15:15-15:45 ***Stress driven diffusion in bone tissue.***
Leslie Banks-Sills

15:45-16:15 ***Adhesion of cells and the influence of cytoskeletal contractility.***
Robert McMeeking

16:15-16:30 Questions and discussion

16:30-16:45 Wrap up and closure

Notes

Mechanics and simulation of ductile fracture

John W. Hutchinson

Abstract

Recent fundamental experiments on the ductility of tough structural alloys reveal that the characterization of ductile fracture must distinguish between deformation under axisymmetric conditions, such as in round bar tensile tests, and deformation dominated by shear. The new data calls for a reassessment of widely used engineering criteria for ductile fracture that accounts for stress state solely through triaxiality. These experiments have motivated new studies of ductile failure under shear, and they have also been the starting point in a recent extension of the Gurson constitutive model of damage and failure of ductile alloys accounting for the possibility of fracture under conditions of pure shear. When properly calibrated against a basic set of experiments, the extended model has the potential to predict the emergence and propagation of cracks over a complete range of stress states. Applications of the extended model will be discussed, including the characterization of a cohesive zone for ductile tearing of large plate structures. In discussing the applications, emphasis will be placed on the appropriate scale of damage characterization in ductile fracture simulations.

Ductile vs brittle fracture behaviors and deformation mechanisms in nanostructured materials

Huajian Gao

Abstract

The rapid development of synthesis and characterization of materials with feature sizes at nanoscale as well as unprecedented computational power have brought forth a new era of materials research in which experiments, modeling and simulations are performed side by side to probe the unique mechanical properties of nanostructured materials. Here we report a number of recent studies on ductile vs brittle fracture behaviors and related deformation mechanisms in nanostructure of materials, including a twin-spacing-induced ductile-brittle transition in nanotwinned nanopillars [1] and crack bridging by nanoscale twins in thin films [2]. In each study, there has been a strong synergy between theory and experiment, with new experimental findings driving advances in modeling and simulations, and new theoretical insights suggesting new experimental studies. The discussions will be organized around the current understandings based on existing experimental and theoretical efforts, as well as the outstanding questions that require further studies in the future.

[1] D.C. Jang, X.Y. Li, H.J. Gao and J.R. Greer, "Deformation Mechanisms in Nanotwinned Metal Nanopillars," 2012, Nature Nanotechnology, Vol. 7, 594–601.

[2] S.W. Kim, X.Y. Li, H.J. Gao and S. Kumar, "In situ Observations of Crack Arrest and Bridging by Nanoscale Twins in Copper Thin Films," 2012, Acta Materialia, Vol. 60, 2959–2972.

Correlating toughness and ductile fracture surface roughness

Alan Needleman

Abstract

Experimental observations have shown that the roughness of fracture surfaces exhibits certain characteristic scaling properties. In particular, the self-affine nature of the roughness of fracture surfaces has been observed in a wide variety of materials and under a wide variety of loading conditions. The initial hope, to relate the scaling properties of the fracture surface roughness to the material's crack growth resistance, has remained unfulfilled. Three dimensional finite deformation analyses of ductile crack growth will be described that address the relation between a ductile material's resistance to crack growth (toughness) and fracture surface roughness. An elastic-viscoplastic constitutive relation for a progressively cavitating plastic solid is used to model the material. Two populations of void nucleating second phase particles are represented, large inclusions with low strength, which result in large voids near the crack tip at an early stage, and small second phase particles, which require large strains before cavities nucleate. The larger inclusions are represented discretely with their spacing introducing a microstructurally based characteristic length into the formulation. The calculations are carried out for small scale yielding conditions and the full statistics of the roughness of the computed fracture surfaces are calculated. Possible relations between toughness and statistical parameters characterizing the ductile fracture surface roughness are explored. This is joint work with V. Tvergaard of the Technical University of Denmark, E. Bouchaud of ESPCI Paris Tech, L. Ponson of Université Pierre et Marie Curie, and A. Srivastava and S. Osovski of the University of North Texas.

Strategies for tough solids

Norman A. Fleck, V.S. Deshpande, G. Noselli, L. St. Pierre and H. Tankasala

Abstract

An examination of the gaps in material property space reveals the opportunity for the invention of composites possessing a high toughness (and high strength, with density in the range 0.1-1 Mg/m^3. Possible toughening strategies are (i) crack deflection into multiple cracks, (ii) plastic dissipation in a layered elastic-plastic solid and (iii) crack blunting and successive crack re-nucleation. Each mechanism is investigated, and the crack nucleation mechanisms is explored experimentally by measurement of the fracture toughness of specimens containing a 2D periodic array of holes. The successive blunting and renucleation of a new crack leads to high macroscopic toughness. This mechanism is explored in more detail for ductile lattice materials, and the dependence of fracture toughness upon relative density (and ductility of lattice) is evaluated.

On coalescence-controlled ductile fracture

Amine A. Benzerga, B. Kondori, L. Morin and J.-B. Leblond

Abstract

In a class of technologically important materials (high-strength steels, magnesium alloys) post-mortem fractography reveals little diffuse damage, if any. The typically ductile fracture surfaces contain shallow dimples, an observation which indicates limited void growth prior to failure. Correspondingly, the effect of stress triaxiality, if at all present, can be smaller than predicted with void growth models. In addition, the opening under triaxial loading of microcracks is observed to be smaller than would be predicted using voided cell model calculations.

In order to rationalize the above experimental observations and related issues, a scenario of ductile fracture is proposed whereby ductility and toughness are determined by the linking of deformation-induced microcracks. Possible mechanisms responsible for the limited void growth are: (i) nucleation-controlled fracture; (ii) participation of a second population of tiny voids; (iii) directionality of growth due to strong plastic anisotropy; and (iv) coalescence-controlled fracture. After briefly discussing each mechanism, emphasis is laid on the latter, as the modeling of void coalescence is essentially in its infancy compared with the level of sophistication of available void growth models. A mathematical framework is presented for the development of effective yield criteria for porous ductile solids near a state of coalescence-induced failure. Two such criteria are derived analytically, one being in closed form, for cylindrical voids of varying aspect ratio. The behavior in the limit of penny-shape cracks is discussed to point out some research directions that are critically needed for the materials of interest.

Notes

Challenges in the modelling of the behaviour of aluminium alloys for structural applications

Odd Sture Hopperstad

Abstract

Aluminium alloys are used in structural applications where light weight is an important design criterion. Examples are bumper beams and crash boxes in automotive structures and mobile protection systems used in international peacekeeping operations. Robust design and production of light but crashworthy structural components in aluminium involve development of alloys and manufacturing processes, structural design and crashworthiness analysis. Optimization of the structural components for strength, energy absorption and light weight, often requires utilization of the material to the verge of strain localization and material failure. It is therefore important to establish accurate, efficient and robust models of material behaviour and fracture at various scales that can be used in the design of aluminium structures and thus reduce the need for extensive and costly test programs. The stress-strain behaviour of an aluminium alloy depends on microstructural characteristics such as solute atoms, hardening precipitates, dislocation density and crystallographic texture, individually or in combination, whereas fracture is influenced by grain structure, particle distribution and, in some alloys, precipitate-free zones adjacent to the grain boundaries. Nano-scale material models have been proposed that are capable of predicting with reasonable accuracy the strength and work hardening of certain classes of aluminium alloys as a function of the chemical composition and heat treatment, while crystal plasticity models may be used to obtain estimates on the plastic anisotropy induced by crystallographic texture. The aim of this presentation is to illustrate some of the challenges in the modelling of the behaviour of aluminium alloys for structural applications with respect to strength and work-hardening, rate sensitivity, plastic anisotropy and fracture.

Polyhedral finite elements in computational solid mechanics

Mark Rashid

Abstract

Polyhedral finite element methods constitute a class of approximation methods that retain most of the favorable properties of conventional finite element methods, but without finite-element-like restrictions on the element geometry and topology. Such schemes offer the promise of greatly simplified automatic mesh generation, even on extremely complex and/or evolving domains. The benefits of such a capability touch a broad range of industrial and research applications, including crack extension, moving interfaces, and complex assemblages of dissimilar materials (e.g. direct simulation of polycrystals). Fully realizing these benefits, however, hinges on success in two areas: 1) the polyhedral element formulation must be tolerant of geometric pathologies; and 2) the mesh-generation approach must handle geometric near-degeneracies in a robust way. Both of these elements present some interesting challenges. With regard to the former, a new approach, the "partitioned element method," will be described, in which the shape functions are defined only discretely, as piecewise-linear functions over a cellular partition of the element. The cells also serve to define the quadrature rule on the element. Thus, the shape functions and the quadrature rule are, in a sense, formulated symbiotically. The computationalgeometry challenges associated with polyhedral mesh generation will also be discussed, with the help of some illustrative example problems. A key issue here is the need to avoid geometric features of the mesh – e.g. edges and facets – that are smaller than a prescribed tolerance. This tolerance is likely to be orders of magnitude larger than "machine epsilon"; thus, some trade-off with geometric precision is inevitable. This tolerance-driven point of view is compelled by the element formulation, and is conceptually distinct, in many respects, from existing notions of robustness in geometric computation.

Effects of Lode angle on yielding and fracture of materials

Ahmed Benallal

Abstract

The objective of this discussion is to have a feed-back from the audience of the Viggo Tvergaard's symposium on the roles played by the third stress invariant on the mechanical behaviour of engineering materials. This is of course a wide topic but the discussion can be focused around the following questions, the list being non-exhaustive :

1) Experimental evidence on the effects of Lode angle on yielding, fracture and other issues. Available data concern concrete materials, metallic alloys and shape memory alloys but other types of material are welcome. Qualitative versus quantitative aspects need also be addressed.
2) Taking this into account, how these effects can be included in constitutive and failure models. Beside the various phenomenological proposals is this feasable through micromechanical approaches ? Some indications already exist in the Rice & Tracey analysis or in Danas & Ponte Castaneda. How about the Gurson approach ? What are the main issues there?
3) What are the main implications of the introduction of the Lode angle especially with respect to localization and rupture?
4) Are there any assessment of these various approaches?

On the strong influence of imperfections upon the quick deviation of a crack loaded in mode I+III from its original plane

Jean-Baptiste Leblond

Abstract

It is well-known that cracks loaded in mode I+III tend to quickly deviate from their original plane when propagating. In a recent paper, Leblond, Karma and Lazarus analyzed the possible bifurcation from co-planar to non-coplanar propagation assuming, all along the crack front, (i) a constant value of the local energy-release-rate G (Griffith's condition), and (ii) a zero value of the local stress intensity factor K_{II} of mode II (Goldstein and Salganik's principle of local symmetry). It was concluded that such a bifurcation does exist for values of the ratio K^0_{III}/K^0_I of the mode III to mode I unperturbed stress intensity factors larger than some threshold depending on Poisson's ratio ν. However, since this threshold is of the order of 0.5 for standard values of ν, this analysis cannot explain the fact that deviations of the crack from its original plane are currently observed for much smaller values of K^0_{III}/K^0_I.

In this work, we explore the possibility that such deviations observed for small values of K^0_{III}/K^0_I might arise, in the absence of any bifurcation, from a strong influence of imperfections upon the propagation path. The idea is that inevitable fluctuations of the fracture toughness G_c within the original crack plane must induce in-plane undulations of the crack front resulting, because of the presence of a nonzero K^0_{III}, in non-zero values of the local K_{II}, implying a future local out-of-plane deviation which might be "unstable" in Cotterell and Rice's sense if the local non-singular stress T_{xx} is positive. Exploration of this idea implies evaluation of the local stress intensity factors K_I, K_{II}, K_{III} and non-singular stress T_{xx} along the front of a semi-infinite crack slightly perturbed within its plane. Both calculations have been performed for a semi-infinite crack in an infinite body in works of Gao and Rice. That of the non-singular stress was however incomplete and is completed here, for arbitrary in-plane perturbations, using Rice's reformulation of Bueckner's theory of 3D weight functions.

Inspection of the results shows that for in-plane sinusoidal undulations of the crack front of sufficient amplitude, the conditions $K_{II} \neq 0$ and $T_{xx} > 0$ are simultaneously met on some parts of the front, implying the possibility of future "unstable" (in Cotterell and Rice's sense) local deviations of the crack from coplanarity, and thus confirming the idea investigated.

A remarkable additional feature of the solution is that the smaller the wavelength of the inplane undulations, the stronger Cotterell and Rice's "instability"; the implication is that out-of-plane deviations of *short wavelength* should initially develop preferentially. This conclusion is compatible with actual observations.

The cohesive band model: A cohesive surface formulation with stress triaxiality

René de Borst, Joris J.C. Remmers, V. Verhoosel, Alan Needleman

Abstract

In the cohesive surface model cohesive tractions are transmitted across a two-dimensional surface, which is embedded in a three-dimensional continuum. The relevant kinematic quantities are the local crack opening displacement and the crack sliding displacement, but there is no kinematic quantity that represents the stretching of the fracture plane. As a consequence, in-plane stresses are absent, and fracture phenomena as splitting cracks in concrete and masonry, or crazing in polymers, which are governed by stress triaxiality, cannot be represented properly. In this paper we extend the cohesive surface model to include in-plane kinematic quantities. Since the full strain tensor is now available, a three-dimensional stress state can be computed in a straightforward manner. The cohesive band model is regarded as a subgrid scale fracture model, which has a small, yet finite thickness at the subgrid scale, but can be considered as having a zero thickness in the discretisation method that is used at the macroscopic scale. The standard cohesive surface formulation is obtained when the cohesive band width goes to zero. In principle, any discretisation method that can capture a discontinuity can be used, but partition-of-unity based finite element methods and isogeometric finite element analysis seem to have an advantage since they can naturally incorporate the continuum mechanics. When using interface finite elements, traction oscillations that can occur prior to the opening of a cohesive crack, persist for the cohesive band model. Example calculations show that the Poisson contraction influences the results, since there is a coupling between the crack opening and the inplane normal strain in the cohesive band. This coupling holds promise for capturing a variety of fracture phenomena, such as delamination buckling and splitting cracks, that are difficult, if not impossible, to describe within a conventional cohesive surface model.

Notes

Crushing of open-cell foams

Stelios Kyriakides, Stavros Gaitanaros, Andrew Barnes, Wen-Yea Jang, Andrew Kraynik, K. Ravi-Chandar

Abstract

Lightweight cellular materials such as foams exhibit excellent energy absorption characteristics and are widely used for impact mitigation in a variety of applications. The lecture will present results from combined experimental and analytical efforts that investigate the crushing behavior of an Al-alloy opencell foam under quasi-static and dynamic loadings. X-ray tomography was used to establish the geometry of the irregular polyhedral cells, ligament length and area distribution, cell anisotropy, density, etc. [1]. Quasi-static crushing was performed under displacement control and the evolution of deformation in the specimen was monitored using X-ray tomography. The response exhibits a relatively stiff linearly elastic regime that terminates into a load maximum; it is followed by an extended load plateau during which localized cell crushing initiates and gradually spreads throughout the specimen. When most of the cells are crushed the densified material stiffens again. Dynamic crushing experiments were performed using a gas gun to accelerate foam specimens together with a backing mass to velocities in the range of 20-160 m/s [3]. The stress at one end is recorded using a pressure bar while the deformation of the entire foam specimen is monitored with high-speed photography. Specimens impacted at relatively low velocities exhibited a response and localized deformation patterns that are very similar to those observed under quasi-static crushing. Interestingly, inertia increased the energy absorption capacity very modestly. By contrast, for impact speeds of 60 m/s and higher the specimens developed nearly planar shocks that propagated at well-defined velocities crushing the specimen. The shock-impact speed Hugoniot was extracted directly from the sequence of high-speed images recorded and this allows calculation of all problem variables without reverting to a constitutive model. The compaction energy dissipation across the shock is found to increase with impact speed and to be significantly larger than the quasi-static one [3].

The experiments are simulated using micromechanically accurate foam models. Skeletal random models are generated from soap froth using the Surface Evolver software. The linear sides of the skeletal microstructure are then “dressed” with appropriate distributions of solid to match those of ligaments in the actual foams and their relative density. The ligaments are modeled as shear-deformable beams with variable cross sections discretized with beam elements in LS-DYNA, while the Al-alloy is modeled as a finitely deforming elastic-plastic material. Utilization of the beam-to-beam contact algorithm of the code is an essential component of the simulation of crushing. Such models were shown to reproduce all aspects of quasi-static crushing faithfully [2]. Results from recent calculations will be shown that reproduce the formation and evolution of shocks including the force acting at the two ends, the shock front velocity, and energy absorbed [4].

[1] W.-Y., Jang, S. Kyriakides. On the crushing of aluminum open-cell foams: Part I experiments. Part II Analysis. Int. J. Solids & Structures 46, 617-650 (2009).
[2] S. Gaitanaros, S. Kyriakides, A.M. Kraynik. On the crushing response of random open-cell foams. Int'l J. Solids & Structures 49, 2733-2743 (2012).
[3] A. Barnes, K. Ravi-Chandar, S. Kyriakides. Dynamic crushing of Aluminum foams: Part I Experiments. In preparation.
[4] S. Gaitanaros, S. Kyriakides. Dynamic crushing of Aluminum foams: Part II Modeling. In preparation.

A coupled framework for climb-assisted glide in discrete dislocation plasticity

Vikram Deshpande

Abstract

It is now well established that the plastic deformation of crystalline solids is size dependent at the micron scale for a range of loading conditions. While there are many underlying reasons for these size effects, attention has been primarily focussed on situations where plastic strain gradients are generated. Models typically tend to over-predict the experimentally observed size effects as they neglect a range of dislocation relaxation mechanisms. These mechanisms include dislocation cross-slip and dislocation climb. Dislocation climb requires the diffusion of vacancies and hence significant amounts of dislocation climb only occur at temperatures above a third of the melting temperature - in these cases mass transport reduces the plastic strain gradients and thereby reducing the effect of specimen size. However, even at lower temperatures, dislocations can surmount small obstacles with the aid of small amounts of climb. This prevents the build-up of large dislocation pile-ups which consequently again relaxes stresses.

The coupling of vacancy diffusion with dislocation motion is a true "multi-scale" problem as vacancy/dislocation interaction is essentially a dislocation core effect. We present a two-dimensional discrete dislocation plasticity framework coupled with vacancy diffusion wherein dislocation motion occurs by both climb and glide. The effect of dislocation climb is explored for a range of problems including size effects in bending of crystals, metal-matrix composites and passivated films. Dislocation climb typically tends to reduce strength enhancements that occur with decreasing size but in some surprising cases can also result in strength increases.

From cavity to Hurst exponent

Erik van der Giessen

Abstract

The safe operation of devices and components in high-temperature environments is severely limited by creep fracture, occurring suddenly after years of stationary loading. This failure process involves a cascade of events across a wide range of length scales: vacancies cluster on grain boundaries, which can lead to stable cavities that grow by grain boundary diffusion and plastic deformation; at a sufficiently high density, the cavities on a grain boundary coalesce to form microcracks; finally, microcracks link-up with each other to form a macroscopic crack, leading to final fracture.

During my post-doc period with him, Viggo introduced me to the world of creep failure in which he built on previous modelling by Ashby, Rice and Needleman of the unit events at the microscopic scale. After several years of collaboration on this, and after a number of PhD students, this talk summarises a model which, by systematic upscaling, spans all length scales from individual cavities up to large macroscopic fracture surface. More specifically I will present unpublished results of the predicted fracture surface roughness in terms of the Hurst exponent.

Some properties of acoustic metamaterials

John R. Willis

Abstract

"Effective constititutive relations" for the dynamics of composites are non-local in space and time, and also display coupling between mean stress and velocity as well as strain, and between mean momentum density and strain as well as velocity. Metamaterials are composites containing resonators, for which these features are particularly pronounced. A consistent framework for the development of such relations, applicable equally to periodic or random media, will be summarised. An outstanding problem concerns the effect of boundaries or, more generally, interfaces, in whose vicinity the effective relations lose validity (or else require some modification). One approach to investigating this is to study the impedance (appropriately defined) of a half-space composed of metamaterial. A start has been made on this; whatever progress has been made by the time of the symposium will be reported.

Multiscale materials modeling: Success stories and current challenges

Javier Llorca

Abstract

A large number of modeling tools are currently available to predict accurately the formation, structure and properties of materials at different time and length scales. They include -among others- quantum mechanics and density functional theory (electronic structure, activation energies, interatomic potentials, etc.), standard and coarse-grained molecular dynamics (thermodynamics, crystalline structure, defect interactions), Monte Carlo methods (kinetics), computational thermodynamics (phase diagrams), phase-field modeling (phase transformation and microstructure development), dislocation dynamics, and a large family of partial differential equations solvers (finite elements, finite differences), which are used to study problems in the continuum (fluid dynamics, solid mechanics, conduction and transport problems, etc.).

These advanced tools have already proven their potential to discover and design materials with improved properties or unexpected structures. The discovery of superconductive cubic Fe at high pressures, new alloy catalysts, or Li-based materials for ultra-fast recharging batteries are examples - among many others- of the potential of computational materials science. Nevertheless, these success stories were possible because the critical structure or properties depended on phenomena with a given time and length scale, which could be simulated using only one of the techniques mentioned above. This is not always the case and, in fact, it is unlikely to occur in materials for engineering applications. For instance, balanced mechanical properties (stiffness, strength, toughness) depend on many different processes which take place along nine or more orders of magnitude in length and time scales. Thus, the next step is to integrate all the available modeling tools into a multiscale strategy capable of simulating processing, structure, properties and performance of engineering materials.

In this presentation, the multiscale modeling roadmap for virtual mechanical testing of structural materials is presented and two success stories related to structural composites [1] and metallic alloys [2-4] are detailed. Then, current challenges of the multiscale modeling strategies for structural materials are highlighted. They include, among others, the homogenization of fracture (and, in general, of localization), coupling atomistic and continuum simulations, and the bridging of time scales.

[1] J. Llorca, C. González, J. M. Molina-Aldareguía, J. Segurado, R. Seltzer, F. Sket, M. Rodríguez, S. Sádaba, R. Muñoz, L. P. Canal. Multiscale modeling of composite materials: a roadmap towards virtual testing. Advanced Materials, 23, 5130-5147, 2011.

[2] A. Arsenlis, M. Rhee, G. homes, R. Cook, J. Marian, A dislocation dynamics study of the transition from homogeneous to heterogeneous deformation in irradiated bcc iron, Acta Materialia, 60, 3748-3757, 2012.

[3] N. R. Barton, A. Arsenlis, J. Marian, A polycrystal plasticity model of strain localization in irradiated iron, Journal of the Mechanics and Physics of Solids, 61, 341-351, 2013.

[4] J. Segurado, R. A. Lebensohn, J. LLorca, C. Tomé. Multiscale modeling of plasticity based on embedding the viscoplastic self-consistent formulation in implicit finite elements. International Journal of Plasticity, 28, 124-140, 2012.

Notes

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Mechanics of hydrogels

Zhigang Suo

Abstract

Hydrogels are used as scaffolds for tissue engineering, vehicles for drug delivery, actuators for optics and fluidics, and model extracellular matrices for biological studies. The scope of applications, however, is often limited by the mechanical behavior of hydrogels. We have recently synthesized a hydrogel of exceptional strechability and toughness (Nature 489, 133, 2012). The hydrogel contains ~90% water and two types of polymers: polyacrylamide chains form a covalent network, and alginate chains associate through ionic bonds. The hydrogel can be stretched beyond 20 times its initial length, and has fracture energy of ~10,000 J/m^2. This exceptional behavior is attributed to the synergy of two molecular processes: crack bringing by the polyacrylamide network, and hysteresis by unzipping the alginate network. Furthermore, the covalent network of polyacrylamide preserves the memory of the initial state, so that much of the large deformation is removed when the load is removed. The unzipped ionic crosslinks cause internal damage, which heals as ionic crosslinks re-zip. This talk describes ongoing work that explores mechanisms of nonlinear rheology and applications of the material.

Gel Mechanics: A thermo-mechanically coupled theory for fluid permeation in elastomeric materials

Lallit Anand

Abstract

An elastomeric gel is a cross-linked polymer network swollen with a solvent, and certain gels can undergo large reversible volume changes as they are cycled about a critical temperature. We have developed a continuum-level theory to describe the coupled mechanical deformation, fluid permeation, and heat transfer of such thermally-responsive gels. In discussing special constitutive equations we limit our attention to isotropic materials, and consider a model based on a Flory-Huggins model for the free energy change due to mixing of the fluid with the polymer network, coupled with a non-Gaussian statistical-mechanical model for the change in configurational entropy - a model which accounts for the limited extensibility of polymer chains. We have numerically implemented our theory in a finite element program. We show that our theory is capable of simulating swelling, squeezing of fluid by applied mechanical forces, and thermally-responsive swelling/deswelling of such materials.

Pressure due to confinement of a bio-membrane undergoing thermal fluctuations

L. Ben Freund

Abstract

The phenomenon of thermal fluctuation of a bio-membrane within a stack of like membranes was introduced in a pioneering paper by Helfrich (1978). Internal energy arises in a representative membrane through elastic resistance to bending deformation, and membrane motion is further restrained through steric interaction with adjacent membranes. Due to reflective symmetry within the stack, analysis of behavior can be reduced to study of a single membrane fluctuating between parallel rigid planes. The phenomenon is re-examined here in order to quantify the dependence of system free energy on size of the gap between membranes. This analysis is based on essentially the same formulation that was used in the original study, and it is found that a statistical analysis based on enforcement of the underlying principles can lead to an exact mathematical solution. On this basis, a self-consistent picture of dependence of free energy on the width of the confining gap that is weaker than has been thought to prevail.

Notes

A gradient crystal plasticity theory at finite strain and its application to three-dimensional simulation of micro-pillar compression

Mitsutoshi Kuroda

Abstract

A finite deformation formulation for higher-order gradient crystal plasticity (Kuroda and Tvergaard, 2008) is reviewed. The formulation does not deviate much from the conventional crystal plasticity theory. A back stress effect and additional differential equations for evolution of the geometrically necessary dislocation (GND) densities are introduced into the conventional theory. The back stress impedes or promotes dislocation motions depending on its sign. As an application of the theory, deformation behavior in single-slip oriented micro-pillars subjected to uniaxial compressive loading is analyzed. In experimental studies, it has been frequently observed that the gauge portion of micro-pillar samples is split into a shear zone and two nearly unstrained dead zones under compressive loading. Here, it is shown that effects of higher-order gradient are essential for the formation of this particular deformation mode of the micro-pillars.

Length scales in crystal plasticity: The dislocation mean free path length

Jeffrey Kysar, Muin S. Oztop, Abdulhamit Sarac, Carl Dahlberg, Christian Niordson

Abstract

We describe measurements of the lower bound on the total density of Geometrically Necessary Dislocations (GND) on individual slip systems of a nickel crystal indented by a wedge. The GND content is measured by high-resolution electron backscatter diffraction (EBSD) with spatial resolutions of 2500 nm, 500 nm, 200 nm, 100 nm, and 50 nm. The multiple length scale measurements demonstrate that the GND density varies quasiperiodically, and the period of the GND variation is a characteristic length scale of crystal plasticity. Since the physical consequence of the formation of the quasiperiodic GND dislocation structure is to limit the mobility of dislocations, the dislocation mean free path length is assumed to scale with the period of the varying GND density. We demonstrate that the dislocation mean free path length becomes shorter as deformation proceeds in a well-defined way. In addition, we demonstrate that there is a distribution of the dislocation free path length and describe measurements of the range. Finally we consider the evolution and self-organization of the GND dislocation structures as deformation proceeds.

Size and rate dependent ductility of thin metallic films

T. Pardoen, M.-S. Colla, M. Coulombier, B. Wang, H. Idrissi, D. Schryvers, F. Mompiou, M. Legros, T.J. Massart, J.-P. Raskina

Abstract

The resistance of thin metallic films to plastic localization is an important issue in flexible electronics, thin coatings on deformable substrates, and several types of MEMS. From a fundamental perspective, thin metallic films often involve nanocrystalline structures which can be easily modified by changing the deposition parameters, offering a wide range of possibilities to study interface dominated plastic deformation mechanisms in nanostructured systems. The resistance to plastic localization is controlled by the strain hardening, strain rate sensitivity, and presence of imperfections. Experimental results obtained using a novel nanomechanical lab-on-chip technique on Al, AlSi and Pd films with thickness between 50 and 500 nm show several types of plasticity mechanisms and size effects affecting the ductility. The Al films, with ~200 nm grain size, demonstrate moderate strain hardening capacity, significant rate sensitivity, intergranular and transgranular dislocation glide, as well as grain boundary migration. The Pd films involve ~30 nm grain size containing a high density of fine coherent ~2-20 nm thick growth twins offering multiple barriers to dislocation motion, and sources for dislocation storage and multiplication. The very high strain hardening capacity coming from the dislocation/twin boundary interactions does not lead to large ductility due to failure mechanisms initiating after 2 to 4 % strain. A strong statistical dependence of the ductility on the overall size of the sample is also observed. An imperfection type localization analysis involving plastic strain gradient effects is performed to rationalize the different contributions to the resistance to necking. The imperfection analysis is successfully validated towards 2D FE strain gradient plasticity based calculations.

A phenomenological model for microstructural evolution during plastic flow

John L. Bassani, Haizhen Pan

Abstract

We consider a class of elastic-plastic materials for which orthotropic symmetry planes characterizing the microstructure evolve with deformation. At finite strain, a multiplicative kinematical decomposition is adopted, and flow rules are defined in the intermediate configuration in terms of a thermodynamically-consistent, non-symmetric stress and one second-order tensor that is sufficient to specify orthotropic symmetry. Microstructural spin is taken to be the difference between the material spin and plastic spin. A key relationship between plastic rate of stretching and plastic spin is derived utilizing representation theory for tensor-valued functions. As a consequence, microstructural evolution arises from non-coaxiality between the plastic rate of stretching and the orthotropic axes, which makes sense. The resulting phenomenological theory extends classical theories of anisotropic plasticity to include the evolution of the orthotropic axes. Only 2 additional material parameters are required for stressing in one of orthotropic symmetry planes, for example for loading in the plane of a textured polycrystalline sheet. Comparisons with experimental data are excellent. Predictions for necking and shear banding display significant effects of microstructural evolution.

On the critical role of the mechanics of interfaces

Marc Geers

Abstract

The challenges in analysing and modelling the mechanics of materials have shifted in the past century from elasticity to plasticity and more recently to damage and fracture. The field of computational mechanics gradually evolved in the past decades, solving geometrically and physically nonlinear problems with a growing complexity. With the maturity attained in computational mechanics, its strong relation with mechanics of materials has moved on the foreground in the scientific developments. Whereas the nonlinear behaviour of single phases is reasonably well understood and modelled by now, many open questions remain on their bonding interfaces. Interfaces are omnipresent in most engineering materials and structures across the scales, and they have a major impact on the resulting mechanical properties, both in the positive and the negative sense.

Interfaces are governing the mechanical material response to a large extent:

- In multi-phase materials, where phase boundaries are known to constrain the deformation of the phases in contact;
- In composites, where they often control the failure behaviour of laminates, multilayered stacks, particulate materials, etc.;
- In polycrystals, where grain boundaries have a marked mechanical influence or in thin films where thin boundary layers largely influence the film mechanics;
- In granular materials, e.g. ceramics, where interfaces control the thermo-mechanical properties under e.g. thermo-shock conditions;
- In particle-filled polymers, where the particle and its interfaces have a significant influence on the overall dynamical properties, e.g. in acoustic metamaterials;
- In coated materials, where the interface between coating and substrate plays a vital role, e.g. in thermal barrier coatings of turbine blades;
- In many applications of the future that rely on the full 3D integration of materials towards multifunctional materials and devices, e.g. stretchable electronics, electronic textiles, printed electronics,

The challenges ahead of us are still numerous. Many of the interfacial models are still in a premature stage of development. The models capturing the physics of plasticity through a grain boundary or at a phase boundary are still limited. The development of multi-scale methods to unravel the mechanics and physics of interfaces has only recently started. Experimental methods to qualitatively and quantitatively characterize the mechanics of interfaces are facing non-trivial questions, since small scale measurement techniques are increasingly important. Many interfacial failure models are largely phenomenological at this stage, and often trigger an intrinsic multi-scale conflict. How to incorporate the underlying physics of failure in a proper manner? Many questions that call for an in-depth discussion session to identify the horizon in mechanics of material interfaces…

Notes

An analytical model of reactive diffusion for transient electronics

Yonggang Huang

Abstract

A remarkable feature of modern silicon electronics is its ability to remain functionally and physically invariant, almost indefinitely for many practical purposes. Here, we introduce a silicon-based technology that offers the opposite behavior: it gradually vanishes over time, in a well-controlled, programmed manner [1]. Devices that are 'transient' in this sense create application possibilities that cannot be addressed with conventional electronics, such as active implants that exist for medically useful timeframes, but then completely dissolve and disappear via resorption by the body. We report a comprehensive set of materials, manufacturing schemes, device components and theoretical design tools for a complementary metal oxide semiconductor (CMOS) electronics of this type, together with four different classes of sensors and actuators in addressable arrays, two options for power supply and a wireless control strategy. A transient silicon device capable of delivering thermal therapy in an implantable mode and its demonstration in animal models illustrate a system-level example of this technology.

Analytical models for dissolution of the constituent materials represent important design tools for transient electronic systems that are configured to disappear in water or biofluids. Here, we present solutions for reactive-diffusion in single- and double-layered structures, in which the remaining thicknesses and electrical resistances are obtained analytically [2]. The dissolution time and rate are defined in terms of the reaction constants and diffusivities of the materials, the thicknesses of the layer, and other properties of materials and solution. These models agree well with the experiments for single layers of Mg and SiO_2, and double layers of Mg/MgO. The underlying physical constants extracted from analysis fall within a broad range previously reported in other studies; these constants can be extremely sensitive to the morphologies of the materials, temperature, and the PH value, concentration, and properties of the surrounding liquid.

[1] Hwang et al., "A physically transient form of silicon electronics," Science, v 337, pp 1640-1644, 2012.
[2] Li et al., "An analytical model of reactive diffusion for transient electronics," Advanced Functional Materials (in press).
[3] Dagdeviren et al., "Transient, biocompatible electronics and energy harvesters based on ZnO," Small (in press).

Surface instabilities of neo-Hookean solids and ruga mechanics

Kyung-Suk Kim

Abstract

Some classical problems of neo-Hookean solid surface instabilities are recently resurfaced due to emergence of needs for nano and biotechnology. In contrast to the classical Biot's solution of linear bifurcation analysis on the surface stability of a flat free surface under lateral compression, a stable branch of creasing followed by snap buckling has been computationally uncovered by Mahadevan's and Suo's groups. The lower limit of the subcritical compressive strain was found to be 35.2% while the critical strain set by Biot is 45.6%. Subsequently Hutchinson and his associates have investigated imperfection sensitivity of the crease-snap limit strain. Here, we introduce a parametric study of creasing with Koiter analysis for a neo-Hookean solid with an exponentially decaying modulus distribution. The parametric study provides various branches of stable or unstable, supercritical or subcritical equilibrium configuration families. These branches delineate flat, wrinkle, instantaneous crease, setback crease and fold crease phases on the plane of the normalized wave-number of the crease or wrinkle periodicity versus the compressive strain. The phase map is called the ruga phase diagram as the Latin word ruga stands for collection of large amplitude wrinkles, crease, ridges and folds. Upon unloading the crease states we could trace the stable branches of creasing down to the subcritical bifurcation limits for different wave-numbers. The parametric study reveals that the subcritical bifurcation limit indeed converges to 35.2% as the modulus decay parameter approaches that of a homogeneous half space. The ruga phase diagram is then used to design experimental procedures to make periodic folds of a graphene sheet attached to a PDMS substrate. Implications and utilities of the ruga phase diagram on biomechanics are also discussed.

Stress driven diffusion in bone tissue

Leslie Banks-Sills, Gustav Lindberg, Per Ståhle, Ingrid Svensson

Abstract

The growth and resorption of bone are governed by interaction between several cells such as bone forming osteoblasts, osteocytes, lining cells and bone resorbing osteoclasts. The cells considered here reside in the periosteum (at the outer boundary of the bone). Further, they are believed to be activated by certain substances to initiate bone growth. The present study focuses on the role that stress driven diffusion plays in the transport of these substances from the medullary cavity to the periosteum. There have been several mathematical models proposed to explain the observed behaviour. A different approach is taken here in which the bone is treated from a macroscopic view point.

Both one and two-dimensional models will be considered. Using the one-dimensional model, an analytic solution is obtained for the concentration at the periosteum of bone nutrients, such as nitric oxide synthase (NOS) or messenger molecules, such as prostaglandin E2 (PGE2), which are absorbed by osteoblasts. Equations for the flux of these nutrients are written for the cross-section of a long bone. The obtained partial differential equation is linearized and solved analytically. The effect of loading frequency, number of cycles and strain level is examined for several experiments that were found in the literature. It is seen that the concentration is greatest on the tensile side of the bone; this location coincides with the greatest amount of bone modeling. Next, a two-dimensional model of the cross-section of a long bone is considered. Calculations of stress driven diffusion are performed under steady state conditions. A sinusoidal time dependence is assumed for the concentration of nutrients. In this way, it was possible to reformulate the problem to determine an analogy with the bending of a plate in the shape of the bone cross-section on an elastic foundation. This problem was solved by means of the finite element method. The concentration of nutrients in the cambium layer of the periosteum was obtained for different choices of load frequencies. The results are compared to experimental findings suggesting increased bone growth occurs in the neighborhood of relatively high nutrient concentration.

Adhesion of cells and the influence of cytoskeletal contractility

Robert M. McMeeking

Abstract

Almost all eukaryotic cells are capable of adhering to an extra-cellular matrix, to other cells, to hard and soft tissue and to artificial substrates, e.g. coated glass slides. Such adhesion occurs by specific and non-specific interactions between substrate ligands and cellular transmembrane protein complexes. An additional phenomenon that is often coupled to cellular adhesion is cytoskeletal contractility driven by protein motors, with the commonest example being that due to myosin cross-bridging with actin filaments. Cases include smooth muscle cells, fibroblasts, endothelial cells and cardiac muscle cells. Observations indicate that the size of adhesive protein complexes, known as focal adhesions, is proportional to the degree of cell contractility, and the magnitude of the forces applied are also similarly controlled. Such phenomena have been incorporated into a chemo-mechanical model for cell adhesions interacting with ligands that are subject to contractile forces from the cytoskeleton. This model has been used successfully to simulate various cellular phenomena. These include the sensitivity of cell contractile forces to substrate stiffness, the orientation of cytoskeletal stress-fibres in smooth muscle cells that are cyclically stretched, and the location of focal adhesions and stressfibers in cells adhering to patterned shapes of fibronectin, a ligand bearing protein. The model is also used to simulate the process of a spherical cell developing adhesion to a flat surface, and the shearing of an adhered cell on a flat surface where the cell body is forced sideways by a blunt tool.

Notes

List of participants

Belgium			
	Thomas Pardoen	Université Catholique de Louvain	thomas.pardoen@uclouvain.be
France			
	Ahmed Benallal	LMT-Cachan	benallal@lmt.ens-cachan.fr
	Jean-Baptiste Leblond	UMPC, Institut Jean Le Rond d'Alembert, Paris	jbl@lmm.jussieu.fr
	Michael Raous	LMA/CNRS, Marseille	raous@lma.cnrs-mrs.fr
Germany			
	Hans Obrecht	TU Dortmund	hans.obrecht@udo.edu
	Bob Svendsen	RWTH Aachen	bob.svendsen@rwth-aachen.de
Italy			
	Lorenzo Bardella	University of Brescia	lorenzo.bardella@ing.unibs.it
Israel			
	Leslie Banks-Sills	Tel Aviv University, Ramat Aviv	banks@eng.tau.ac.il
Japan			
	Mitsutoshi Kuroda	Yamagata University, Yonezawa	kuroda@yz.yamagata-u.ac.jp
Netherlands			
	Marc Geers	Eindhoven University of Technology, Eindhoven	m.g.d.geers@tue.nl
	Erik van der Giessen	Zernike Institue for Advanced Materials, Groningen	E.van.der.Giessen@rug.nl
Norway			
	Odd Sture Hopperstad	Norwegian University of Science and Technology, Trondheim	odd.hopperstad@ntnu.no
Saudi Arabia			
	Choon Fong Shih	King Abdullah University of Science & Technolgy	shih@kaust.edu.sa
	Li Cheng	King Abdullah University of Science & Technolgy	lily6888@gmail.com
Spain			
	Pilar Ariza	University of Seville	mpariza@us.es
	Javier Llorca	Polytechnic University of Madrid	javier.llorca@imdea.org
Sweden			
	Jonas Faleskog,	KTH, Stockholm	faleskog@kth.se
	Matti Ristinmaa	Lund University	matti.ristinmaa@solid.lth.se
	Bertil Storåkers,	KTH, Stockholm	bertil@kth.se
	Per Ståhle	Lund University	per.stahle@solid.lth.se
	Mathias Wallin	Lund University	mathias.wallin@solid.lth.se
Switzerland			
	William Curtin	EPFL, Lausanne	william.curtin@epfl.ch
UK			
	René de Borst	University of Glasgow	Rene.DeBorst@glasgow.ac.uk
	Vikram Deshpande	University of Cambriidge	vsd@eng.cam.ac.uk
	Norman Fleck	University of Cambridge	naf1@eng.cam.ac.uk
	John Huber	University of Oxford	john.huber@eng.ox.ac.uk
	John Willis	University of Cambridge	jrw1005@cam.ac.uk

USA

Lallit Anand	MIT, Cambridge	anand@mit.edu
John Bassani	University of Pennsylvania, Philadelphia	bassani@seas.upenn.edu
Amine Benzerga	Texas A&M University, College Station	benzerga@tamu.edu
Ben Freund	University of Illinois at Urbana-Champaign	lbf@illinois.edu
Huajian Gao	Brown University, Providence	huajian_gao@brown.edu
Yonggang Huang	Northwestern University, Evanston	y-huang@northwestern.edu
John W. Hutchinson	Harward University, Cambridge	hutchinson@husm.harvard.edu
Kyung-Suk Kim	Brown University, Providence	kyung-suk_kim@brown.edu
Stelios Kyriakides	University of Texas at Austin	skk@mail.utexas.edu
Jeffrey Kysar	Columbia University, New York	jk2079@columbia.edu
Robert McMeeking	University of California, Santa Barbara	rmcm@engineering.ucsb.edu
Alan Needleman	University of North Texas, Denton	needle@unt.edu
Mark Rashid	University of California, Davis	mmrashid@ucdavis.edu
Zhigang Suo	Harvard University, Cambridge	suo@seas.harvard.edu
Michael Thouless	University of Michigan, Ann Arbor	thouless@umich.edu

Denmark

Joe Alexandersen	Technical University of Denmark	joealex@mek.dtu.dk
Casper S. Andreasen	Technical University of Denmark	csa@mek.dtu.dk
Danial Ashouri Vajari	Technical University of Denmark	dvaj@mek.dtu.dk
Niels Bay	Technical University of Denmark	nbay@mek.dtu.dk
Christian Berggreen	Technical University of Denmark	cbe@mek.dtu.dk
Esben Byskov	Aalborg University	eb@civil.aau.dk
Henrik Carlsen	Technical University of Denmark	hc@mek.dtu.dk
Michele Cerullo	Technical University of Denmark	mcer@mek.dtu.dk
Philippe Couturier	Technical University of Denmark	phicout@mek.dtu.dk
Salim El-Naaman	Technical University of Denmark	saeln@mek.dtu.dk
Hans Nørgaard Hansen	Technical University of Denmark	hnha@mek.dtu.dk
Jan Høgsberg	Technical University of Denmark	jhg@mek.dtu.dk
Henrik Myhre Jensen	Aarhus University	hmj@agse.dk
Freja N. Jespersen	Technical University of Denmark	frnj@mek.dtu.dk
Steen Krenk	Technical University of Denmark	sk@mek.dtu.dk
Mark Laier-Brodersen	Technical University of Denmark	mlai@mek.dtu.dk
Brian Nyvang Legarth	Technical University of Denmark	bnl@mek.dtu.dk
Britta Lindgreen	NOV Flexibles	blindgreen0510@gmail.com
Tore Lucht	MAN Diesel & Turbo	Tore.Lucht@man.eu
Erik Lund	Aalborg University	el@m-tech.aau.dk
Lars P. Mikkelsen	Technical University of Denmark	lapm@dtu.dk
Kim Lau Nielsen	Technical University of Denmark	kin@mek.dtu.dk
Christian Niordson	Technical University of Denmark	cn@mek.dtu.dk
Niels Olhoff	Aalborg University	no@m-tech.aau.dk
Niels L. Pedersen	Technical University of Denmark	nlp@mek.dtu.dk
Pauli Pedersen	Technical University of Denmark	Pauli@mek.dtu.dk
Preben T. Pedersen	Technical University of Denmark	ptp@mek.dtu.dk
Pia Redanz	Det Norske Veritas	pia.redanz@dnvkema.com
Ann Bettina Richelsen	Technical University of Denmark	abri@mek.dtu.dk
Ole Sigmund	Technical University of Denmark	Sigmund@mek.dtu.dk
Bent F. Sørensen	Technical University of Denmark	bsqr@dtu.dk
Viggo Tvergaard	Technical University of Denmark	viggo@mek.dtu.dk
Grethe Winther	Technical University of Denmark	grwi@mek.dtu.dk
Sanita Zike	Technical University of Denmark	zike@dtu.dk