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Mechanics of Materials

Organised by
Reinhold Kienzler (Bremen)
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January 22nd – January 28th, 2006

Abstract. All up-to-date engineering applications of advanced multi-phase materials necessitate a concurrent design of materials (including composition, processing routes, microstructures and properties) with structural components. Simulation-based material design requires an intensive interaction of solid state physics, material physics and chemistry, mathematics and information technology. Since mechanics of materials fuses many of the above fields, there is a pressing need for well founded quantitative analytical and numerical approaches to predict microstructure-process-property relationships taking into account hierarchical stationary or evolving microstructures. Owing to this hierarchy of length and time scales, novel approaches for describing/ modelling non-equilibrium material evolution with various degrees of resolution are crucial to linking solid mechanics with realistic material behavior. For example, approaches such as atomistic to continuum transitions (scale coupling), multiresolution numerics, and handshaking algorithms that pass information to models with different degrees of freedom are highly relevant in this context. Many of the topics addressed were dealt with in depth in this workshop.

Mathematics Subject Classification (2000): 74-XX.

Introduction by the Organisers

The workshop *Mechanics of Materials*, organised by Reinhold Kienzler (Bremen), David L. McDowell (Atlanta) and Ewald A. Werner (München) was held January 22nd–January 28th, 2006. The workshop attracted some 40 participants with a wide geographic spread. Special attention was devoted to increasing the participation of younger members of the related research community.
Mechanics of Materials is a broad, interdisciplinary subject that focusses on the intersection of Applied Mathematics, Continuum Mechanics, Material Physics and

applications. To address important, emerging topics related to these interdisciplinary areas, several themes were pursued in distinct sessions, each with keynote addresses and extended discussions. The following main topics were treated:

- Emerging topics at the interface of Mechanics of Materials and Materials Science
- Inhomogeneous materials and phase transformations
- Configurational Mechanics
- Atomistic and discrete modelling approaches to defects and defect structures
- Mathematical modelling new materials and engineering applications
- Elasticity, Plasticity and time dependent material behavior

Although these fields appear to be quite unconnected, certain physical properties and numerous mathematical approaches were identified as common structures. This includes basic balance and conservation laws as well as variational principles for establishing and solving the evolving partial differential equations. Bridging scales from electrons to macroscopic structures by various consistent methods we were able to arrive at a more complete picture of modelling material behavior and the associated mathematical challenges.

The unique atmosphere at the Institute offered an extraordinary opportunity for intense, amiable exchange of currently emerging, detailed and conceptual ideas. The significant amount of time devoted to fruitful discussion is certainly an element that made this meeting in Oberwolfach distinct from other outstanding technical venues. Many new collaborative relationships were initiated.

The following abstracts very well summarize both the keynote lectures and the additional contributions to the discussion.

It was our great pleasure to celebrate during an informal gathering the 50th anniversary of Horst Lippmann as participant, organizer and long-term intellectual contributor to many Oberwolfach workshops.

Workshop: Mechanics of Materials

Table of Contents

Abstracts

State of the art in engineering creep mechanics and open questions

Holm Altenbach
(joint work with Konstantin Naumenko)

The research in engineering creep mechanics is focussed on the description of creep of various materials (i.e. the time-dependent microstructural changes and the phenomenological behavior) and the analysis of structural elements under creep conditions. In this sense one has to take into account creep, relaxation and other effects. The equations allowing the description of the material behavior and the analysis of structural elements should be useful in the case of uniaxial and multi-axial stress states. In addition, the stress states can be inhomogeneous and anisotropic. Up to now (as was shown earlier [1, 2]) sometimes one gets significant disagreements between the results of the simplified (engineering) analysis and the improved estimations. The explanation of these discrepancies is one of the main research directions in engineering creep mechanics.
The division of the creep behavior into three states (primary, secondary and tertiary creep) is accepted by the scientific community. During the last years the materials science based approach was influenced by the publications of Ashby, Nabarro and others. The structural mechanics approach was summarized, for example, by Betten, Hayhurst, Skrzypek and Hyde. At present, the induced anisotropy and non-proportional loading is mostly discussed in the literature.
Our investigations are directed toward the creep-damage behavior of thin-walled structural elements (beams, plates and shells). The performed numerical calculations show effects which cannot be described by the classical theory of Euler-Bernoulli-beams or Kirchhoff-plates. In addition, the calculations based on 2D finite elements are in a significant disagreement with 3D calculations. The reasons are the thickness integration, the 3D constitutive and evolution equations and the 2D structural mechanics equations [3, 4].
The state of the art in engineering creep mechanics can be sorted into four groups:

- empirical models ("curve fitting")
- materials science based models (mechanism related equations)
- micromechanical models (representative volume homogenization)
- continuum mechanics based models (balance equations).

They all show advantages and disadvantages. For example, the first approach is very simple, but the extension of the models is often impossible. The materials science based models are mostly one-dimensional and based on scalars. The micromechanical models are founded on an idealized microstructure. The continuum mechanics models are fruitful, since they are able to represent the three-dimensional behavior. Using tensors of different ranks the analysis of the creep damage behavior is possible and the extension, for example, from the full isotropic

case to various anisotropic states is possible. As was shown in [5, 6] the continuum mechanics approach allows for a sound theoretical analysis of isotropic and anisotropic creep-damage.
From the analysis of an example (multi-pass weld metal) and the results of previous publications the following open questions can be formulated:

- How can the approach used in the analysis of transversally isotropic material behavior be extended to the orthotropic case?
- How can the secondary anisotropic equations be extended to the tertiary creep regime?
- How should the identification procedures be realized?

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Modeling dislocations and disclinations with finite micropolar elastoplasticity

Douglas J. Bammann
(joint work with John D. Clayton, David L. McDowell)

Aspects of a constitutive model for characterizing crystalline metals containing a distribution of dislocation and disclination defects are presented [1, 2, 3, 4]. Kinematics, balance laws, and general kinetic relations are developed from the perspective of multiscale volume averaging upon examination of a deforming crystalline element containing a distribution of displacement discontinuities in the form of translational and rotational lattice defects, i.e., dislocations and disclinations. The macroscopic kinematic description is characterized by a three-term multiplicative decomposition of the deformation gradient. The micro-level description follows from an additive decomposition of an affine connection into contributions from populations of dislocations and disclinations to the distortion of the lattice directors. Standard balance equations apply at the macroscopic scale, while momentum balances reminiscent of those encountered in micropolar elasticity (i.e., couple stress theory) are imposed at the micro-level on first and second order moment stresses associated with geometrically necessary defects. Thermodynamic

restrictions are presented, and general features of kinetic relations are postulated for time rates of inelastic deformations and internal variables. Micropolar rotations are incorporated to capture physics that geometrically necessary dislocations stemming from first order gradients of elastic or plastic parts of the total deformation gradient may alone be unable to reflect, including evolution of defect substructure at multiple length scales and incompatible lattice misorientation gradients arising in ductile single crystals subjected to nominally homogeneous deformation.
During large plastic deformations of ductile fcc metals grain subdivision and dislocation substructure formation substantially affect slip system activity, strain hardening, stored lattice energy, and texture evolution in single and polycrystals. Also measured within pure ductile metals and certain alloys at large deformations and/or high temperatures are long range internal stress fields associated with misoriented subgrain boundaries. The formation of cells of relatively small misorientation organized collectively into larger cell blocks, with average misorientations between blocks usually significantly greater in magnitude than those between cells. Upon increasing applied strain, cell block sizes generally decrease at faster rate than do cell sizes. In the context of our theory, the disclination concept can be used to capture the gradients of lattice rotation at the cell block boundaries that arise from the organization and superposition of relatively small misorientations between the cells, reflected here by geometrically necessary dislocations. Additionally, when the kinetics of evolution of statistically stored defects, geometrically necessary dislocations, and geometrically necessary disclinations are properly coupled, cells and cell blocks will emerge in single crystals upon homogeneous loading, as observed in the aforementioned experiments, and the subdivided crystal will attain an energetically favorable configuration (i.e., a local minimum in free energy over its entire volume). We suggest that a lack of local convexity or, more precisely, lack of cross-quasiconvexivity in the terminology of Carstensen et al. [5] stems from the superposition of free energy wells associated with different mechanisms, in our case associated with generation and interaction of defect densities of various origins (e.g. populations of geometrically necessary and statistically stored dislocations and disclinations).

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Modelling martensitic transformation at different length scales

Marcel Berveiller

Transformation induced plasticity (TRIP) occurs when a martensitic phase change takes place in an elastic-plastic parent phase (so called austenite). Due to internal stresses produced by the (incompatible) transformation strain, an additional plastic flow occurs (in the austenite as well as inside the martensite). Improvement of mechanical strength and simultaneously large ductility of TRIP steels are due to this martensitic (Ms) transformation [1]. The behavior of a Representative Volume Element undergoing Ms transformation and plastic flow is described from a scale transition point of view based on classical micromechanics and thermomechanics of moving boundaries. We present the core of two micromechanical models able to describe the TRIP phenomenon coupled with plastic flow.

Crystallographic model for TRIP materials: At the microscopic level, the transformation mechanism is represented by moving boundaries, the boundary being the interface between the austenitic matrix and growing martensitic domains. Let $\varepsilon^{\mathrm{t}}(r)$ be the transformation field equal to known uniform values: $\varepsilon^{\mathrm{t}} = \varepsilon^{\mathrm{t}i}$, $i = 1$ to 24 for 24 variants inside the martensitic domains. The volume average of the inelastic strain rate $\varepsilon^{\mathrm{tp}}(r)$ over the RVE volume V is given by:

$$\dot{E}^{\mathrm{tp}} = (1-f)\bar{\dot{\varepsilon}}^{\mathrm{pA}} + f\bar{\dot{\varepsilon}}^{\mathrm{pM}} + \sum_i \varepsilon^{\mathrm{t}i}\dot{f}^i\,, \tag{1}$$

where $f = \sum f^i$ is the total volume fraction of martensite and f^i represents the volume fraction of variant i. The evolution equation for the plastic flow ($\dot{\varepsilon}^{\mathrm{p}}$) inside the austenite and the martensite may be deduced from the classical flow rule or in the frame-work of crystal-plasticity [1], if the corresponding driving forces are given (Cauchy stress inside austenite and martensite). For the evolution of the volume fractions, the associated driving forces have to be deduced from a thermodynamical approach. Let $w + \varphi$ be the density of elastic and chemical energies. The Helmholtz free energy of the whole RVE is given by $\Phi = \frac{1}{V}\int\limits_V (w+\varphi)\mathrm{d}V$ and its time derivative is:

$$\dot{\Phi} = \frac{1}{V}\int\limits_V (\dot{w}+\dot{\varphi})\mathrm{d}V + \frac{1}{V}\int\limits_A [w+\varphi]\omega_\alpha n_\alpha \mathrm{d}A\,, \tag{2}$$

where A is the (moving) interface between austenite and martensite and $\omega_\alpha\, n_\alpha$ is the normal velocity of the interface.

Using Hadamard's condition, $[v_i] = -[u_{i,k}]n_k\omega_\alpha n_\alpha$, the intrinsic dissipation D is given by [2]:

$$D = \frac{1}{V}\int\limits_V \sigma : \dot{\varepsilon}^{\mathrm{p}}\mathrm{d}V - \frac{1}{V}\int\limits_A \frac{1}{2}\left((\sigma^+ + \sigma^-) : [\varepsilon^{\mathrm{t}}] + [\varphi]\right)\omega_\alpha n_\alpha \mathrm{d}A\,. \tag{3}$$

The volume part corresponds to the dissipation by plastic flow and the second term represents the surface dissipation. If the martensitic domain can be represented by an ellipsoidal inclusion with fixed half-axes, the driving force F for a growing ellipsoidal inclusion is given thanks to Eshelby's tensor S by [3]:

$$F = \sigma^- : \varepsilon^{\mathrm{t}} - B(T - T^0) + \frac{1}{2}\varepsilon^{\mathrm{t}} : C : (I - S) : \varepsilon^{\mathrm{t}}\,, \tag{4}$$

where σ^- is the (uniform) stress inside the inclusion and $B(T-T^0)$ corresponds to the linearised form of the change of chemical energy. Based on this driving force and on the resolved shear stress on the slip systems in austenite and martensite, the behavior of the single crystal and the polycrystal may be deduced by classical scale transition techniques.

In order to derive a **physically well founded simplified model**, we propose in a second part to model the behavior of the (polycrystalline) Representative Volume Element by considering the material as a non-linear two-phase composite with evolving microstructure. The behavior of the evolving composite is deduced from a micromechanical approach (non-linear self consistent approach) in the context of the deformation theory like Hencky-Mises for plasticity. In that case, the equations of the problem are given by the field equations $\operatorname{div}\sigma = 0$ and $\varepsilon = \operatorname{sym}\operatorname{grad} u$ and the behavior $\sigma = l^{\mathrm{M}} : (\varepsilon - \varepsilon^{\mathrm{t}})$ inside the martensite and $\sigma^{\mathrm{A}} = l^{\mathrm{A}} : \varepsilon$ inside the austenite, where ε^{t} describes the mean transformation strain over the volume of martensite with volume fraction f. The macroscopic behavior $\Sigma = L : (E - E^{\mathrm{t}})$ is deduced from a self consistent scale transition model [4], where L and E^{t} are respectively the overall secant modulus and the global transformation strain. ε^{t} and f are given from thermodynamical considerations.

For isotropic and incompressible behavior (L, l^{M}, and l^{A} depend only on the corresponding (non-linear) shear modulus μ, μ^{M}, μ^{A} and $\varepsilon^{\mathrm{t}}_{kk} = 0$), two equations for μ and E are deduced from the model [5]:

$$f\frac{5\mu}{3\mu + 2\mu^{\mathrm{M}}} + (1 - f)\frac{5\mu}{3\mu + 2\mu^{\mathrm{A}}} = 1\,, \tag{5}$$

$$E^{\mathrm{T}}_{ij} = \frac{5\mu^M}{3\mu + 2\mu^M} f\varepsilon^{\mathrm{t}}_{ij}\,. \tag{6}$$

The last formula corresponds to the so called Greenwood-Johnson effect [6], where the macroscopic strain created by $f\,\varepsilon^{\mathrm{t}}$ is much larger than $f\,\varepsilon^{\mathrm{t}}$, since in general $\mu^{\mathrm{M}} > \mu$. This relatively compact model is easily to be integrated into a finite element code.

For both models the theoretical results are in good agreement with the experimental ones and show the complementarities of the two approaches.

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Texture based material models

Thomas Böhlke

From the numerical point of view, large scale FE computations based on the Taylor model are very time-intensive and storage-consuming, if the crystallographic texture is approximated by several hundreds of discrete crystals. The presentation focuses on the problem of approximating a given crystallite orientation distribution function [3] by a small set of texture components [2]. The equivalence of this task to a Mixed Integer Quadratic Programming problem (MIQP) is shown [1]. The Taylor model in its standard form [4, 5], which is based on discrete crystal orientations, has the disadvantage that the anisotropy is significantly overestimated, if only a small number of crystal orientations is used. Therefore a modified Taylor model is discussed which allows to reduce the overestimation. The peak intensity is reduced by modeling the isotropic background texture by an isotropic material law. Furthermore, an extension of the widely used Mises-Hill anisotropic plasticity model is suggested and discussed. In a first step the Mises-Hill anisotropy tensor - which specifies the quadratic flow potential - is expressed in terms of the 4th-order moment tensor of the crystallite orientation distribution function. It is well known that specific anisotropies of polycrystalline metals generally cannot be modeled by quadratic flow potentials. Motivated by this fact the concept of anisotropic equivalent stress measures is generalized by incorporating the higher-order moment tensors in a second step.

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Analysis of thin coatings containing two types of transforming inclusions

Helmut J. Böhm
(joint work with F. Dieter Fischer)

Thin layers are studied that consist of an elastic matrix in which two or more populations of elastic spheroidal inhomogeneities are embedded. The mechanical contributions to the energetics of the growth and shrinking of the inhomogeneities by phase transformations are considered, the latter being described by phase-wise homogeneous stress-free transformation strains. Mean-field approaches are an obvious option for estimating the strain energy densities of such systems, which provide the macroscopic mechanical contribution to the energetics of the phase transformations. A Mori–Tanaka expression for the strain energy densities of two-phase systems was given e.g. by Mura [1]. The Transformation Field Analysis (TFA) of Dvorak et al. [2] is well suited for handling multi-phase transformation problems in a mean field framework, and a version of the TFA employing Mori–Tanaka approximations [2] is brought to bear on the present problem. Three types of macroscopic boundary condition are considered, viz. free macroscopic deformations, fully constrained macroscopic deformations and "layer like" constraints. The latter consist of fully constrained in-plane plus free out-of-plane macroscopic strains and correspond to a thin layer perfectly bonded to a rigid substrate. Whereas the strain energy density pertains to the macroscopic energetics of phase transformations, the mechanical driving force at the interface contributes to the evolution of shape of inhomogeneities. On the basis of Eshelby's expressions for the fields in dilute matrix–inclusion systems [3, 4] the position-dependent stress and strain jumps at the interface can be obtained following [5]. These jumps, in turn, allow the evaluation of the mechanical driving force [6] at any point on the surfaces of spheroidal inhomogeneities embedded in a matrix [7]. In general, such formalisms cannot follow the evolution of the shapes of inhomogeneities, because in most cases they quickly deviate from spheroids. However, "snapshots" can be generated that point out trends. The method can be extended to non-dilute inhomogeneities in a "Mori–Tanaka sense", in which case it provides estimates on the ensemble average of the local mechanical driving forces acting on the interfaces.
The TFA-based mean field approach is applied to studying thin layers consisting of a $Ti_{0.34}Al_{0.66}N$ matrix containing transforming spherical TiN and AlN particles. For this system the transformation strains of TiN and AlN are of opposite signs and different magnitudes [8]. "Isotropized" approximations to the elastic moduli of the phases (all three of which show f.c.c. symmetry) are employed.
For the $Ti_{0.34}Al_{0.66}N$ system the macroscopic boundary conditions markedly influence the predictions for the dependence of the strain energy density on the phase volume fractions. The results on the mechanical driving force indicate that (as expected) initially spherical inhomogeneities remain spherical for free and fully constrained macroscopic boundary conditions, but become non-equiaxed for the "layer like" constraints.

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A consistent Eulerian formulation for finite thermo-elastoplasticity

Otto T. Bruhns

Recently it has been demonstrated that, on the basis of the separation $\mathbf{D} = \mathbf{D}^e + \mathbf{D}^p$ arising from the split of the stress power and two consistency criteria for objective Eulerian rate formulations, it is possible to establish a consistent Eulerian rate formulation of finite elastoplasticity in terms of the Kirchhoff stress and the stretching, without involving additional deformation-like variables labelled "elastic" or "plastic". It has further been demonstrated that this consistent formulation leads to a simple essential structure implied by the work postulate, namely, both the normality rule for plastic flow $\mathbf{D}^p$ and the convexity of the yield surface in Kirchhoff stress space. Here, we attempt to place such an Eulerian formulation on the thermodynamic grounds by extending it to a general case with thermal effects, where the consistency requirements are treated in a two-fold sense. First, we propose a general constitutive formulation based upon the foregoing separation as well as the two consistency criteria. This is accomplished by employing the corotational logarithmic rate and by incorporating an exactly integrable Eulerian rate equation for $\mathbf{D}^e$ for thermo-elastic behaviour. Then, we study the consistency of the formulation with thermodynamic laws. Towards this goal, simple forms of restrictions are derived, and consequences are discussed. It is shown that the proposed Eulerian formulation is free in a sense of thermodynamic consistency. Namely, a Helmholtz free energy function may be found such that the restrictions from the thermodynamic laws can be fulfilled with positive internal dissipation for arbitrary forms of constitutive functions included in the constitutive formulation. In particular, that is the case for the foregoing essential constitutive structure in the purely mechanical case. These results eventually lead to a complete constitutive theory for coupled fields of deformation, stress and temperature in thermo-elastoplastic solids at finite deformations.

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Multiscale modelling of defects in crystals

John D. Clayton

Two complimentary approaches to describing the mechanics of crystalline materials containing distributed defects are discussed. In the first approach, a continuum model of finite micropolar elastoplasticity is formulated to capture the physics of distributed dislocations and disclinations. In the second approach, asymptotic homogenization methods permit the calculation of effective mechanical properties (e.g. strain energy, stress, and stiffness) of a representative crystalline element containing statistically periodic defect structures. Fundamental nonlinear-elastic mechanical behavior of crystalline materials at the length scale of a macroscopic continuum is described, given a-priori a complete characterization of discrete atomic interactions. The atomistic-continuum scaling technique complements the micropolar continuum theory, as the former approach may conceptually be used as a tool

to develop the latter, specifically to support formulation of free energy potentials accounting explicitly for the presence of crystal defects.
Our continuum framework [1, 2] is founded upon two major kinematic assumptions, the first being a three-term decomposition of the average deformation gradient for a crystal element, with the intermediate term, non-standard in the literature [3], accounting for the presence of defects that affect the average lattice arrangement and internal residual stresses within the crystalline volume element. Also introduced in this decomposition are the elastic deformation representing both the recoverable lattice stretch associated with the average applied stress acting on the element and rigid-body rotations of the lattice, as well as the plastic deformation accounting for the partition of fluxes of mobile defects that leaves the lattice unperturbed.
The second major assumption is an additive decomposition of a linear connection describing spatial gradients of the slip directions and lattice director vectors between neighboring crystalline elements. Christoffel symbols of this connection describe gradients of the director vectors due to first-order gradients in the lattice deformation, following [4]. A micromorphic variable [5, 6] participates in the connection as well, describing the following physics: a micro-rotation associated with disclinations, an isotropic micromorphic expansion associated with point defects, and a general micromorphic strain that may be used to represent arbitrary lattice director deformations when superposed with the other terms. Dislocation and disclination density tensors then follow from the torsion and curvature, respectively, of the connection, the latter vanishing when the connection is integrable.
Regarding thermodynamics, we make the following general assumption regarding the dependency of the Helmholtz free energy function for the crystalline volume element. The covariant elastic strain tensor is included to model the change of average elastic energy density with a change of external loads. The left stretch tensor associated with the intermediate deformation map is incorporated to reflect contributions to the free energy from residual microelasticity within the volume element, and may be non-negligible when the deformation within the volume element is heterogeneous [7]. The elastic energies due to net lattice curvatures in the volume element induced by geometrically necessary dislocations and disclinations are reflected, respectively, by the inclusion of the corresponding rank-two tensors of defect density. Notice that when the intermediate mapping and disclinations vanish, the formulation agrees with constitutive assumptions made in previous theories [8] in the absence of disclinations. Scalar parameters are incorporated to model elastic self-energy of the statistically stored dislocation density and the statistically stored disclination density. The macroscopic Cauchy stress obeys the standard linear and angular momentum balances and reflects the average traction carried by a local crystalline volume element in the current configuration. Microforces reflect higher-order moments of the microscopic traction distribution supported by the volume element. Contravariant variations of these forces satisfy coupled microscopic momentum balances [1], analogous to the micropolar elastic balance laws suggested by others [5, 9].

The asymptotic homogenization technique forwarded here [10] falls into the category of spatially decoupled multiscale methods. In this approach, discrete calculations are conducted at the atomistic level, with each characteristic volume element of atoms subjected to periodic boundary conditions. Asymptotic homogenization methods [12] are concurrently employed to deduce the macroscopic tangent stiffness associated with the mechanical response of the ensemble. The Cauchy-Born approximation [12] is invoked for imposition of the bulk continuum deformation, with the fine-scale deformation of the atoms identified with the inner displacements in the asymptotic solution. The present approach is ideal for addressing the response of microstructures containing spatially periodically-distributed defects, in contrast to coupled methods [13] that appear better suited to addressing more localized defect configurations. This is because only one or a few defects need be simulated explicitly at the atomistic level within the context of the periodicity assumption invoked in our homogenization scheme.

Our framework was implemented numerically and applied to study the nonlinear elastic response of BCC tungsten (W) containing periodically distributed vacancies, screw dislocations, screw dislocation dipoles, and low-angle twist boundaries (the latter described via disclination concepts [1]). It was found that defect energies associated with vacancies, screw dislocations, and screw dislocation dipoles tended to increase with applied uniaxial stretching, while energies of twist boundaries tended to decrease with stretch. Elastic stiffness in the direction of stretch tended to decrease with increasing dislocation content, and increase with twist grain boundary area. Anisotropy of the elastic constants of W, nominally isotropic, was also demonstrated in the presence of defects and deformations. The model was implemented in a limited fashion to study the elastic-plastic response of W containing fixed distributions of [111](110)-screw dislocations. An oscillatory stress-strain response due to motion of atomic planes across Peierls barriers was demonstrated, and influences of dislocations on elastic moduli and strain energy densities were apparent from the multiscale calculations.

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Multiscale modelling in materials: atomic/continuum, dynamic, and discrete/continuum methods

William A. Curtin

Direct coupling of different modelling methods corresponding to different spatial resolutions can be necessary for problems in which a phenomenon at a small scale, e.g. crack growth by atomic-scale material separation, must be retained with full resolution in some local region of space but where driving forces for that phenomenon are caused by behavior in the surrounding regions, e.g. stresses generated by arrays of dislocations, where a less-detailed description is an acceptable approximation. The less-detailed description involves fewer overall degrees of freedom, leading to computational tractability, but must faithfully retain the important physical phenomena that influence the smaller-scale behavior. The key in such modelling is to create seamless interfaces between different methods and different scales. The interfaces must of course transmit the proper mechanical forces. In addition, mobile material defects – point defects, dislocations, etc. – must be able to move from one region to another without the introduction of artifacts. However, the methods typically have different constitutive behaviors or energy functionals, reflecting the different degrees of freedom involved, and can be non-linear, non-local, long-ranged, and/or dynamic. The coupling is thus more subtle than merely "grading" the system from one energy functional to another over some region. And, without attention to detail the coupling can often create artifacts that strongly limit the ability of the multiscale model to be useful and predictive. Here, we describe a hierarchical set of coupling methodologies for problems in the mechanics of materials with the ultimate goal of coupling atomistic, mesoscale dislocations, and continuum crystal plasticity within a single framework.

The first method is the coupling of a full atomistic region to a hyperelastic continuum region within a quasistatic framework without artifacts at the coupling interface [1]. This problem has been tackled by many workers in the last decade, with a variety of elegant formulations. However, many such formulations lead to artifacts/defects at the interface, the origins of which lie in the local/non-local mismatch between atomistic and continuum energy functionals. Methods to avoid artifacts inevitably sacrifice the existence of a single energy functional for the coupled system in favor of force-based analyses. This method is then augmented to seamlessly couple an atomistic region to a continuum region containing discrete dislocation plasticity, including the ability to pass dislocations across the atomistic/continuum boundary from one region to the other [2]. The discrete dislocation method eliminates all atomistic degrees of freedom but retains the dislocation cores as defects residing within an elastic continuum. Plasticity in the continuum then stems from motion of the dislocations, rather than through effective viscoplastic constitutive laws. Although current methods are reasonably successful for 2d plane strain models, in which the dislocations remain straight and are effectively point defects in 2d, the development of 3d models is a challenge.

The second method is atomistic/continuum coupling for finite-temperature, dynamic problems. Here, equilibrium and non-equilibrium phenomena are in direct competition. Dynamic events, such as crack growth or dislocation emission, generate non-equilibrium deformation waves that must propagate out of the atomistic regime and into the continuum without reflection at the interface, which would lead to artificial heating of the atomistic region. However, in the absence of such events, maintenance of equilibrium conditions in a canonical ensemble is critical for obtaining both the correct thermodynamics and the correct thermally-activated nucleation rate of the dynamic events. Elegant methods to handle seamless wave propagation have been developed and applied to a number of problems, but only at 0K and often for specialized atomic interactions. Methods to effectively thermostat a coupled atomistic/continuum domain have also been developed, but they do not prevent interface reflections. The use of an atomistic boundary region obeying Langevin dynamics is shown to address both problems adequately and also permit a decoupling of time scales [3], at the expense of suppression of wave propagation in the continuum.

The fourth method is the coupling of a discrete-dislocation plasticity region to a continuum crystal plasticity region. Discrete dislocation models can represent regions of material up to 10s of microns in size, but larger scales remain computationally prohibitive at present. However, the size scales at with dislocation models are necessary to account for "plasticity size effects" are on the order of 10 microns, suggesting that crystal plasticity at larger scales could be an adequate approximation. In this coupling, however, the transition is from a discrete system of defects (the dislocations) to a set of field equations for the plastic strains. It can be envisioned that suitably averaging can be done to relate a dislocation flux to a plastic strain rate, allowing for coupling of the defect flow. However, the loss of the dislocations is accompanied by a loss of their long-range stress fields and hence the problem has significant subtleties. As a precursor to full solution of this problem, we investigate the coupling of discrete diffusion to continuum diffusion, where discrete entities are tied to a field equation but the diffusing entities do not carry long range stress fields or singularities. We consider the specific case of kinetic Monte Carlo modeling of diffusion on a lattice coupled to a region described by the continuum diffusion equation. With the existence of a field equation, traditional domain decomposition ideas emerge as feasible, but with one discrete domain wherein suitable averaging of concentrations and fluxes yields boundary conditions for the continuum domain. We present one possible approach to this type of problem, along with appropriate convergence criteria and minimization of domains over which iterative approaches are needed [4].

In summary, multiscale modeling is a rich area at the intersection of physics, mechanics, mathematics, and materials science. We have identified relevant classes of multiscale problems that are attractive to materials scientists but that currently pose various theoretical difficulties that may be overcome by the construction of a broader mathematical framework for multiscale modeling.

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Asymptotic homogenization for elastic media with evolving microcracks

Cristian Dascalu

(joint work with E. Agiasofitou, G. Bilbie)

In this work, an asymptotic homogenization technique is used to describe the overall behavior of a damaged elastic body with a locally periodic distribution of growing micro-cracks that is loaded in tension. The microstructural deterioration is represented, at the macroscopic level, by a local internal variable which is the micro-crack length. An evolution damage law is deduced, through asymptotic homogenization, by assuming a microscopic fracture criterion of Griffith type. Finite element solutions are presented in order to illustrate this new approach. We show that the model leads to damage localization and macro-fracture nucleation.
Many papers have been devoted to the overall behavior of micro-fractured solids (see for instance Nemat-Nasser and Horii [1] for a review). Almost all these works are confined to the case of stationary cracks. As exceptions one can cite Prat and Bazant [2] or Caiazzo and Constanzo [3], which take into account the fracture evolution. Our aim is to model such phenomena by using a different method, with a good mathematical basis, that of asymptotic homogenization [5]. This method has been used for stationary micro-cracks by Leguillon and Sanchez-Palencia [4]. Our work is an extension of their results for evolving micro-cracks. We consider tension loadings and parallel micro-cracks oriented normal to the direction of loading. The mean orientation of a real system of micro-cracks, which are activated by such loadings is expected to be close to the normal direction. We assume traction-free conditions on crack faces.
Starting from the energy balance over elementary volumes we deduce a macroscopic damage evolution law, in which the micro-crack length naturally appears as a damage variable. The equilibrium equations are coupled with the damage evolution law, in a quasi-static system. In order to allow the classical homogenization procedure, we consider explicit time integration of the damage law, so the system becomes discrete in time and at every time instant the equilibrium equations are linear. For the corresponding time-continuous system we obtain an explicit expression of the tangent matrix and we analyze failure indicators, like the loss of ellipticity of the equilibrium equations. It is proved that the overall response involves softening for large micro-crack lengths.

Finite element solutions are obtained for two-dimensional geometries. The influence of the micro-cracks evolution on the homogenized mechanical response is analyzed through the obtained numerical solutions. We show that damage localization occurs prior to macro-crack nucleation. The macroscopic model involves an internal length (cell size), so mesh-independence is expected for the numerical solution. Extended proofs and more results will be presented in a future paper of the authors [6].

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Two-phase deformations of elastic solids: constitutive equations, strains, equilibrium and stability

Alexander B. Freidin
(joint work with Leah Sharipova, Elena Vilchevskaya, Yibin Fu, Igor Korolev)

In the talk we give a brief summary of the results obtained by our 'phase transitions team' during last years. Some of the recent publications are listed below. If phase transformations take place in a deformable body, the interface between two different phases can be viewed as a surface across which the displacement is continuous but the deformation gradient suffers a discontinuity. Equilibrium interfaces can exist not in any elastic material: it is known that a strain energy function must be nonconvex in some meaning. Another limitation is put on deformations. The fact that the conditions on the interface can be satisfied not for any deformations leads to the notion of phase transition zones (PTZs) formed by all strains which can exist on the equilibrium phase boundaries in a given material. The PTZ is determined entirely by the material properties, i.e. by the strain-energy function. The PTZ construction allows us to categorize strain-energy functions with respect to the existence of two-phase deformations and the type of interfaces in dependence on strain state. The PTZ can be used as a guide in searching for the appropriate constitutive equations, if the interfaces appearing for different deformation paths are known from experiments.
We examine a number of strain energy functions in both finite and small strains cases and construct corresponding PTZs. We show what types of the interfaces

are possible and demonstrate a variety of phase transformation behaviors as well as common features. We develop a procedure to examine the stability of two-phase deformations. Considering examples of spherically-symmetric two-phase deformations in various non-linear elastic materials, we study non-uniqueness and stability of the solutions obtained within the frameworks of the PTZs.
Then the nucleation of new phase areas is studied considering the case of small strains. We show that nuclei of different shape can appear on different deformation paths as well as at loading and unloading paths. We construct nucleation (transformation) surfaces and relate them with the PTZs. A model is developed for heterogeneous deformation due to multiple appearance of new phase areas. Two cases are examined dealing either with ellipsoidal nuclei or with newly appearing phase layers. An effective field approach is used to take into account the interaction of ellipsoidal nuclei at the initial stage of the transformation. Parameters of two-phase structure are found in dependence on average strains. Average stress-strain diagrams depending on the path of the phase transformation are constructed. Average and local strains are related with the PTZ.
We also study phase transformations in an inclusion under external stresses transmitted by a linear elastic matrix. Energy preferences of various two-phase states and one-phase states are investigated in dependence on the type of boundary conditions, the relative size of the inclusion, and relationships between the elastic moduli of the phases. Finally, the interaction between a crack and the phase transforming inclusion is discussed.
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Microstructure design using statistical correlation functions

Hamid Garmestani

A methodology for microstructure design is developed and applied to multi-phase microstructures using statistical continuum mechanics theory linking mechanical, magnetic, and transport properties to microstructures represented by statistical correlation functions. Texture and composite volume fractions are considered as one-point functions and grain boundary character distribution and particle to particle and the effect of precipitates can be introduced using pair correlation functions and higher order statistics. In this work, homogenization techniques based on statistical continuum mechanics are used to calculate effective properties on the knowledge of the N-point Distribution Functions. The evolution of the microstructure using the two-point correlation functions is compared to experimental results. The effect of second phase/particle and pore distribution is also shown to be well-represented by these distribution functions. The results are presented in the form of texture evolution for each of the phases and for the distribution of the multi-phase materials for a variety of initial conditions and deformation modes.

Microstructure Sensitive Design: Prior work produced results for elastic and inelastic properties for composites and polycrystalline materials [1, 2, 3, 4]. A framework for Microstructure Sensitive Design for textured polycrystalline materials using one-point orientation distribution function [5]. This formulation was extended to composites using pair correlation functions [6].

Recently a methodology was developed by Adams et. al. [1] that uses a spectral representation as a tool to allow the mechanical design to take advantage of the microstructure as a continuous design variable. This new approach, called microstructure-sensitive design (MSD) uses a set of Fourier basis functions to represent the microstructure (e.g. single orientations) as the material set [1]. The combination of all these elements of microstructure states can be used to construct the property enclosure for any particular structure. The procedure in this methodology can be summarized in the following:

- Microstructure representation: The microstructure and its details are represented by a set of orthogonal basis functions χ_n .

$$F(\chi_n, C_n) = \sum_n C_n \chi_n \,, \tag{1}$$

  where C_n are the coefficients, determined for each individual microstructure.

- Properties and constraints: The properties and constraints are represented in the same orthogonal space

$$P(\chi_n, p_n) = \sum_n p_n \chi_n \,. \tag{2}$$

- Coupling: The properties and constraints can represent hyper planes in the property enclosure which is defined as a universe of all variation in the inter relation among several properties for the same microstructure.

- Designer materials: Intersection of these planes defines the universe of all materials and microstructure (distributions) appropriate for design. This is similar to how Ashby's diagrams are being used in design [2].

In a related work, a complete investigation was performed in the use of two-point correlation functions for microstructure representation and reconstruction in nano-composite materials [7]. Two-point correlation functions are measured using both microscopy (Transmission Electron) and scattering techniques. The use of scattering techniques can provide 3-dimensional information on two-point statistics; whereas, in the case of microscopy, such information can only be obtained through the tedious task of serial sectioning. Scattering data (as opposed to imaging techniques) suffers from the basic disadvantage in that it does not provide a micrograph from the microstructure. A methodology for microstructure reconstruction has been reevaluated and optimized to provide an image from the two-point correlation functions. Microstructures of co-polymer nano-composites have been analyzed using both microscopy and x-ray scattering techniques to evaluate the distribution of the nano-cobalt particles. Empirical forms of the two-point probability functions for two-phase composites are also investigated in this work. Additionally, alternate forms of the two-point correlation functions were introduced that incorporate both periodicity and randomness. A modified form of the probability function is introduced that can provide a tool to examine the degree of randomness and periodicity. The results show the potential of these functions in the evaluation of microstructures and acquiring higher order details not available previously. These functions are then used to reconstruct the microstructure of these composites. The methodology introduces a revolutionary advance in the use of two-point functions from scattering techniques: Not only two-point correlations functions are measured and evaluated using simple empirical forms, a methodology is introduced that the corresponding microstructures can be reconstructed. The present form of the formulation can only address the statistical isotropic microstructures. The potential for such techniques to be extended in a self-consistent procedure to address the anisotropic forms of the microstructures are discussed.

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Computational models for spatial and temporal multi-scale modeling of composite and polycrystalline materials

Somnath Ghosh

Understanding the role of the material microstructure, at the length scale of constituent heterogeneities like grains, polycrystalline aggregates, fibers and inclusions, on the deformation and failure characteristics of the material is critical to the reliable design of components. Such an understanding requires an analysis framework that can predict inhomogeneities in time-dependent plastic flow under fatigue and creep conditions. Naturally, that sets a requirement for representing the real microstructure and defects, within the analysis tools. A robust design methodology must also link variabilities involved at all length scales that can affect the components in service performance.

A multiple scale computational model is developed for composite materials to concurrently predict evolution of variables at the structural and microstructural scales, as well as to track the incidence and propagation of microstructural damage [1, 2, 3]. The microscopic analysis is conducted with the Voronoi cell finite element model (VCFEM) while a conventional displacement based FEM code executes the macroscopic analysis [4, 5, 6, 7]. Adaptive schemes and mesh refinement strategies are developed to create a hierarchy of computational sub-domains with varying resolution. Such hierarchy allow for differentiation between non-critical and critical regions, and help in increasing the efficiency of computations through preferential zoom-in regions. Coupling between the scales for regions with periodic microstructure is accomplished through asymptotic homogenization, whereas regions of nonuniformity and non-periodicity are modeled by true microstructural analysis with VCFEM. An adaptive Voronoi cell finite element model is also developed for micromechanical analysis. Microstructural damage initiation and propagation in the form of debonding and particle cracking are incorporated. Error measures, viz. a traction reciprocity error and an error in the kinematic relation, are formulated as indicators of the quality of VCFEM solutions. The complete process improves convergence characteristics of the VCFEM solution.

In the second part of this contribution, a computational technique for multi-time scaling of the crystal plasticity is developed for prediction of deformation subject to multi-cycle loading. The crystal plasticity model involves microstructural characterization and incorporation of crystallographic orientation distribution to models, based on accurate microstructural data obtained by orientation imaging microscopy. The crystal plasticity models use thermally activated energy theory

for plastic flow, self and latent hardening, kinematic hardening, as well as yield point phenomena. The multi-time scaling is based on a homogenized with the asymptotic expansion method that is generally introduced for spatial homogenization for heterogeneous materials. In the formulation, the governing equations are divided into two initial-boundary value problems with two different time scale. One is a long time scale problem for describing the smooth averaged solution (global problem) and the other is for the remaining oscillatory potion (local problem). In the global problem, long time increments, which are longer than a single cycle period can be used and this multi-time scaling becomes an effective integrator. Several numerical examples seve to validate this work.

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Configurational forces in ferroelectrics - interaction between defects and domain walls

Dietmar Gross
(joint work with Ralf Mueller)

The applicability of ferroelectric materials under cyclic loading is limited by the so-called electric fatigue effect. Macroscopically, electric fatigue is characterized by a gradual decrease of the mechanical output for a fixed cyclic electric excitation which may lead to a total electric failure of a component. Its origins on the microscale are suspected in electro-mechanical mechanisms which are not yet fully understood. Experimental observations support the hypothesis that the most important micro mechanism is the blocking of domain walls, i.e. hindered domain switching, by defects of different kind, such as point defects and their agglomerates or volume defects. In case of point defects, oxygen vacancies are probably the sources which interact with the domain wall and the external loads. Since a direct experimental verification of this hypothesis is difficult, numerical simulations may provide a qualitative and quantitative understanding of interaction effects between defects and domain walls. In order to model this scenario, configurational forces

acting on the defects and vice versa on the domain wall are introduced and explained as an appropriate theoretical concept which can be realized numerically. Once the coupled field equations are solved by Finite Elements, the configurational forces are calculated to investigate possible motions of the defect and the domain wall, respectively. Various numerical simulations are presented which demonstrate the effect of the kind of defect, the defect position and concentration on the driving force acting on the domain wall. The results are in qualitative good agreement with experiments and indicate that the defects in fact form a barrier which, if high enough, leads to a blocking of the domain wall. In order to overcome these obstacles, higher external fields are necessary to move the domain wall again. Other examples show the effect of repeated domain switching on the defect distribution.

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Multiscale modelling of shape memory alloys

Klaus Hackl

In order to formulate a physically well motivated mechanical model for shape-memory alloys, it is required to gain deeper understanding of the material due to its complexity. This means primarily not only to account for the macroscopic characteristic along with their phenomenological description, but to take care of the behavior on microscopic scales as well. Within our work we consider four scales: the atomic scale determines the number of martensite variants and the corresponding transformation strains to be taken into account. On the microscopic scale we assume a laminated martensitic microstructure within a single-crystalline domain.

On the mesoscopic scale we combine a large number of single-crystals with different crystallographic orientations to define a polycrystal. Here the texture defined by the orientation-distribution of the various martensitic domains constitutes the fundamental quantity which has to be modeled. Finally the meso-macro transfer is done via appropriate averaging techniques.

In all cases we use energetic formulations based on the free energy $\Psi(\mathbf{F}, \mathbf{K})$ of the material and on a dissipation-functional $\Delta(\mathbf{K}, \dot{\mathbf{K}})$. Here $\mathbf{F}$ is the deformation-gradient and $\mathbf{K}$ denotes a specific set of internal variables describing the actual crystallographic variant, i.e transformation-strain, chemical energy and so on. We determine the evolution of $\mathbf{K}$ via minimization of the sum of elastic power and

dissipation.

$$L = \frac{d}{dt}\Psi + \Delta \to \min\,. \tag{1}$$

The microstructure of a single crystal as well as the texture of a polycrystal can now be described by a probability-distribution, a so-called Young-measure, $\lambda_{\mathbf{K}}$ of the internal variables and additional quantities $\mathbf{p}$, which define the geometry of the microstructure. Via a subsequent minimization process it is now possible to obtain relaxed potentials $\Psi^{\mathrm{rel}}(\mathbf{F}, \lambda_{\mathbf{K}}, \mathbf{p})$ and $\Delta^{\mathrm{rel}}(\lambda_{\mathbf{K}}, \mathbf{p}, \dot{\lambda}_{\mathbf{K}}, \dot{\mathbf{p}})$. The argument in (1) yields now evolution equations of the form

$$q_{\mathbf{K}} = -\frac{\partial \Psi^{\mathrm{rel}}}{\partial \lambda_{\mathbf{K}}} \in \frac{\partial \Delta^{\mathrm{rel}}}{\partial \dot{\lambda}_{\mathbf{K}}}\,, \qquad \mathbf{q} = -\frac{\partial \Psi^{\mathrm{rel}}}{\partial \mathbf{p}} \in \frac{\partial \Delta^{\mathrm{rel}}}{\partial \dot{\mathbf{p}}}\,, \tag{2}$$

where $q_{\mathbf{K}}$ and $\mathbf{q}$ are the corresponding thermodynamical driving-forces.
The models are capable of reproducing all essential effects in the material behavior of shape memory alloys such as pseudo elasticity and pseudo plasticity. Comparing our models to results from synchrotron diffraction experiments good agreement is observed between experimentally and analytically obtained orientation distribution functions.

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Theory of materials: experimental facts and constitutive modelling

Peter Haupt

The theory of materials includes the *experimental identification* of material properties, the *material modelling* and *test calculations* in order to verify and validate the constitutive equations. A material model is a relation between strain and stress processes. In view of the experimental identification, a basic problem arises at this point: it is only possible to control and measure finite displacements; strains and stresses cannot be measured directly. That means: only a quite incomplete picture of the multidimensional world of continuum mechanics is experimentally observable. Common solutions to this problem are experiments on test specimen of very simple geometry and loading, such as tension tests on bars with constant cross section or tension and torsion of thin-walled tubes. In these situations homogeneous states of stress and strain occur and are directly controllable. Before constructing a constitutive model, the experimental data can be classified from

a general point of view. Four possibilities can be distinguished [1]: the observed material behavior may be

- rate-independent without a hysteresis
- rate-independent with a hysteresis
- rate-dependent without an equilibrium hysteresis
- rate-dependent with an equilibrium hysteresis.

In view of the construction of material models these 4 categories correspond to 4 different theory classes of material behaviour, namely

- Elasticity
- Plasticity
- Viscoelasticity
- Viscoplasticity.

These 4 classes of constitutive theories are related to different kinds of material memory, which characterizes the influence of the past history of the input process on the present response of a material body: An elastic material body is not able to memorize the process history except its reference configuration. Viscoelastic and plastic materials show fading and permanent memory properties, respectively. As the general case, the response of a viscoplastic material depends on the process history in such a way that both effects of fading as well as permanent memory occur. These general arguments suggest representation techniques to set up stress functionals. The theory of materials provides general methods and special tools to design quite simple or more detailed constitutive models within these 4 categories. The further development of those methods and tools is a still ongoing process. In this context the technique, usually applied to represent the different grades of memory behaviour is the theory of internal variables.

A constitutive model contains material parameters; their numerical values quantify the intrinsic material properties. The material parameters must be determined from experimental data. In some special cases the material parameters can be directly identified according to their physical meaning. In general, however, they must be identified indirectly utilizing methods of nonlinear optimization.

The conception of a constitutive model on the basis of experimental data is explained as an example for the application of the general theory of materials. For the underlying research project see [2] and [3].

To collect an appropriate set of experimental data, experiments of tension, torsion and combinations of tension and torsion are carried out. The investigated material is a black-filled rubber, industrially applied in tires. Under the general assumption of incompressibility and isotropy, which is realistic in this case, the applied deformation (tension and torsion of a circular cylinder) is a solution of the local equilibrium conditions for any particular material behavior. Therefore, the performed one- and two-dimensional experiments are qualified to give information about the intrinsic material properties.

The experimental results suggest rate-dependence and a very small equilibrium hysteresis which can be neglected. Thus, a material model of nonlinear viscoelasticity is designed on the basis of a rheological model, consisting of nonlinear spring

and damping elements. Following the experimental data, process-dependent viscosities are introduced. This leads to the possibility to represent nonlinear rate-dependence and to model the influence of the deformation process on the relaxation during subsequent hold times.
Numerical simulations on the basis of identified material parameters demonstrate the success of the identification process and the ability of the constitutive model to reproduce the phenomena, which are experimentally observed.

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Some new relations in wave motion

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(joint work with Reinhold Kienzler)

G.B. Whitham [1] has developed a variational approach to study linear and also nonlinear wavetrains and its many ramifications and applications in a variety of fields, including modulation theory. The essence of Whitham's approach consists in postulating a Lagrangian function for the system under consideration, specializing this function for a slowly varying wavetrain, averaging the Lagrangian over one period and, finally, to derive variational equations for this averaged Lagrangian. Since the average variational principle is invariant with respect to a translation in time, the corresponding energy equation was derived, and since it is also invariant to a translation in space, the 'wave momentum' equation was also established. Kienzler and Herrmann [2] have shown that the two relations may be derived also by calculating the time rate of change of the average Lagrangian and the spatial gradient of the same function. It is also possible to obtain the energy equation and the three 'wave momentum' equations through a simple operation by applying the grad operator in four dimensions of space-time. This has been carried out for elastodynamics by Kienzler and Herrmann [3].
The purpose of this contribution is to consider not only the grad operator as applied to the average Lagrangian, but additionally also the div and curl operator to a 4-dimensional *Lagrangian Vector*. In the first of these two cases a conservation law for the *wave virial* was derived, while in the second case merely a balance equation for the *wave curl* was obtained because it did not appear possible to remove a non-vanishing source term, when rotation in space and time was considered. Rotation in space, whilst keeping the time axis fixed, led to a conservation law for

isotropic materials. To illustrate the general relations, several two-dimensional (in t, x) examples were presented.
It is recalled that the grad operator (translation) leads in fracture mechanics to the J-integral, the div operator (self-similar expansion) yields the M-integral and the curl operator (rotation) results in the L-integral, as discussed in [2, 3]. Details of the derivation may be found in [4].
Whitham has shown that his variational formulation of dispersive wave motion for linear uniform problems may be extended to non-uniform (nonhomogeneous and/or time-dependent) media and also to non-linear problems. It would indeed be a tempting task to extend the essential contents of the present contribution along those two directions cf., e. g., [5].
As regards the value and usefulness of conservation and balance laws in a general way, reference may be made to an evaluation of such laws by Olver [6]. It may suffice to mention here the applicability of conservation (and balance) laws in numerics. Being incorporated into various algorithms, the accuracy of the numerical results can be validated by checking whether or not the conservation laws are satisfied identically. If the equations are not satisfied, so-called spurious material nodal forces occur in finite-element calculations, which can be used to improve the finite-element mesh by shifting the nodes in such a way as to eliminate the spurious forces, cf. Braun [7], Müller and Maugin [8], Steinmann et al. [9].

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Description of industrially used rubber materials within the finite element method

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Industrially used filled rubber materials show large deformation capability, highly nonlinear material behavior as well as complicated inelastic effects, namely hysteresis even in stationary cycles, and a distinct softening induced by the loading-history, which is called Mullins effect. These characteristics entail high efforts of

an efficient description in the framework of continuum mechanics. Thus, the development of models suitable for those materials and the implementation of those models into the finite element method are complicated.
Moreover, the Mullins effect is sensitive to the relative orientation of the directions of the prestraining in the past and the present straining. Thus, the material evolves a distinct strain-induced anisotropy. This attracts attention even in the case of the simple shear deformation mode, provided that a loading sequence according to Muhr [1] is carried out. In contrast to multiaxial tension tests such a shear experiment is a reliable and easily feasible way to detect strain-induced anisotropy. Those shear processes indicate, that anisotropy occurs in the simulation of many industrial components with shear deformations as the most typical deformation mode and affects those applications considerably. If the component is loaded periodically with positive as well as negative shear angles but with different intensities in these two directions, the shear stiffness is expected to be different in the two shear directions. Of course, the extent of anisotropy depends on the used material and the intensity of the loading.
Considering the demands of an important class of industrial applications, the so called MORPH constitutive model (MOdel of Rubber PHenomenology [2]) is used to simulate rubber material behavior within the frame of the finite element method. The model focusses on stationary processes of technical components with inhomogeneous distributions of stress and strain.
The physical motivation of the model is the so called theory of self-organizing linkage patterns [3]. This approach is based on the theory that, during an external deformation, a self organization process of physical linkages starts on the molecular level. This leads to a separation of comparatively spacious, stiffened areas with to a great extend softened layers in between. Such a distribution of physical linkages is called linkage pattern and it is interpreted as the origin of the influence of the loading history to the momentary material behavior.
In its simplest form the MORPH constitutive model contains eight material constants. Their identification works fast and automatically. The strong nonlinearities as well as the hysteresis and even the softening effects are simulated reliably and close to reality.
To describe the anisotropic Mullins effect a tensorial history function is defined [4], which is based on second-order tensors, which are calculated using ellipsoid representations of all right Cauchy-Green tensors in the past, belonging to the same material point. This way, the anisotropic softening is reproduced in good correspondence to the experimental data.

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Constitutive modelling of anisotropic hyperelastic materials by polyconvex strain energy functions

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(joint work with Alexander E. Ehret)

Soft biological tissues as well as many engineering materials, as for example fiber-reinforced or calendered rubber-like elastomers, are characterized by strong anisotropy and are able to undergo large elastic deformations. In the constitutive modeling these features should be taken into account in an adequate manner. In the present contribution we discuss various hyperelastic anisotropic constitutive models with the focus mainly on the issue of polyconvexity of anisotropic strain energy functions [1]. Polyconvexity ensures ellipticity or the so-called Legendre-Hadamard condition. It implies positive definiteness of the acoustic tensor so that the speed of displacement waves is always real for any direction of propagation. Furthermore, in combination with coercivity, polyconvexity guarantees the existence of the global minimizer of the total elastic energy of the body which is of decisive importance in the context of a boundary value problem [2]. To benefit from these positive features we propose a class of polyconvex anisotropic strain energy functions. They are given by a series represented by some convex scalar functions. Each term of this series a priori satisfies the condition of the energy and stress free natural state so that no additional restrictions have to be imposed. Special cases of the proposed hyperelastic model based on power [3] and exponential [4] function representations show very good agreement with experimental data.

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Fatigue strength calculations based on the weakest-link concept

Frank Jablonski

Surface hardened steel, e.g. case-hardened or laser-hardened, is widely used in the field of machine building, especially when low abrasion is required. The experimental determination of the strength of surface-hardened parts under cyclic loading is quite cost intensive due to the expenditure of material and testing time. The influence of material, load type, stress multiaxiality, size effect, mean stresses, residual stresses and surface properties causes a broad scatter of the fatigue strength of these parts. This scatter can be described by means of the Weibull distribution.
To reduce the number of experiments, a calculation method is developed which is based on Weibull's weakest link concept [1]. This method allows to compute the failure probability and the failure location of machine parts which are loaded in the transition region to the fatigue limit. Fatigue failure of machine parts with inhomogeneous material properties under inhomogeneous stress conditions may occur either at the material's surface or inside the material. Therefore, a separate treatment of the surface and the volume of the material is necessary. Moreover, the effects of residual stresses and mean stresses are to be considered.
The essential quantities in the presented model are the distribution of Vicker's hardness and the exponents of the Weibull distribution of the surface and the volume. Also the residual stress state is important. Due to the fact that the experimental determination of residual stresses - e.g., with X-ray diffractometry - is only possible at free surfaces, an additional numerical iteration is needed to obtain an equilibrium state for the residual stresses. The surface roughness and surface oxidation depth are included by means of diminution factors for the surface strength. The local strength is characterized with Murakami's relation between hardness and fatigue limits [2, 3]. The multiaxiality of the stress state is considered by equivalent stresses; for example von Mises, Tresca or Dang Van's criterion [4]. By integrating the survival probabilities of the surface and the volume, the survival probability of the entire part is calculated, which allows to compute the fatigue limit. The necessary parameters have to be determined from reference specimens. The model is successfully examined by comparing experimental and calculated results for case-hardened and laser-hardened specimen established with both smooth and notched specimen under different loading conditions. Details of the procedure presented may be found in [5] and [6].

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Mechanics of ion-bombardment of semiconductor materials

Harley T. Johnson

Ion-bombardment is a widely used processing tool in microelectronics, and it is increasingly used as a fabrication tool for nanotechnology. The target material, often a semiconductor such as silicon or germanium, is significantly affected mechanically by the incident ion irradiation. While the process has been studied in detail experimentally, computationally studies are needed to fully investigate the mechanisms behind these effects. In the present work, molecular dynamics (MD) is used to reveal detailed mechanisms underlying the effects of ion-bombardment. The results of the MD studies are interpreted spatially and temporally over many orders of magnitude. Interpreting the results in this way, and connecting the atomistic data to continuum experimental observations, presents many challenges that can be related more generally to a range of important mechanics problems; here the analysis is applied to study two specific mechanics problems associated with ion-bombardment. First, the simulations are used to explain the role of ion-bombardment in developing near-surface stress in the target material. Second, the results are applied to investigate the self-assembly of nanoscale surface features under the appropriate ion-bombardment conditions.

Stress development due to ion bombardment arises from several atomistic mechanisms that are readily observed by computer simulation. Experimentally, stress is measured in ion-bombarded thin film structures through wafer curvature measurements, which sense an in-plane stress averaged over the thickness of the film [1]. Direct MD simulations of the ion-bombardment process show that the actual stressed layer in the target material is only a few nanometers thick [2]. In this stressed layer, the material is heavily damaged and even amorphous when the process is carried out at temperatures in the range of room temperature or lower. The results of the MD work show that the damage itself contributes to the development of stress in the material, since the amorphous material, unconstrained by the underlying crystalline material, would have a lower density. In addition to the microstructural changes, the effect of ion implantation contributes significantly to the development of stress: the added material itself causes additional compressive stress. The simulations reveal one other interesting but transient feature of stress development in ion-bombarded materials: the initial stress that develops is tensile in nature, due to the tendency of the topmost atoms in the nearly single-crystalline target to reconstruct. Finally, the simulations reveal the onset of steady

state stress in the system. In the few-nanometer-thick damaged layer at the surface, the stresses in a medium energy ion-bombarded semiconductor material are on the order of several GPa.

Under certain ion-bombardment conditions, the spontaneous formation of nanoscale ripples and dots is observed experimentally [3, 4]. In the present work, molecular dynamics simulations are used together with continuum surface evolution models to uncover the atomistic origins of this behavior. The instability yields reproducible, uniform, ordered arrays of nanostructures, including either well defined lines or dots on semiconductor surfaces that may be useful in nanoelectronics, optoelectronics, or nanomechanical applications requiring surface patterning. Until now, only phenomenological continuum models have been used to interpret the widely seen experimental results, [5, 6], and no models have achieved the predictive ability needed to shed light on the basic physics and mechanics or to bring the process into use as a potential nanomanufacturing method. Here, a large database of molecular dynamics results as a function of variables including temperature, stress, incident angle, energy, and surface characteristics is collected; the results are then incorporated into continuum surface evolution models. The studies reveal the atomistic mechanisms by which medium energy ions incident on an initially flat surface preferentially amplify surface roughness, even as thermally activated mass transport tends to smoothen surfaces out to longer length scale features [7]. Numerous possible stabilizing and ordering mechanisms occurring at the atomistic scale are considered including viscous relaxation, sputtered atom redeposition, and other short time scale correlations between change in surface height and spatial derivatives of the local surface morphology. The key conclusion is that existing models fail to include the effects of mass redistribution due to individual ion impacts; this subtle, local feature leads to significant long range effects, such as the experimentally observed saturation in ripple amplitudes that occurs after extended sputter erosion of a surface.

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Zanaboni's treatment of Saint-Venant's principle

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A simplified proof is presented of a basic inequality employed by Zanaboni in his treatment [2, 3, 4] of Saint-Venant's principle for an arbitrary shaped anisotropic linear elastic body in equilibrium under zero body force and self-equilibrated loads distributed over a part of an otherwise free surface. Of his main conclusions, those of interest here may roughly be expressed as:

(1) The stored energy in the part of the body sufficiently remote from the load surface tends to zero.
(2) The decay rate for cylindrical bodies is exponential.

Basic inequality: Let Ω_1, a bounded three-dimensional region with Lipschitz smooth boundary $\partial\Omega_1$, be occupied by a linear anisotropic nonhomogeneous elastic material in equilibrium subject to zero body-force and self-equilibrated loads P_i over a part $\Gamma \in \partial\Omega_1$ of the otherwise free surface. A second body Ω_2 of the same elastic material is bonded to Ω_1 across the interfacial surface $\Sigma \subset \partial\Omega_1 \setminus \Gamma$, so that the resulting displacement and traction are continuous across Σ and $\partial\Omega_2 \setminus \Sigma$ is free. Let $\Omega = \Omega_1 \cup \Omega_2$ and suppose that $u_i^{(1)}, e_{ij}^{(1)}, \sigma_{ij}^{(1)}$ and u_i, e_{ij}, σ_{ij} are the displacement, strain, and stress in Ω_1 and Ω respectively. Denote the corresponding internal energy in Ω_1 when isolated by:

$$V_{\Omega_1}(u^{(1)}) = \frac{1}{2}\int_{\Omega_1} c_{ijkl} e_{ij}^{(1)} e_{kl}^{(1)}\, dx, \tag{1}$$

where the elastic moduli c_{ijkl}, common to both Ω_1 and Ω, possess both major and minor symmetries and are positive-definite.
The principle of minimum strain energy applied to Ω_1 regarded as an isolated body yields:

$$\begin{aligned}
\int_\Gamma P_i u_i^{(1)}\, dS &= \int_{\Omega_1} c_{ijkl} e_{ij}^{(1)} e_{kl}^{(1)}\, dx \\
&\geq 2\int_\Gamma P_i u_i\, dS - \int_{\Omega_1} c_{ijkl} e_{ij} e_{kl}\, dx \\
&= \int_\Omega c_{ijkl} e_{ij} e_{kl}\, dx + \int_{\Omega_2} c_{ijkl} e_{ij} e_{kl}\, dx \qquad (2) \\
&\geq \int_\Gamma P_i u_i\, dS, \qquad (3)
\end{aligned}$$

where the last inequality,which demonstrates that additional material stiffens a body, was derived by Zanaboni but again by a different method.
Zanaboni's basic inequality is given by (2) which for later purposes may equivalently be written:

$$V_{\Omega_2}(u) \leq V_{\Omega_1}(u^{(1)}) - V_\Omega(u). \tag{4}$$

Positive-definiteness of the elasticities and (4) imply that:

$$V_\Omega(u) \leq V_{\Omega_1}(u^{(1)}). \tag{5}$$

Zanaboni completed the proof of Conclusion 1 by successive bonding of a sequence of further bodies to Ω subject to the same load on Γ. This generates a monotonic non-decreasing bounded below sequence of energies that by Cauchy's theorem leads to the desired result.

Decay in cylindrical bodies: For convenience, we suppose that the surface Γ is planar and enclose within Ω_1 a prismatic cylinder C_1 of length l with Γ as its base; while Ω is enclosed within a prismatic cylinder C_2 of length L whose base contains Γ. The cylinders C_1, C_2 are subject to the loads P_i over Γ but are otherwise free. From (5) and dual extremum principles with $L \to \infty$ we obtain the decay estimate:

$$V_{\Omega_2}(u) \leq \int_\Gamma P_i P_i \, dS \exp\{-2\mu_2^{\frac{1}{2}} l\} \left[c_0 \mu_2^{\frac{1}{2}} \left(1 - \exp\{-2\mu_2^{\frac{1}{2}} l\}\right)\right]^{-1},$$

where μ_2 is the second eigenvalue in the free membrane problem for Γ and c_o is a positive constant. This represents the required estimate derived without using differential inequalities.

Concluding remarks: Insofar as the method relies upon dual extremum principles it may be extended to other theories possessing analogous properties. Furthermore, while the above treatment compares internal energies between bodies of different sizes, a possible alternative approach involves enlarging a body through accretion of additional material and investigation of the roles of the energy-momentum tensor and chemical potential.

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Residual stress and machining distortion

Christian Krempaszky

To obtain materials/components covering a wide range of conditions with characteristic mechanical properties, quenchings in connection with special heat treatments are of particular engineering importance. In addition to strength demands, a reduction of the production costs of forged parts by eliminating processing steps is essential. In this course a direct age version of IN 718 has been proposed for which an increase of strength is possible by precipitation strengthening during cooling from the forging temperature. The mechanical and thermal treatments

inevitably result in residual stresses and distortions in the treated parts, which result from coupled thermo-mechanical interactions during the usually rapid cooling from sufficiently high temperatures down to room temperature [1, 2]. Due to the macroscopic portion of the residual stress state, machining of slender forged components may lead to severe distortion of the component. In the worst case, the dimensional accuracy of the pre-finished component is not achieved.
Within the scope of the presentation, the residual stresses in forged plate-like components are investigated with the focus on the distortion of the component during machining. To predict the transient thermal stresses during quenching and the resulting residual stress state a semi-analytical plate model is set up following the ideas of Landau et al. [3]. Based on these results the redistribution of the residual stresses and the corresponding distortion due to machining are estimated. Additionally, an approximative solution of the plate approach is proposed using the finite element method. To verify the theoretical predictions of the residual stress state and the corresponding distortion resulting from machining, the component distortion is determined by experiment considering turbine disks of the Ni-base superalloy IN 718.

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Determination of ductile damage parameters from measured deformation fields

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(joint work with M. Springmann, M. Scherzer)

Ductile damage mechanics describes the non-linear deformation process, failure and fracture within the framework of a continuum theory. For its application and acceptance it is of great importance to determine the abundant number of material parameters in such models. The material parameters of damage models are usually gained from the force-displacement curves of simple tensile experiments via empirical (best fit) methods. However, the complexity of the problem requires more comprehensive information from the experiment than a simple force-displacement curve. On this account more advanced identification algorithms are needed to exploit supplementary information, which may be obtained from measured inhomogeneous deformation fields. Furthermore, to identify the damage parameters of ductile materials, experiments with homogeneous stress and strain

distributions are neither capable nor sufficient. A significant influence of the damage parameters occurs only after large deformations, which lead unavoidable to inhomogeneous stress and strain fields, as e. g. in necking regions.
This work comprises the development, implementation and application of methods for the parameter identification of damage mechanical constitutive laws. Ductile damage is described by extension of the von Mises yield condition with the Gurson-Tvergaard-Needleman as well as with the Rousselier model. The classical Rousselier model is complemented by accelerated void growth and void nucleation. The non-linear initial boundary value problem for hyperelastic-plastic large deformations is solved by the finite element system SPC-PMHP, which was developed in the frame of the special research program SFB393 on parallel computers [1, 2]. The aim is, to identify the material parameters from locally measured displacement fields and measured force-displacement curves. For this purpose, the inverse boundary value problem has to be solved. A non-linear optimization algorithm is used, which renders a suitable multi-objective function to a minimum by means of the gradient based method of Levenberg & Marquardt. The gradients with respect to the material parameters are implicitly calculated by means of a sensitivity analysis (Mahnken & Stein) from the current finite element solution. Furthermore, the point of localization of deformation in the specimen is compared with the loss of ellipticity of the boundary value problem in the numerical analysis. For this reason, during the FEM-computations the acoustic tensor is monitored in the whole specimen during the deformation process. Several numerical experiments are performed in order to check the efficiency of the identification algorithms. A useful strategy to identify the material parameters was found by careful numerical studies [3, 4].
A special experimental set-up was developed to perform tensile experiments with notched flat bar tension specimens. In order to measure the local displacement fields at the specimen surface, the object grating method was used. The method was applied to the steel StE 690. The hardening and damage parameters for both damage models could be identified. More detailed information can be found in the PhD-thesis of M. Springmann [5].

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On the kinetics of the pseudoelastic hysteresis loop

Khanh Chau Le

Shape memory alloys such as NiTi or CuZnAl, due to their specific crystal lattices, may have more than one stable equilibrium state. In these materials the coexistence of phases (or phase mixing) is possible under particular thermal or loading conditions. If the resistance to the nucleation and motion of phase interfaces is negligible and hence the dissipation is zero, phases are arranged in a microstructure that minimizes energy of the system. However, in real materials, there are many barriers and obstacles hindering the creation and motion of phase interfaces, and, if their resistance is large, the low energy states may not be attained at all. This resistance to the creation and motion of phase interfaces can only be overcome at some energy expenses. Consequently, the rearrangement of phases and the accompanying energy dissipation should be governed by the laws of non-equilibrium thermodynamics. It is commonly argued in the material science community that, in order to describe the drastic phase rearrangement during the yield or the recovery, additional kinetic relations governing the evolution of phases are needed.

Abeyaratne and Knowles [1] were among the first to have proposed an initiation criterion and a kinetic relation in addition to the well-known balance equations of continuum mechanics. Within the one-dimensional model of quasi-static motion of bars under tension, the proposed relations close the system of equations governing the evolution of phases and are consistent with the laws of thermodynamics. Unfortunately, this theory is unable to describe many well-known features of the hysteresis loops observed in experiments. This is due to its two deficiencies: i) the free energy does not include the surface energy (or the coherency energy) of phase interfaces, ii) the dissipation potential is not a homogeneous function of the first order with respect to the volume fraction rate, so the theory is not rate-independent. The proposed initiation criterion associated with the Maxwell line is neither confirmed by experiments on internal yield or recovery [2].

A fundamental understanding of the initiation of phase transition has been achieved by Fu et al. [2] and Huo and Müller [3]. By including the coherency energy of phase interfaces into the free energy of the system, the correct formula for the driving force was derived. This leads to the diagonal line connecting the upper left with the lower right corner of the hysteresis loop, at which the nucleation of new phase begins. The existence of this line was confirmed by the experiments reported in [2]. However, since the kinetic equation is absent in [2, 3], it is not clear why does the stress-strain curve prefer moving along the horizontal yield or recovery line for the given loading path. The explanation based lonely on the energy consideration and stability requirement was not convincing.

The aim of this short note is to fill the logical gap in the above mentioned studies [2, 3]. We propose a simple kinetic relation consistent with the second law of thermodynamics. This relation is obtained from the dissipation potential which is proportional to the magnitude of the volume fraction rate times the newly formed

volume fraction. We will show that the theory is rate-independent, but history dependent, and that it can describe all features of hysteresis loops observed in experiments. For simplicity, the analysis of hysteresis is provided for the piecewise linear stress-strain curve and simple loading paths. However, it will be clear from this analysis that hysteresis loops can be simulated for a rather general non-monotone stress-strain curve and arbitrary loading programs.

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Open and recently answered questions in the configurational mechanics of solids

Gerard A. Maugin

Mechanics of materials on the material manifold, also called " configurational" or "Eshelbian" mechanics (after J.D.Eshelby) provides a natural and safe basis for the formulation of the thermomechanics of forces driving evolving defects and material inhomogeneities [1, 2, 3, 4, 5]. Fully expressed on this material manifold, it exploits a parametrization of space-time in terms of material coordinates X and Newtonian time t. A strong and vivid scientific and engineering activity has developed in this modern framework including a rationalization of the construction of driving forces and new computational techniques [6] where the notion of spurious material forces is fully exploited. Like in all rapidly developing fields (this, essentially since the late 1980s) with many faceted applications , a large number of questions is raised, some of them having already received a definite answer and others still waiting for the most reasonable answers. Five of these questions recur on the scientific scene mainly due to a lack of common understanding These questions have been briefly enunciated and answered.

The main ingredient in the material mechanics of materials is the statement of the "balance of material (also called canonical or pseudo) momentum", and its related jump relation at a discontinuity surface. Hence the first question.

Question 1: Can we formulate the balance equation of canonical momentum without specifying the energy density? Some school (M.E. Gurtin and co-workers) claims that that equation can be postulated independently of the usual balance equations of continuum physics, including that of linear momentum and independently of any specified material behavior, and thus granting to that equation the status of a "new law" of physics. Another, more modest view (held by the author and many others) is that the balance of canonical momentum is intimately related

to a basic invariance of physics (translational invariance on the material manifold, in other words the property of material homogeneity): the existence of material forces reflects a breaking of this symmetry. Material inhomogeneity per se, but also field singularities and some dissipative effects "materialize" in this breaking of symmetry. We may speak of pseudo-inhomogeneity effects [7]. The latest works by the author (e.g. [8]) show how far one can go in the formulation of the balance of canonical momentum; As a matter of fact, it is possible, even in the presence of complex dissipative effects, to formulate simultaneously canonical expressions for the balance of material momentum and of a special energy density (product of thermodynamic temperature and entropy) without specifying the explicit dependence of the free energy density, thus for an infinitely large class of material behaviors. Though, these equations are not formally independent of the usual balance equations written in most general terms. The same holds good a priori for the associated jump relations. QED.

Question 2: What is the energy to be considered in the Eshelby stress? In many practical problems one distinguishes between different thermodynamical situations, among these, isothermal evolution and adiabatic conditions are the most common ones. This is critical in studying various discontinuity surfaces (phase-transition fronts, shock waves). But the Eshelby stress tensor which provides the "flux" in the balance of canonical momentum involves such an energy. Accordingly, one must pay special attention to which energy density (e.g., free or internal) the Eshelby stress incorporates, as a pseudo-material force of different types may appear as a source in the balance of canonical momentum and its associated jump relation [9, 10].

Question 3: Is there any confusion in the literature between the conservation of material momentum and an equation governing a microstructure? Brief answer: Yes!

Question 4: Are equations governing evolving surfaces independent of the balance of canonical momentum? Answer: no, evolving interfaces break translational material symmetry!

Question 5: What happens in the dual space of wavelike solutions where relevant entities are the material wave vector K and the angular frequency ω, remembering that a phase is naturally defined by the invariant relation (K.X-ωt)? Answer in a forthcoming work [11].

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Atomistic simulations of disclination structures and evolution in fcc metals

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(joint work with D.E. Spearot, K.I. Jacob, M.A. Tschopp)

The role of interfaces (e.g., grain boundaries) in continuum level defect field theory is often minimized. In order to incorporate low and high angle boundaries (grain and sub-grain), it is necessary to develop appropriate kinematics (tangent spaces and deformation mappings for characteristic defects), thermodynamics (free energy) and kinetics (evolution). Treatment of the disclination character of high-angle boundaries can be rigorously pursued as an undergirding element of generalized dislocation-disclination defect field theory of crystals, starting with atomistic calculations. In this work we explore the structure of grain boundaries in fcc Al and Cu bicrystals using a 0 K conjugate gradient energy minimization of EAM potentials, with equilibration of an NPT ensemble at finite temperature for a full range of <001> and <110> misorientation axis symmetric tilt boundaries. Both CSL character and disclination structural units are identified. Emission of the first dislocation is characterized for each boundary misorientation. For dissociated grain boundaries (low to moderate stacking fault energy, e.g., Cu), a new mechanism is found for eradication of the extended intrinsic stacking fault (disconnection). It is found that for some boundaries, secondary rather than primary slip systems are activated first. Finally, possible directions for informing continuum models are briefly discussed. A simple model for grain boundary strength (first dislocation emission event) is found that depends not only on misorientation angle and favorable lattice orientation (primary dependence), but also on a measure of nanoporosity or free volume obtained by averaging the solution over a certain interface strip. A general kinematic and thermodynamic framework for coupled disclination and dislocation defect populations is briefly discussed, based on our recent works [1, 2, 3]. A strategy is suggested for informing such a continuum theory based on microscopic phase field models and discrete dislocation-disclination dynamics. Outstanding issues include:

(1) rendering of dislocations
(2) dislocation/disclination interactions
(3) forms of interaction terms in thermodynamic free energy
(4) mobility characteristics and single defect/many body kinetics

Explanation: Understanding of the role of grain boundaries in deformation and fracture of polycrystalline metals is still incomplete. Numerous authors have suggested over the years that coincident site lattice (CSL) boundaries, special boundaries with characteristically lower excess energy, may contribute to enhanced deformation and fracture resistance. However, attempts to quantify dependence of mechanical behaviors in terms of the CSL boundary index (number of overlapping atoms in the unit cell of interpenetrating lattices with misorientation) have not provided satisfactory generality of correlation with strength or fracture resistance. Moreover, studies of the dependence of dislocation nucleation mechanisms on CSL boundaries have typically been limited in scope.

Molecular statics (0 K) calculations of grain boundary structure have been performed in this study using a sequence of lattice translations, atom extraction to avoid overlap, conjugate gradient energy minimization, followed by finite temperature equilibration to achieve stable, minimum energy structures. Comparisons with HRTEM experiments and ab initio results confirm the algorithm. The embedded atom potential (EAM) is used for both both fcc Cu and Al [4]. Certain high angle boundaries in low stacking fault energy metals show a dissociated structure, with extended intrinsic stacking faults (ISFs) emanating from disclination structural units. The dissociated structure of such boundaries is typical of low intrinsic stacking fault energy fcc crystals, and limits applicability of the structural unit model proposed by Sutton and Vitek [5] which estimates grain boundary energies for special and intermediate boundaries based on the energies of summations of repeating structural units. We show [6, 7, 8, 9] that these dissociated structural units, otherwise labeled as "disconnections" by Hirth et al. [10] possess certain distinct characteristics in terms of dislocation nucleation. Specifically, it is found for a 53.1 deg. Near Σ_{11} CSL symmetric tilt boundary about the <110> misorientation axis in Cu that under tensile load, the ISF must constrict towards the interface until a pair of partial dislocations separated by an extrinsic stacking faulty (ESF) is emitted from the interface at the intersection of the ISF with the structural unit. Subsequently, a pair of partial dislocations is emitted on the opposite side of the interface; finally, following emission of the trailing partial dislocation, the ISF is eradicated. In this way, the disconnection is removed [8].

A model for strength of grain boundaries is developed that combines lattice orientation (with non-Schmid effects on dislocation nucleation after Ogata et al. [11] and interface structure (expressed through a coordination number-based measure of nanoporosity) to propensity to nucleate a dislocation [9]. The importance of this result is that CSL both misorientation and grain boundary structure must be considered. The model does not appear to work for a <110> boundaries with a very high misorienation angle, but suffices for all others. This indicates that a disclination-based representation of grain boundaries is critical to framing physically-based polycrystalline plasticity theories.

It is contended that such results may contribute necessary thermodynamic characterization and understanding of kinematical mechanisms to continuum phase field and other continuum field theories for combined dislocation-disclination kinematics

and kinetics. A comprehensive kinematical defect field theory that reflects both disclinations and dislocations has been recently developed that may ultimately accept these results (cf. [1, 2, 3]).

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Computational modelling of growth and remodelling of biological tissues

Andreas Menzel

Biological tissues posses various substructures on different scales of observation. Apart from highly anisotropic response, the adaptation of these materials results in reorientation of such substructures according to the applied loading directions. Different continuum theories have been proposed in the literature to capture related growth and remodelling phenomena; the reader is referred to the contributions [1, 6, 11] and references cited therein. Special emphasis on the incorporation of effects stemming from additional mass sources and mass fluxes as well as on numerical applications has been placed in [2, 3, 7, 8]. Here, we are particularly interested in the modelling of fibre reorientation during growth and remodelling of soft tissues loaded under tension. Two orthogonal fibre families are thereby incorporated into a continuum model and allow interpretation as phenomenologically representing bundles of collagen fibres. As such, the proposed framework extends previously developed formulations accounting for transversally isotropic response;

see [4, 5] where stress-driven models are developed or the kinematics-based ansatz in [9, 10]. The overall framework is inspired by the works [12, 13], namely that the fibres are aligned in a time dependent manner so that both fibre families reorient with respect to principal stretch directions - the strain energy accordingly approaching an extreme value. The developed algorithm fits nicely into, for example, common nonlinear finite element codes. Concerning future research, the following (open) problems - among other related topics - might be of interest:

(i) design of relevant experimental setups and comparison of measured data with simulation results
(ii) numerical elaborations on different fibre reorientation models
(iii) analysis of (deformation dependent states of) commutative stress and stretch tensors for fibre family directions which do not coincide with principal stretch directions
(iv) further investigations on the incorporation of residual stresses
(v) comparison of stress-driven growth formulations with energy-driven growth approaches
(vi) incorporation of forces related to inhomogeneities of the material into growth evolution equations.

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Phase diagrams modified by interfacial penalties

Ingo Müller

The conventional forms of phase diagrams are constructed without consideration of interfacial energies and they represent an important tool for chemical engineers and metallurgists. If interfacial energies are taken into consideration, it is intuitively obvious that the regions of phase equilibria must become smaller, because there is a penalty for the formation of interfaces. We investigate this phenomenon qualitatively for a one-dimensional model, in which the phases occur as layers rather than droplets or bubbles. The modified phase diagrams are exhibited for the case of full miscibility in the low temperature phase and for the case of a miscibility gap in the liquid phase.

Modeling of spinodal decomposition and coarsening in AgCu: a quantitative approach

Wolfgang H. Müller
(joint work with Thomas Böhme)

Experimental investigations show that the microstructure of solders changes over time. In order to estimate the reliability and the lifetime of microelectronics it is important to predict the rate of microstructural changes. Starting with an overview on coarsening phenomena as observed in lead-free solder alloys this paper concentrates on the theoretical description of phase separation and subsequent phase growth that occurs in various solid binary alloys. Here the mixture decomposes into its equilibrium mass concentrations $c_{\alpha/\beta}$ which are determined by the common tangent rule: $\frac{\partial\psi(c,T)}{\partial c}|_{c=c_\alpha/c_\beta} = \frac{\psi(c_\beta,T)-G(c_\alpha,T)}{c_\beta-c_\alpha}$. Furthermore phase separation can be distinguished into two different processes, namely nucleation and spinodal decomposition, which are defined by aspects of thermodynamical stability [1]. Indeed, one can find three areas of stability in the Gibbs free energy density curve $\psi(c,T)$:

$$\frac{\partial^2\psi(c,T)}{\partial c^2}\begin{cases} <0 & \text{, unstable} \\ >0 \wedge c\in\{[c_\alpha,c_1^{\mathrm{sp}}]\vee[c_2^{\mathrm{sp}},c_\beta]\} & \text{, metastable} \\ >0 \wedge c\notin\{[c_\alpha,c_1^{\mathrm{sp}}]\vee[c_2^{\mathrm{sp}},c_\beta]\} & \text{, stable} \end{cases} . \tag{1}$$

Here $c_{1/2}^{\mathrm{sp}}$ denote the so called spinodal concentrations determined by the inflection points $\partial^2\psi(c,T)/\partial c^2 = 0$. According to Eq (1) classical Fickean diffusion, spinodal decomposition or nucleation occurs if the initially (homgeneous) mass concentration c is outside or within the unstable/metastrable area.

In order to simulate phase separation and coarsening an extended diffusion equation of the phase field type is presented which can be interpreted as a generalization of the well known Cahn-Hilliard equation. It takes diffusion of the

FICKean type, surface tensions along the phase boundaries as well as local mechanical stresses into account, [2]:

$$\begin{aligned}\frac{\partial c}{\partial t} &= \frac{\partial}{\partial X_i}\Big[M_{ij}\frac{\partial}{\partial X_j}\Big(\frac{\partial \psi}{\partial c} - 2A_{kl}\frac{\partial^2 c}{\partial X_k \partial X_l} - \frac{\partial A_{kl}}{\partial c}\frac{\partial c}{\partial X_k}\frac{\partial c}{\partial X_l} \\ &\quad -2\frac{\partial A_{kl}}{\partial \varepsilon_{mn}}\frac{\partial c}{\partial X_k}\frac{\partial \varepsilon_{mn}}{\partial X_l} - \frac{\partial^2 a_{kl}}{\partial \varepsilon_{op}\partial \varepsilon_{mn}}\frac{\partial \varepsilon_{op}}{\partial X_k}\frac{\partial \varepsilon_{mn}}{\partial X_l} - \frac{\partial a_{kl}}{\partial \varepsilon_{mn}}\frac{\partial^2 \varepsilon_{mn}}{\partial X_k \partial X_l}\Big)\Big]. \end{aligned} \tag{2}$$

The symbols X_i and t denote the reference position and the time. Furthermore the required material parameters ψ, M_{ij}, A_{kl}, a_{kl} and C_{ijkl} must be specified for a chosen material and can be determined either from the literature/databases or from calculations based on the embedded atom method which is suitable for describing atomic interactions in metals [3]. Note that the stiffness coefficients C_{ijkl} yield the strains ε_{kl} solving the elastic problem.

In a first step of investigations it is considered the one-dimensional and stress-free case, where Eq (2) reduces to

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial X}\left[M(c)\frac{\partial}{\partial X}\left(\frac{\partial \psi(c)}{\partial c} - 2A(c)\frac{\partial^2 c}{\partial X^2} - \frac{\partial A(c)}{\partial c}\left(\frac{\partial c}{\partial X}\right)^2\right)\right]. \tag{3}$$

Eq (3) represents a nonlinear partial differential equation of 4th order which describes the temporal development of different equilibrium phases in a binary alloy. As an example this equation is (numerically) solved by means of discrete FOURIER transforms [4], and results are illustrated for the FCC-structured lead-free solder alloy AgCu.

Finally we turn attention to the formation of scallop-shaped intermetallic compounds observed at the interface between solder material and substrate. A LSW-based ansatz is used [5], and evaluated for various solders (SnAgCu + In, SnAgCu + In + Nd), that allows the prediction of the development of the mean grain radius followed by exemplary results for Cu_6Sn_5 scallops on Cu substrate.

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Extraction of constitutive properties of composite panels in interlaminar shear

Jonas M. Neumeister

A doubly notched specimen is used to test shear properties in the test region between the notches. This configuration produces non-uniform stress fields. By superimposing bending moments over each notch giving equally poor stress fields, but of opposite sign, the net stress remains unchanged, but very uniform (combined) stress fields are obtained. Treating the notches as sharp cracks, appropriate combination of normal (N) and bending (M) loading is achieved for cancellation of the arising stress intensity factor, i.e. $K_{\mathrm{I}}^{\mathrm{tot}} = K_{\mathrm{I}}^{\mathrm{N}} + K_{\mathrm{I}}^{\mathrm{M}} = 0$. This is accomplished by a fixture with two specimen holders loading it isostatically where the mutual proportion of loadsets (N & M) is adjusted by varying the angle between specimen and external load. This **I**nclined **D**ouble **N**otch **S**hear test (IDNS) is used to study the strengths, moduli and general constitutive behavior of several composite laminates. Its advantages over existing shear tests are confirmed, and very uniform strainfields are monitored optically. By using tilted notches even the (minor) K_{II} component is minimized.
Cyclic loading with increasing peak shear strain of a carbon-epoxy composite reveals non-linearity already at low stresses, notable inelastic strains, widening hysteresis loops, large failure strains ($> 7\,\%$), high strength ($> 120\,\mathrm{MPa}$) and a decaying elastic (reloading) modulus (by $12\,\%$) quite early in the tests. Such material behavior could not be observed previously in shear, since no test could provide equally uniform conditions in a test region.

How big is big enough?

Martin Ostoja-Starzewski

While the entire field of continuum solid mechanics relies on the separation of scales, there is a need for definite statements regarding the size of the Representative Volume Element (RVE). In the relatively much smaller, but rapidly growing field of stochastic solid mechanics there is a need for results on the connection of the Statistical Volume Element (SVE) to the relevant microstructural length scale, and on the formulation of random fields. Strictly speaking, the SVE should involve a scale-dependent homogenization carried out on a mesoscale, an intermediate scale separating the microscale (level of micro-heterogeneities) from the macroscale (level of macroscopic response). As the mesoscale grows, the SVE tends to the RVE. This occurs in terms of two hierarchies of bounds stemming from Dirichlet and Neumann boundary value problems on the mesoscale, respectively [1, 2]. Since, generally, there is no periodicity in real random/heterogeneous media, the RVE can only be approached approximately (e.g. within 5% accuracy) on mesoscales, i.e. length scales finite relative to the microscale. The key question is: On what mesoscale is the RVE attained within a prescribed accuracy for a specific type of a random microstructure? We review recent results and

outstanding challenges in this field, using first-order continuum approximations, in the settings of linear elasticity, physically nonlinear elasticity, finite elasticity, elasto-plasticity, rigid-plasticity, thermoelasticity, and permeability in random composites [3, 4, 5, 6]. More information can be contained in such a homogenization process when a higher-order continuum is employed, and this, of course, comes at a cost of greater complexity, e.g. [7].

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Computation methods for higher-order continua

Jerzy Pamin

The higher-order continuum theories are necessary to explain and simulate the physical behaviour of materials with microstructure. In particular, size effects evidenced at all levels of observation as well as localization and softening phenomena, which have their origin in the micro/meso-structure of materials, but are revealed in the macroscopic response, require enhanced continuum theories. The theories incorporate intrinsic length parameters and the gradient terms represent the microstructural interactions in phenomenological modelling.

A review of numerous gradient-enhanced models is performed for instance in [1, 2, 3]. The theories can be classified in two groups: 1) models based on Mindlin gradient continuum, involving higher order stresses in balance and evolution equations, e.g. [4], and 2) models in which the classical equilibrium/motion equations are augmented by an additional differential equation of plastic consistency or variable averaging, e.g. [5, 6].

Computational implementation of the gradient theories requires a proper linearization and discretization of two- or three-field governing equations written in a weak format. The approximation functions must satisfy increased continuity requirements. Finite element methods based on continuous or discontinuous Galerkin

approximation [7, 8] as well as meshless methods can be used. It is noted that discretization itself does not regularize the mathematical model.
In the research the attention is limited to linear kinematics and isothermal conditions. Finite element and element-free Galerkin implementation of the gradient-dependent plasticity theory [5, 9] is presented among others in [10, 11, 12], while computational gradient-enhanced damage theories are covered e.g. in [6, 13, 14]. Simulations of strain localization and failure in quasi-brittle and geotechnical materials (concrete, soil) under static and dynamic loading can then be performed. Benchmark examples include the simulation of static failure and standing localization waves in tensile bars, shear band formation in biaxially compressed specimens, slope stability analysis, the Brazilian split test, cracking in plain and reinforced concrete beams under monotonic and reversed loading and three-dimensional fracture tests.
The lack of pathological discretization sensitivity is verified. It is noticed that in the regularization of localization problems strain-like quantities should be averaged. The future of localized failure simulations seems to belong to gradient-enhanced models combined with extended finite elements to model displacement discontinuities (macrocracks), cf. [15].

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Modelling of new materials in medical technology and biomechanics

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(joint work with Markus Böl)

General concept. It is well-known that rubber-like polymers consist of long-chain macromolecules which are attached to each other at certain points. Several authors have studied the material behavior of this network by means of molecular-dynamics (micro mechanical) simulations (see e.g. [1]). Such a procedure is, however, extremely expensive from the computational point of view and makes the numerical investigation of engineering structures practically impossible. For this reason we follow here a so-called meso-mechanical approach based on the finite element method. In comparison to a classical continuum mechanical modelling this has the advantage that the physical understanding of the material behavior and the knowledge about that from other disciplines (e.g. chemistry, physics) can be much better incorporated.
The proposed concept uses the idea of representing the polymer network by means of an assembly of non-linear truss elements (see also [2]). Each truss element models the force-stretch behavior of a certain group of chains. The truss elements are configured in such a way that six of them form a cell of tetrahedral shape. The embedded tetrahedral elements serve to model the hydrostatic pressure built up in the network. Applying a random assembling procedure we are in the position to model arbitrary geometries. Alternative finite element-based approaches have been suggested e.g. in [3].
The total Helmholtz free energy function (per reference volume) upon which the finite element formulation is constructed reads

$$(1) \qquad W = \underbrace{\frac{K}{4}\,(J^2 - 1 - 2\ln J)}_{W_{\text{tetr}}} + \sum_{j=1}^{6} \underbrace{\frac{f_{\text{chain}}}{A_{0j}\,L_{0j}}\,k\,n_j\,\theta\,\left(\frac{\lambda}{\sqrt{n_j}}\,\beta_j + \ln\frac{\beta_j}{\sinh\beta_j}\right)}_{W_{\text{truss}\,j}}$$

Here K refers to the macroscopic bulk modulus. J is a short hand notation for the determinant of the deformation gradient $\mathbf{F}$. It can be concluded that the first part of W is or purely macro mechanical nature. It suffices to model the near-incompressible behavior of rubber with sufficient accuracy. $f_{\text{chain}} = N/N_{\text{truss}}$ (ratio of number of chains with respect to number of trusses per reference volume)

is a measure for the size of the chain bundle, n_j the number of chain links, θ the absolute temperature, k Boltzmann's constant and β_j the inverse Langevin function. Usually f_{chain} is an extremely high number, e.g. 10^{15}. The micro-macro transition happens at the point where it is assumed that the stretch λ of the truss is equal to the stretch of the corresponding chain (bundle). It is important to emphasize that due to this assumption the length and the cross-section of the truss cancel out of the formulation. They do not have any influence on the final result. In comparison with classical continuum mechanically-based finite element simulations the new approach does not require more degrees-of-freedom.

Soft tissue. Biomaterials, e.g. soft tissue, are certainly different from rubber. However, it is accepted that the micro structure of these materials, whether they are artificial or natural, is very similar to the one of rubber-like polymers. It therefore suggests itself to use and extend the proposed model in the context of biomechanics and medical technology.

Muscle. A good example for that is a skeletal muscle which can be considered as a fibre-reinforced soft tissue. The muscle contraction mechanism has been already investigated in the mentioned fields. Authors of these disciplines (see e.g. [4]) usually develop one-dimensional relations for the active force (contraction force) in dependence of length or stretch, time and contraction velocity:

$$F_{\text{act}} = F_{\text{iso}}\, f_\lambda\, f_t\, f_v \tag{2}$$

The isometric force F_{iso} is determined by means of experimental results. It can be referred to the total muscle or to a single muscle fibres. One of the most difficult points is the realistic modelling of muscle activation which is linked to the Calcium concentration and finally to the state of the muscle action potential. Obviously the Calcium concentration is not homogeneous in the muscle. Despite of this fact many authors model the activation process simply by means of a function of time. This alone shows that the numerical simulation of muscle contraction must be much further developed. In the present work we enrich the soft tissue network by additional truss elements which stand for muscle fibre bundles. We implement the above relationship into these elements. The fibre and "chain" elements are attached to each other only at the nodes. This is already sufficient to model the interaction between active (muscle fibres) and passive (soft tissue) forces. Future work should be directed into a much more realistic mathematical description of the activation processes which can be e.g. performed by considering the diffusion process of the Calcium ions inside the muscle. Further it has to investigated in which way the active force depends on the stretch which can be interpreted here as ratio between the sarcomere length in the deformed configuration with respect to the sarcomere length in the undeformed configuration.

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Postbuckling response and ultimate strength of a rectangular elastic plate using a 3-D Cosserat brick element

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Use is made of a 3-D Cosserat brick element [1] which admits full material and geometric nonlinearity to determine the postbuckling response of a rectangular plate and its ultimate strength. Examples are discussed which show that existing approximate solutions are more limited than originally anticipated.

Buckling of plates and shells has been a topic of great interest for a number of years. Although the determination of the bifurcation (onset of buckling) of plates is well known, for the postbuckling response the deformed shape must be treated as a curved shell even when the reference shape was a flat plate. Moreover, the nonlinear equations also include the influence of bending on the membrane stresses that are the primary cause for buckling. The main objective of this work is to analyze the postbuckling response of a square plate and the ultimate strength of a rectangular plate. Specifically, it is shown that the approximate analytical solutions discussed in Timoshenko and Gere [2] are more limited than originally anticipated and that the postbuckling process associated with the ultimate strength of the plate is different from that presumed in the simple analysis.

Here, attention is focused on an isotropic elastic rectangular plate with length L, width W and thickness H. The plate is modeled using 3-D Cosserat brick elements [1]. The Cosserat element has 8 nodes with 24 degrees of freedom, it includes both material and geometric nonlinearities and it is invariant under superposed rigid body motions. The main difference between the Cosserat point approach and standard finite element formulations appears in the constitutive equations for the element. In the Cosserat approach these equations are hyperelastic with the intrinsic director couples being determined by algebraic equations in terms of derivatives of a strain energy function. In contrast with standard finite element formulations, the Cosserat approach needs no integration through the element region to determine the constitutive response.

The first example considers axial compression of a square plate with no lateral deformation. The results of the Cosserat element show that the approximate analytical expression discussed in [1] is more limited than originally anticipated. Specifically, the Cosserat solution predicts a snap-through phenomena as the mode shape changes abruptly.

The second example shows that as a rectangular plate is compressed in uniaxial stress the development of lateral tension causes the plate to divide into subdivisions which are rectangular instead of square, as predicted by the linearized theory. The ultimate strength of the plate occurs when the subdivision yields before the plate further subdivides elastically. This postbuckling process is different from that presumed in the simple analysis described in [1].

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On anisotropic formulations for finite strain plasticity and the plastic spin

Carlo Sansour

The multiplicative decomposition of the deformation gradient into elastic and inelastic parts can be considered nowadays as classical. A closer look at the literature, however, reveals that applications of the decomposition at a macroscopic level have been popular in the purely isotropic case. It is only recently that some anisotropic formulations are emerging. In fact, when it comes to anisotropy, the decomposition gives rise to ambiguities and can be a source of confusion. These ambiguities start with issues like the adequate formulation of the strain energy function and the choice of the so-called structural tensors which identify the anisotropy at hand. They continue with the question whether invariance conditions are to be imposed on such a function. Likewise, it is not evident from the outset, which stress quantity should be considered in the flow rule.
Let $\mathbf{F}$ be the deformation gradient and $\mathbf{F} = \mathbf{F_e}\mathbf{F_p}$ its multiplicative decomposition. We can define two inelastic rates by $\dot{\mathbf{F}}_\mathbf{p} = \tilde{\mathbf{L}}_\mathbf{p}\mathbf{F}_\mathbf{p} = \mathbf{F}_\mathbf{p}\mathbf{L}_\mathbf{p}$. $\mathbf{l_p} = \mathbf{F}\mathbf{L_p}\mathbf{F}^{-1} = \mathbf{F_e}\tilde{\mathbf{L}}_\mathbf{p}{\mathbf{F_e}}^{-1}$. Further, let $\mathbf{C}$ and $\mathbf{C_e}$ be tensors of the right Cauchy-Green type. Further a structural tensor is defined as $\mathbf{M} = \mathbf{v} \otimes \mathbf{v}$, where $\mathbf{v}$ is a privileged direction of the material. Now, let ψ define the free energy function. It is evident that ψ must depend on the elastic strain tensor $\mathbf{C_e}$. The anisotropy must be included through appropriately defined structural tensors. If we assume ψ to depend on $\mathbf{C_e}$ and $\mathbf{M}$ as well: $\psi = \hat{\psi}(\mathbf{C_e}, \mathbf{M})$, then contribution of the stresses to the reduced dissipation inequality takes the form:

$$D = \boldsymbol{\tau} : \mathbf{l_p} = \boldsymbol{\Xi} : \mathbf{L_p} = \tilde{\boldsymbol{\Xi}} : \tilde{\mathbf{L}}_\mathbf{p}, \tag{1}$$

where $\boldsymbol{\tau}$ is the Kirchoff stress tensor, $\boldsymbol{\Xi}$ is the material Eshelby-like tensor, and $\tilde{\boldsymbol{\Xi}}$ is Mandel's stress defined at the intermediate configuration. However, $\psi = \hat{\psi}(\mathbf{C_e}, \mathbf{M})$ is not invariant to superimposed rotations on $\mathbf{F_p}$.

Such an invariance can be achieved by transforming the structural tensors to the intermediate configuration. A reasonable transformation is a mixed-variant one as proposed in [1]:

$$\tilde{\mathbf{M}}^i_{\mathbf{e}} = \mathbf{F}_{\mathrm{p}}\mathbf{M}^i_{\mathbf{e}}\mathbf{F}_{\mathrm{p}}^{-1}\,, \quad i = 1,2,3\,. \tag{2}$$

The invariance requirement, however, alters the form of the mechanical contribution to the reduced dissipation equation. Eq. (1) will be modified. If we write the new equation in the form

$$D = \boldsymbol{\Gamma} : \mathbf{L_p} = \tilde{\boldsymbol{\Gamma}} : \tilde{\mathbf{L}}_{\mathbf{p}} = \boldsymbol{\gamma} : \mathbf{l_p}, \tag{3}$$

where Γ is a material stress-like tensor, and $\tilde{\boldsymbol{\Gamma}}$ and $\boldsymbol{\gamma}$ are its counter parts defined at the intermediate and the current configurations. It can be shown that $\tilde{\boldsymbol{\Gamma}}$ retains symmetry.

In addition, the fact that the stress tensors under consideration, in general, need not be symmetric necessitates a special treatment of the flow function, where representation theorems of tensor valued function with non-symmetric arguments are invoked. It is shown that the corresponding resulting rate, as defined at the actual configuration, is not symmetric any more. Accordingly, the rate naturally includes a plastic material spin. Moreover, we deal with the theoretically interesting question of how to define spin-free rates. It is also demonstrated that the flow function must depend not only on the stress tensor together with adequate structural tensors, but also on the deformation itself in form of one of the right Cauchy-Green tensors $\mathbf{C}$ or $\mathbf{C_e}$. However, this surprising dependency, which must obey a specific form, can be justified as physically meaningful. Various numerical examples of large plastic deformations of structural components are presented, that underpin the capabilities of the formulations. Numerical examples of large scale anisotropic computations of structural components will be presented as well.

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Multi-scale modelling of Pb-free solders

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(joint work with Jicheng Gong, Changqing Liu, Paul P. Conway)

Miniaturization of SnAgCu solder joints for electronic package results in the diminishment of the number of grains within a single joint, sometimes down to only one or two grains per joint. In this case, solder joints exhibit an anisotropic creep

behavior. Moreover, the crystal structure of beta-Sn (matrix of SnAgCu eutectics and Sn dendrites) is a contracted version of a diamond cubic, one leading to a body-centered tetragonal structure, which enhances this non-uniform character. These factors affect the character of creep and consequently determine reliability of solder joints for electronic packages. In this study, a crystal visco-plasticity model is developed to capture an anisotropic behavior of SnAgCu solder joints in cases of single-, bi- and multi-crystals. In order to simulate responses of solder joints under thermal cycling, a multi-scale finite element modelling is performed. In a global model, responses of joints in a flip chip package are simulated. Then results for displacements are adopted in the sub-model of a single joint. The obtained results are compared with those based on the traditional isotropic constitutive descriptions.

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Non-local modeling of crack propagation in metal matrix composites

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(joint work with Frederik Reusch, Christian Hortig)

The numerical analysis of ductile damage and failure in engineering materials and metal matrix composites is often based on a micromechanical description of the damage and failure process [1, 2, 3]. In particular, such failure involves (i), void nucleation at second-phase inclusions, (ii), growth of nucleated and existing voids via inelastic deformation of the matrix, (iii), void coalescence leading to crack initiation, and (iv) crack growth leading to specimen fracture. In the current work, we discuss a recently developed ductile damage formulation based on the modeling of void coalescence as a statistical process. The statistics here are in turn based on a Green distribution for the likelihood of coalescence of two voids [4, 5], with void nucleation and growth representing the corresponding point source processes. Averaging over this distribution leads to a non-local model of ductile damage and in particular void coalescence depending on the statistical average separation between neighboring voids. This model has been implemented into a finite element simulation of crack initiation and propagation in two- and three-dimensional metal matrix composites. A stability analysis of the corresponding boundary-value problem for the standard and non-local damage models allows the determination of the region of parameter space where the statistical non-local approach yields a regularization of the boundary-value problem. This in turn can be used as a criterion for adaptive mesh refinement. Application of this approach to the simulation and prediction of ductile crack propagation in Al-SiC metal matrix composites demonstrates its efficiency, robustness and reliability.

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Mechanical models for the analytical determination of the macroscopic material behaviour of textile reinforced concrete

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(joint work with Mike Richter)

Textile reinforced concrete (TRC) is a composite of a so called fine grained concrete matrix and a textile reinforcement which is used in the field of civil engineering for the fabrication of new structural elements and the strengthening of existing constructions [1]. The textile reinforcement consists of rovings. A roving is a bundle of huge number of continuous filaments. The failure mechanisms of TRC are very complex. Most important are the matrix cracking, the debonding of the roving from the matrix and the breaking of the filaments and rovings [6]. The macroscopic material behaviour can be classified in a linear elastic part for low loadings, the micro cracking and the macro cracking. The final failure of the composite occurs by the breaking of the rovings. To model this complex material behaviour the heterogeneous structure of TRC is analysed on the mesoscopic level. Then the macroscopic material behaviour, characterised by the overall elasticity tensor $\overline{\mathbf{C}}$, is obtained by the process of homogenisation. In this paper only analytical approaches are discussed.

For a low macroscopic loading the material behaviour is approximately linear elastic. Basis of the analytical determination of the overall elasticity tensor is the micro mechanical solution of the average strain in a single inclusion embedded in an elastic matrix according to Eshelby [2]. This solution leads to an equation for the overall elasticity tensor $\overline{\mathbf{C}}$:

$$\overline{\mathbf{C}} = \mathbf{C} + \sum_{\alpha=1}^{n} f_\alpha \left((\mathbf{C}^\alpha - \mathbf{C})^{-1} + \mathbf{S}^\alpha : \mathbf{D} \right)^{-1}. \tag{1}$$

Herein are $\mathbf{C}$ the elasticity tensor of the concrete matrix, $\mathbf{C}^\alpha$ the elasticity tensor of the inclusion α and $\mathbf{D}$ the compliance tensor of the matrix. $\mathbf{S}^\alpha$ is the Eshelby tensor and f_α the volume fraction of the inclusions α. This solution neglects any interactions between the inclusions and is called the solution for dilute distributions

or simple the dilute solution. In extension of the presented dilute solution for multi directional reinforcements an effective field approximation (EFA) is used [3]. This approach considers the interaction between the different orientated rovings in an average sense. Now the different orientated rovings are assumed to be in a matrix with the still unknown average matrix strain $\overline{\varepsilon}^m$. This problem can be solved analytically and leads to an equation for the direct computation of the overall elasticity tensor [6]:

(2)
$$\overline{\mathbf{C}} = \mathbf{C} + \sum_{\alpha=1}^{n} f_\alpha \left(\mathbf{C}^\alpha - \mathbf{C}\right) : \left\{ \mathbf{K}^\alpha + \sum_{\beta=1,\beta\neq\alpha}^{n} f_\beta \left(\mathbf{K}^\beta - f_\beta \mathbf{1}\right)^{-1} : \left(\mathbf{K}^\alpha - f_\alpha \mathbf{1}\right) \right\}^{-1}$$

with

(3)
$$\mathbf{K}^\alpha = \left(f_m + f_\alpha\right)\mathbf{1} - f_m \mathbf{S}^\alpha : \left(\mathbf{1} - \mathbf{D} : \mathbf{C}^\alpha\right).$$

Compared to eq. (1) in eq. (2) now the differently oriented rovings are coupled. f_m is the volume fraction of the matrix.

If the matrix stress exceeds a critical value micro cracks are developing. The additional strain due to the micro cracks $\overline{\varepsilon}^c$ can be expressed by the definition of a forth order tensor $\mathbf{J}^c$ and the prescribed macroscopic strain $\varepsilon^{\mathbf{0}}$ [4]. In the sense of the analytical homogenisation it is assumed, that there are no direct interactions between the micro cracks among themselves and between micro cracks and rovings, but the application of the effective field approximation allows the consideration of these interactions in an average sense. Hence, the additional strain due to the micro cracks is given as

(4)
$$\overline{\varepsilon}^c = \mathbf{J}^c : \overline{\varepsilon}^m.$$

The coordinates of $\mathbf{J}^c$ can be obtained by integration over the crack opening displacement [6] which is known from fracture mechanical solutions.

For the characterisation of the actual state we define a model parameter f_c, called *crack density parameter* as the product of the total number of cracks per unit area and the squared half crack length [4, 6]. Therewith we can describe the evolution of the micro cracks with only one parameter, and the tensor $\mathbf{J}^c$ depends on f_c. Using this parameter we don't need to know the lengths and the distribution of the cracks. However, the calculation of stress singularities is not possible.

In the mechanical model it is assumed, that the micro cracks cumulate to macro cracks if the micro crack density reaches a critical value. After initiation of the macro cracking the bond behaviour between roving and matrix dominates the overall macroscopic material behaviour. For the modelling of the bond behaviour a slip based bond model with a multiple linear shear stress-slip relation is used [5, 6]. A multiple linear approach allows the closed form analytical solution of the bond problem. At least three linear sections are necessary to consider the perfect bond zone, the partly damaged bond zone and the complete debonded zone. The exact function of the shear stress-slip relation can be determined by pullout experiments.

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Dislocation dynamics

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Bridging the gap between dislocation physics and continuum theories has become possible with the advancement in computational technology with bigger and faster computers. To this end, over the past two decades various discrete dislocation dynamics models have been developed. The early discrete dislocation models were two-dimensional and consisted of periodic cells containing multiple dislocations whose behavior was governed by a set of simplified rules (e.g. Lepinoux and Kubin, 1987 and Needleman and van der Giessen, 2001). These simulations, although served as a useful conceptual framework, were limited to two-dimensional space and, consequently, could not directly account for such important features in dislocation dynamics as slip geometry, line tension effects, multiplication, certain dislocation intersections and cross-slip. During the 90's, development of new computational approaches of dislocation dynamics (DD) in three-dimensional space generated hope for a principal breakthrough in our current understanding of dislocation mechanisms and their connection to continuum theories (e.g. Kubin, 1993, Zbib et al. 1996, 1998). In these new models, dislocation motion and interactions with other defects, particles and surfaces are explicitly considered. The discrete dislocation dynamics model we have developed has been utilized by a number of researchers to investigation many complicated small-scale crystal plasticity phenomena that occur under a wide range of loading and boundary conditions (Zbib and Khraishi 2005), and covering a wide spectrum of loading and boundary conditions. Some of the major phenomena that we have addressed include:

- The role of dislocation mechanisms in strain hardening (Hiratani and Zbib 2002).
- Strength in nanolaminates and nanocomposites (Zbib et al. 2005).
- Dislocation-defect interaction problems, including dislocation–void interaction, and dislocation-SFT/void-clusters interaction in irradiated materials (Diaz de la Rubia, Zbib et al. 2000; Khraishi, Zbib et al. 2002, Wirth et al. 2001; Hiratani and Zbib, 2003).

- The effect of particle size on hardening in metal-matrix composites (Khraishi and Zbib, 2002).
- The role of various dislocation patterns such geometrically necessary boundaries (GNB's) in hardening phenomena (Khan, Zbib et al. 2001, 2003).
- The role of dislocation mechanisms in increased strength in nano-layered structures (Zbib and Diaz de la Rubia 2002).
- High Strain Rate Phenomena and shock wave interaction with dislocations (Shehadeh et al., 2002-2005).

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