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Mechanics of Materials: Multiscale Design of Advanced Materials and Structures

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Abstract. Materials can now be designed and architectured like structural components for targeted mechanical and physical properties. Structures and microstructures should not be studied independently and their design will benefit from a multiscale approach combining nonlinear continuum mechanics approaches and physical descriptions of elasticity, viscoplasticity, phase transformations and damage of microstructures, at various scales. The aim of the workshop was to gather outstanding junior and senior researchers in the various branches of mathematics, physics and engineering sciences suited to address the question of design of materials and structures by means of multiscale discrete and continuum approaches to their constitutive behavior. Examples include atomic or macroscopic lattices, random or periodic cellular materials, smart materials like shape memory alloys, 3D woven composites, acoustic and electromagnetic metamaterials, etc. Modern continuum mechanics relies on sophisticated constitutive laws for anisotropic materials exhibiting elastoviscoplastic behavior, still a field of intense research with new mathematical concepts. In particular size-dependent properties are addressed by resorting to generalized continua such as gradient or micromorphic and phase field models. The latter are attractive for the simulation of microstructure evolution coupled with mechanics, due to thermodynamic and metallurgical processes and damage. Scale transition and homogenization methods for continuous and discrete systems are required for the determination of effective material and structural behavior. Metamaterials are architectured materials specifically designed to achieve certain propagation and dispersion properties of elastic and plastic waves. Optimization strategies for the design of optimal architectures are involved in the design process. Target functions for optimization are now based on multicriteria (stiffness, strength, thermal expansion, transport properties, anisotropy etc.).

Mathematics Subject Classification (2020): 74-XX, 65-XX, 49-XX, 35-XX.

Introduction by the Organizers

The workshop *Multiscale design of advanced materials and structures* attracted 43 participants with broad geographic representation (Germany, USA, Austria, France, Italy, Czech Republic, Switzerland, The Netherlands, Spain, Poland). This workshop comprised a well balanced blend of researchers with backgrounds in mathematics, mechanics and materials science. The organizers successfully recruited a significant number of younger representatives of the mentioned research communities.

The sequence and duration of the sessions were defined on Monday morning. They were moderated by session chairs and each consisted of 4-6 extended lectures (20 to 30 minutes each, including discussion) presented to all participants of the workshop. Two general lectures were scheduled to introduce two main branches of the program, namely the mathematical and physical aspects of the mechanics of heterogeneous materials, by G. Milton, and the multiscale computational mechanics and physics of materials, by L. Capolungo. Ample time was devoted to discussion, both during and following presentations. The format of the sessions (subject to hard stops for lunch and dinner), including coffee breaks, gave the flexibility to maximize productive discussion. Reports from the session chairs were summarized and discussed extensively on Friday morning and are summarized in this report. A DB strike lead to a more complicated situation on Friday for travelers trying to reach airports and train stations!

The organizers regard this particular workshop as extremely successful in the topical area of mechanics of materials, for several reasons. First, a number of young participants were involved and highly active in presentations and discussions, representing the next generation of applied mathematicians tackling problems in mechanics of materials. Computational mechanics applied to materials was well-represented. Some young and some experienced researchers discovered the Oberwolfach Stimmung for the first time and appreciated it. Second, the discussions were detailed and deep into the subject, with many useful points and counterpoints discussed. We believe that this workshop has launched many potentially fruitful couplings of researchers, and has defined some specific target areas as goals for mathematics, mechanics and materials science.

Tradition was respected with the usual long walk to Sankt-Roman, and its famous Schwarzwälderkirschtorte, during a rainy Wednesday afternoon, and with a piano concert on Thursday night thanks to the MFO Steinway grand piano.

Materials can now be designed and architectured like structural components or civil engineering structures for targeted mechanical and physical properties. Structures and microstructures should not be studied independently and their design will benefit from a multiscale approach combining modern nonlinear continuum mechanics approaches and physical descriptions of elasticity, viscoplasticity, phase

transformation and damage of microstructures, at various scales. The aim of the workshop was to gather outstanding junior and senior researchers in the various branches of mathematics, physics and engineering sciences suited to address the question of design of materials and structures by means of multiscale discrete and continuum approaches to their constitutive behavior. Examples of architectured materials and structures include atomic or macroscopic lattices, random or periodic cellular materials, smart materials like shape memory alloys, 3D woven composites, acoustic and electromagnetic metamaterials, etc. Modern continuum mechanics relies on sophisticated constitutive laws for anisotropic materials exhibiting elastic-viscoplastic behavior, still a field of intense research with new mathematical concepts. In particular, size-dependent properties are addressed by resorting to generalized continua such as gradient or micromorphic and phase field models. The latter are attractive for the simulation of microstructure evolution coupled with mechanics, due to thermodynamic and metallurgical processes and damage. Predicting instabilities is still the main challenge by detecting symmetry breaking conditions at various scales from local buckling phenomena in a truss to macroscopic strain localization and fracture of heterogeneous materials. Scale transition and homogenization methods for continuous and discrete systems are required for the determination of effective material and structural behavior. Efficient numerical techniques are thriving from FE to FFT methods. They incorporate stochastic aspects of morphology of phases and local properties thus allowing for a statistical analysis of overall responses. Envisaged physical phenomena at the constituent level are plasticity, viscoplasticity, crystal plasticity and twinning, diffusive and displacive phase transformation in solids. Metamaterials are architectured materials specifically designed to achieve certain propagation and dispersion properties of elastic and plastic waves. Tailoring band gaps in the frequency domain is the challenge of the corresponding design. Although periodic patterns dominate in this field, random sets may have attractive properties to widen the frequency spectrum. Multimodal databases produced from experimental observation and numerical simulation serve as the basis for the understanding of complex deformation and damage mechanisms and for the construction of overall reduced order metamodels required for the design process. Multimodal experimental data include field measurements of displacement, elastic strain, crystal lattice or fiber orientation, phase morphology evolution by means of optical, X-ray, electron tomography and diffraction available in labs or in international facilities. Multimodal numerical data emerge from large scale full field simulations of representative volume elements of materials or structures. These simulations are used to solve initial boundary value problems of continuum mechanics and physics, by means of finite element or FFT methods, or the evolution of discrete systems such as molecular dynamics or discrete dislocation dynamics.

The exploration and interpretation of databases from a range of models and experiments at various length and time scales can benefit from modern model reduction techniques and machine learning tools. Combining physical, mechanical,

mathematical knowledge and artificial intelligence is required to accelerate design processes and increase the reliability of prediction by appropriate uncertainty quantification. Optimization strategies for the design of optimal architectures for targeted properties are required in the design process. Target functions for optimization are now based on multicriteria (stiffness, strength, thermal expansion, transport properties, anisotropy etc.). Sophisticated mathematical and simulation methods are available from level set to phase field techniques. Multiscale optimization for composite design is even more challenging to reach the desired target properties.

1. Design of materials and structures

Chair: Dennis Kochmann (March 4th, morning session)

The quest for materials with optimized, extreme, or peculiar properties has been a challenge for centuries, originally stemming from the optimization of fabrication routes for traditional materials and more recently also applying to the creation of novel architected materials or metamaterials with as-designed properties and functionality. *Well-studied problems* were reviewed in this session and included, among others, the properties of cellular solids (i.e., two-phase composites in which one phase is solid and the other is void), whose analysis has resulted in the class of extremal composites, which are mathematically rooted in the soft modes of the elasticity tensor and admit beneficial properties such as fluid-like behavior (e.g., pentamode materials), insulation against shear waves (e.g., unimode materials for seismic insulation) or extremal elastic properties. Cellular solids also include beam-, plate-, and shell-based architected materials, which have been optimzed for high stiffness-, strength-, and toughness-to-weight ratios, have enabled the design of mechanical waveguides that exploit wave dispersion to direct stress waves along pre-defined paths or attenuate waves at specific frequency. Besides beam-based structures, a recent advance has been the use of spinodal-type cellular architectures, which admit tuning of the effective elasticity and nonlinear response through the choice of anisotropy in the underlying Gaussian random fields. A further example is the link between microstructural features (such as the statistical information contained in the grain size distribution and texture of a polycrystal) and the effective mechanical response of materials (such as the stress-strain response of polycrystalline metals), which calls for techniques to understand the aforementioned link and to invert it towards the design of materials with optimal properties.

2. Constitutive laws for crystalline materials

Chair: Thomas Hochrainer (March 4th afternoon, session)

Crystal plasticity modelling plays a central role in the nonlinear mechanics of materials. It tackles the difficult problem of the transition from dislocation mechanics to continuum plasticity, a still widely open question. Six talks were presented on this topic.

Several presentations were dedicated to the discrete dislocation dynamics, a computational methods to predict the motion, multiplication and interaction of individual dislocations in a micrometer-sized box, based on the elasticity theory with defects and special interaction rules. The method can be used to predict the overall response of the volume element to macroscopic loading.

Katrin Schulz proposes a data-based derivation of internal stresses for the coarse-graining in dislocation-based plasticity. This can be regarded as a way of extracting information from huge data produced by DDD in the form of complex dislocation entanglements. Thomas Hochrainer then presents another tool in this endeavour: A translation invariant approximation of the Koopman operator for analysing discrete dislocation data. Yaovi Amouzou-Adoun also relies on DDD simulations of cyclic plasticity to predict size effects and construct a strain gradient continuum plasticity model. He shows that a strain gradient crystal plasticity model can be calibrated to reproduce, at least qualitatively, the size effects observed during cyclic shearing.

Anter El-Azab tackles a novel aspect of dislocation dynamics, namely mesoscale plasticity of inhomogeneous alloys, linking chemistry and dislocation dynamics. The interaction of dislocations with solute atoms is a fundamental aspect of mechanical metallurgy. It plays a role in solution hardening in alloys and in static and dynamic strain ageing.

Finally, David McDowell presents a comprehensive thermodynamical framework to formulate the constitutive equations of crystal plasticity by means of nonequilibrium statistical mechanics of thermally activated dislocation ensembles and internal state variable theory.

An important feature of dislocation based plasticity is the stochastic aspects of slip avalanches and strain burst in crystals. Jaime Marian presents stochastic solvers for crystal plasticity in order to match plastic and numerical discreteness.

3. Multiscale and multiphysics approaches

Chair: Javier Segurado (March 5th morning, session)

Six talks including discussion were presented, with very different scopes but all of them covering multiscale aspects.

The first talk was an introductory lecture by Laurent Capolungo from Los Alamos NL (USA). The talk focused on (1) showing the technological needs for fundamental scientific developments (2) describing the overall multiscale modeling paradigm and (3) emphasizing some of the epistemic gaps that require more attention to enable phenomenology free constitutive modeling. It was suggested that many times models are pushed too far away from the limits of their applicability, driven by the need of studying the response in critical and out-of-equilibrium situations. A general conclusion was that there is a critical need to establish rigorous mathematical linkages between microstructure configurations, energy barriers, internal stress and entropic contributions to kinetic factors. They were many comments and questions. To give one example, one question dealt with a mesoscopic

approach to retrieve a GND distribution in nano-laminates, which may go beyond a continuum model.

The second talk was presented by Mischa Blaszczyk, PhD student at Institute of Mechanics of Materials, Ruhr-Universität Bochum and entitled "A fully coupled multiscale model of cancellous bone considering mechanical, electric and magnetic effects". The motivation behind this multiscale and multiphysical modeling of bone study was the osteoporosis, leading to bone disease worldwide. The model is solved using two scales (FE2) and including electric and magnetic effects at the two scales while a two-phase material was defined on the microscale (cortical bone and bone marrow). Ostheoporosis effects were included explicitly in the definition of the RVEs. The numerical results show a drastic reduction of the magnetic field strength resulting from a small mechanical impact for later stages of the disease, which is in conformity with experimental research. Regarding questions, there was an interest of knowing if magnetic fields relaxation times are not an obstacle for identifying ostheoporosis from magnetic measurements.

The third talk was a study of the chairman, Javier Segurado from "Universidad Politécnica de Madrid" and IMDEA-Materials Institute (Spain), and was chaired by David McDowell. The title was "Elastic interactions in Object kinetic Monte Carlo for defect evolution: radiation defect migration". First, an FFT based approach was presented to introduce the elastic fields caused by any type of dislocation, point defects, solute atoms and second phases in OkMC simulations. The model was applied to study the migration of prismatic loops and self-interstitials in iron, accounting for their mutual interaction and the presence of other immobile dislocations. The second part of the talk presented a method to use non-regular grids in FFT solvers to improve the resolution near dislocation cores in the computation of the elastic fields produced by dislocation and other defects. During the discussion, he was asked whether the non-regular technique corresponded to a "mesh refinement" or if it was a transformation of the physical space. It was explained that the method was just a translation of the discretization points to better represent the solution, but all the operators were defined at the material points.

The fourth talk was presented by Liming Xiong, from Iowa State University (USA) and was entitled "Concurrent Atomistic-Continuum Simulation of Plastic Flow in Heterogeneous Alloys". In this talk, L. Xiong presents a concurrent atomistic-continuum (CAC) methodology and its applications in modeling the dislocation-mediated plastic flow. One main unique feature of CAC is to retain the microscale dislocation slip, the atomic-scale diffusion and kink dynamics on the dislocation line, as well as the nanoscale grain boundary (GB) structure evolution all within one model. The applicability of CAC is demonstrated through: (i) modeling the dislocation loop nucleation and growth from atomistic to microscale; (ii) characterizing the core structure/stress heterogeneity induced by atomic-level diffusion along a micrometer-long dislocation line; (iii) quantifying the stress concentration induced by the slip-GB reaction. The main outcome of this talk is to

provide the community with an alternative vehicle to bridge atomistic with continuum by formulating the local stress-/GB-state based metrics of slip transfer that can be informed into higher scale models, as DD or CPFE. One main remaining question is about how to consolidate the CAC simulation results into constitutive rules or slip transfer metrics that can be used at the engineering scale. At the end of the talk, the extension of CAC to finite-temperature through phonon density states-based algorithm was also discussed.

The fifth talk was presented by Barbara Zwicknagl, from Humboldt-Universität zu Berlin (Germany). The tile of the work was "Geometry of needle-like microstructures in martensites". In their work, the modeling of needle-like microstructures – which are often observed experimentally near macro-interfaces in certain shape-memory alloys – was analyzed. In particular, the focus lied on the tapering length scale of the needle. It was shown that linearized elasticity is not able to predict the value of the tapering length. In the questions, it was discussed the need or not of including explicitly and interfacial energy in the formulation.

The last talk of the session was presented by Christian Wieners from Karlsruher Institut für Technologie (KIT) in Germany. His talk initiated an open discussion about waves in materials with heterogeneous microstructures. First, some known results were summarized, including the response of linear waves in 1D and some general marks about the 2-scale simulation. Then, the framework of the homogenization of Maxwell equations was reviewed to explore if there exist some unified approach for electro-magnetic and for elastic waves. As result, it was shown that density in a two-scale problem can be directly replaced by the average in the microstructure. Finally, several open remarks were made around the conditions for a FE2 formulation of wave propagation.

4. Numerical methods and models for plasticity and damage

Chair: Stéphane Berbenni (March 5th, afternoon session)

Damage was first envisaged at interfaces in dual phase steels in the form of thin ductile martensitic layer undergoing large plastic deformation and leading to grain boundary sliding. The finite element simulation results can be compared with experimental strain field measurements. Open questions remain regarding the identification of physical parameters for interface damage mode initiation and propagation, the effect of bi-cristallography between Martensite and Austenite (KS or NW orientation relationships). Simulations at lower scales (atomistics) could be used to derive physically based cohesive laws.

Quasi-brittle damage was also considered in polycrystals using the phase field method combined with elasticity. Open questions remain regarding the tractability of 3D simulations, on the proper choice of non-convex energy functionals. Intersting outcomes could be the prediction of the effect of grain size distribution on cracking.

A mathematical point of view was then given to handle non convexities in rate-independent systems. Several algorithms, including viscosity regularization, were then proposed.

An alternative to finite element simulation is the use of spectral methods. FFT-based methods have become very popular for the simulation of plastic deformation in microstructures. Is it possible to go beyond periodic boundary conditions? Periodic boundary conditions introduce a bias in the case on non-periodic images of microstructures. Some proposals were made to extend spectral methods to account for Dirichlet boundary conditions.

A FFT-solver was also applied to mesoscale field dislocation mechanics introducing dissipative mechanisms and defect energy. The existence of a back-stress was demonstrated in a simple shear test under cyclic loading. Open questions are related to the implementation of non-quadratic energy potential (logarithmic of power law) in the FFT scheme, and to the introduction of a grain boundary behaviour in such a discrete scheme.

New perspectives in quasi-brittle damage and fracture modelling are brought by the so-called peri-dynamic approach which includes nonlocal kernel interactions between material points with an horizon range. Point-wise discretisation eases dynamic fracture simulations and makes the model a promising approach.

5. Phase transformation and thermodynamics

Chair: Thomas Antretter (March 6th, morning session)

The five talks of this session dealt with modeling and experimental determination of energetic and dissipative stresses in plastic deformation (by T. Böhlke), a new look at twin branching in shape memory alloys (a 1D continuum model and energy dissipation effects, by S. Stupkiewicz), and thermomechanical coupling of phase transformations and constitutive laws to describe microstructural evolution (by M. Flachberger). S. Mesarovic presented advances on continuum modelling of sintering processes in metals. The question of recrystallisation was addressed by A. Ask, with a Cosserat continuum representation of crystal plasticity and grain boundary migration. Finally, T. Antretter exposed a chemo-mechanically coupled model of bainitic transformation in steels.

The discussions around the 5 talks of this session were focused on several critical issues in materials and interface mechanics:

- Energy storage and dissipation in plasticity of metals
- Computational description of interface processes: orientation, lattice growth and sliding
- Computational approach to phase transformations on the microscale and their continuum representation

In spite of the complexity of the problems, significant progress has been made in the last decade. Specifically, the power of the phase field computational approach has been demonstrated on a large span of length scales. Given correct mathematical formulation and sufficient computational power, predictive simulations of a variety of complex physical processes are feasible.

Nevertheless, several open problems emerged from discussion:

- What are the possible methods of distinguishing energy storage and dissipation in plasticity? Is there a clear relation between this problem and configurational and vibrational entropy production in plastic deformation.
- The question of representing relative misorientation of crystals at interfaces within the phase field model remains open. Such representation must be computationally efficient and represent the underlying physics correctly. This is particularly relevant for anisotropic grain growth.
- While the problem of connecting heterologous (lattice and mass) continua in the phase field framework appears resolved in principle, details of interface processes: lattice growth and sliding need to be calibrated to the sharp interface formulation (which is the basis for interpretation of experiments).
- The role of dissipation in continuum representation of discrete phase transformation events (twin branching) requires quantification.
- When many variants of microstructures appear equally energetically favorable, computational distinction between them is an open problem. The problem of bainite microstructures is the specific example of this difficulty.

6. Fundamentals of continuum theories including gradient approaches

Chair: Arash Yavari (March 7th, morning session)

The six talks were related to problems in finite plasticity, crystal plasticity, compatibility equations of anelasticity in a Eulerian setting, coupling of Cahn-Hilliard equation with heat equation, a rigorous formulation of nonlocal hyperelasticity, Korn inequalities for general incompatibilities, and universal deformations in nonlinear elasticity and anelasticity. These are all important problems with direct applications in the design of new materials and structures.

We anticipate that the following will represent immediate research challenges worthy of investigation. The results of these studies will be presented in a future Oberwolfach meeting.

- Making connections between compatibility equations in the Lagrangian and rate formulations of anelasticity
- A notable limitation of the model proposed by Jebahi et al. is that it cannot mimic scaling relationships with exponents less than 1, which are generally predicted by DD observed in several small-scale experimental investigations. This limitation underscores a significant challenge and opens a critical avenue for further research within the domain of strain gradient plasy. It raises pivotal questions about the capabilities of existing strain gradient plasticity models to fully encapsulate the nuances of size effects. As such, this area remains ripe for innovation, invitivancements that can bridge persisting gaps and provide a more comprehensive understanding of material behaviors at small scales.
- Push and understand the case of generalized Korn's inequalities in the context of non-constant coefficients. This is crucial in considerations from viscoelasticity.

- Deriving a coupled heat equation using a given free energy (that is a function of a phase field, velocity and velocity gradient, and temperature) and the first and second laws of thermodynamics and ring it with the proposed heat flow equations.
- Using the proposed nonlocal hyperelastic elasticity in solving some concrete problems. One can start with simple problems that have already been investigated using other nonlocal theories, e.g., beading formulated using Eringen's nonlocal theory.
- Solving Ericksen's open problem: Find all the constant-principal invariant universal deformations of homogeneous incompressible isotropic solids. This has been an open problem since the 1950s.
- Working on several semi-inverse solutions in the mechanics of growth, remodeling, and visco-anelasticity.

7. Heterogeneous and architectured materials

Chair: Thomas Böhlke (March 7th, afternoon session)

The keywords of this session were: computational homogenization, higher-order asymptotic homogenization, deep material networks, topology optimization.

The main topics and advances dealt with computational homogenization (coupled linear problems). Based on homogenisation methods, the elastic and acoustic properties of metamaterials can be manipulated with locally resonant metamaterials (local resonance regime). The solid-fluid interaction was included by V. Kouznetsova in the approach. Filtering of vibrational frequencies and negative reflection were discussed for practical metamaterial design. The flexibility, efficiency and accuracy of scale bridging techniques for nonlinear thermo-mechanical behavior were reviewed. As an example, the generation of virtual open-cell-like structures is discussed and used for solid-fluid-type simulations. The combination of numerical scale bridging with an analytical macroscale model shows advantages when the macroscale approach captures the main features of the macroscopic material behavior.

In the context of higher order multiscale asymptotic homogenization of periodic microstructures, first and higher order boundary corrections were recalled. Non-periodic boundary conditions, in particular Dirichlet and mixed boundary conditions, are discussed. The results show much better accuracy than the approaches without higher order corrections. Outstanding issues relate to the following points: Boundary layer effects for any shape of the boundary and any cut of the boundary, the extension to small strain elastoplasticity (some mathematical attempts exist), computations at the macroscale with strain gradient effective medium are needed in some cases.

M. Schneider showed that Deep Material Networks (DMN) offer a numerically efficient alternative to FE^2 or FE-FFT approaches for modeling the macroscopic nonlinear behaviour of fiber-reinforced polymers. DMNs are represented by a hierarchy of laminates, where the local properties of the laminates (volume fraction, laminate orientation) are identified by off-line linear elastic training. Based on the

training restricted to the elastic fields on the microscale, the nonlinear material behaviour can be predicted with surprising accuracy even for non-proportional deformation paths in viscoelasticity and (visco)plasticity. Current research questions are: Are Deep Material Networks expressive, i.e., may the homogenization function of any (two-phase) microstructure be approximated by a hierarchy of laminates? Is there an improved design of Deep Material Networks (e.g., different building blocks, different hierarchy) which is expressive? Is there an underlying theory which explains why elastic training suffices for inelastic applications? Can this insight be used to improve the selection of the training data?

A material design approach based on variable stiffness design was shown to provide an alternative approach to shape optimisation. The transition between single and multi-scale problems is discussed, specifically for truss structures, and a two-stage optimisation algorithm was introduced by M. Doskar, including a manufacturing tolerant design.

8. General discussion and prospects for a future Workshop

Vivid discussions took place on fundamental aspects of continuum mechanics, plasticity and damage of materials. It is remarkable that the relation of plasticity and damage to thermodynamics was at the center of discussions several times during the symposium. There are still largely open questions regarding the theoretical and experimental determination of stored energy, dissipation rate the formulation of thermodynamically consistent theories, with significant advances reported at the Workshop. Non-convexities in inelasticity and damage still remain challenging mathematical, physical and computational issues.

Composite materials and metamaterials were explored in great detail with the promising optimal design guideline, opening a new era in engineering sciences including mathematical and materials science aspects.

Large scale multiscale computational methods are ubiquitous and require adequate error estimations and analysis of convergence as illustrated in a few cases, for a broad scope of discrete or continuous, physical and mechanical approaches.

Emergent topics that were discussed include the use of machine learning (ML) and its applications. If large datasets are available, then tools such as neural networks, variational autoencoders, or image/video diffusion models can be used to (i) learn the forward homogenization problem of predicting the effective properties of a given structure as a surrogate homogenization model, and (ii) to tackle the inverse design problem of predicting structures with given effective properties. Existing approaches are promising but only the tip of the iceberg, so that it is an ongoing challenge to fully leverage ML-based tools for the forward and inverse homogenization problems. It is expected that many more such strategies may be exploited in the future. If datasets are small, ML tools can still be used such as the application of Gaussian regression – both for forward and inverse homogenization but also for intermediate steps (e.g., for predicting material microstructures for given statistical microstructural information).

There is tremendous interest for reducing the complexity of a microstructure to low-dimensional microscale descriptors, which can be achieved through mathematical morphology or ML tools. Especially when using experimental data as the starting point, datasets are naturally limited, so that multi-modal approaches that take into account both experimental and simulated data are promising. Furthermore, open challenges of course also pertain to fundamental questions in the design of materials, e.g., the full exploration of extremal materials and their properties, and the search for optimal microstructures that attain property bounds. When it comes to the design of materials with extreme properties, another challenge is the extension from periodic designs to spatially graded ones, for which classical homogenization approaches may not apply and multiscale techniques become necessary (e.g., including multiscale topology optimization schemes).

There is still a work to be done on multiphysical models involving different scales (for problems as additive manufacturing or corrosion), concurrent approaches for two-scale simulation beyond mechanical behavior (e.g. in batteries).

Open problems in computational homogenization still remain: incorporation of (thermo-)viscous dissipation into the computational homogenization framework for elasto-acoustic metamaterials and the extension of the range of applicability of the computational homogenization framework to the cases where the strict confinement of the resonance in a longwave host medium does not hold and has to be relaxed. What are the most suitable theoretical, numerical and algorithmic settings for computational homogenization, when accuracy, efficiency, and flexibility of application are considered simultaneously? Are these strategies straightforwardly extendable to multiphysics (electro-magneto-mechanical; thermo-mechanical; chemo-mechanical) settings? In two-scale problems, how can local microscopic fields be reconstructed from efficient, perhaps ML-based, macroscale descriptions?

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Workshop: Mechanics of Materials: Multiscale Design of Advanced Materials and Structures

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Abstracts

Dialogue strain gradient crystal plasticity and discrete dislocation dynamics: kinematic hardening modeling.

Yaovi Armand Amouzou-Adoun
(joint work with Mohamed Jebahi, Samuel Forest, Marc Fivel)

The study of size effects requires the introduction of internal length scales as classical plasticity theories fall short in modeling these effects. Strain gradient (crystal) plasticity (SG(C)P) emerges as a powerful framework for investigating the size-dependent behavior of materials at small scales [1]. In order to have physically informed SGCP theories, dialogue with discrete dislocation dynamics (DDD) is a suitable approach. The latter method is able to model size effects in a quite natural way [2]. Using DDD, a shearing problem of a two-dimensional strip with infinite length in x-direction and a small width h in y-direction, is treated. DDD revealed a strengthening phenomenon with the apparent higher-order yield stress evolving as $h^{-0.2}$ and a strong kinematic hardening. The strengthening is explained here are as consequence of a micro-plasticity process rather than a delay of the onset of plastic flow. Inspired by the main results with DDD, a SGCP model is developed in order to model the higher-order kinematic hardening behavior. The present model is based on multi-kinematic decomposition strategy to decompose the plastic slip gradients into recoverable and non-recoverable parts [3]. Within this framework, the defect energy density is articulated through a combination of quadratic and less-than-quadratic functions, providing a robust basis for capturing complex material behavior. By manipulating specific model parameters, the scaling exponent factor r in the scaling relationship (h^{-r}) can be easily adjusted within the interval $[1.0, 2.0]$, demonstrating the model flexibility in representing size effects over a range from linear to quadratic scaling. However, the inability of SGCP theories to mimic scaling relationships with exponents less than 1 as obtained with DDD and/or experiments seems to be a notable limitation. Fig. 1 shows the comparison of SGCP and DDD predictions for the shearing problem. The different plastic regimes were successfully modeled by the proposed SGCP in terms of the micro-plasticity process, the kinematic hardening and also the presence of the uncommon type III (KIII) kinematic hardening of Asaro. Only, the scaling law does not fit. It raises pivotal questions about the capabilities of existing strain gradient plasticity models to fully encapsulate the nuances of size effects. As such, this area remains ripe for innovation, inviting advancements that can bridge persisting gaps and provide a more comprehensive understanding of material behaviors at small scales.

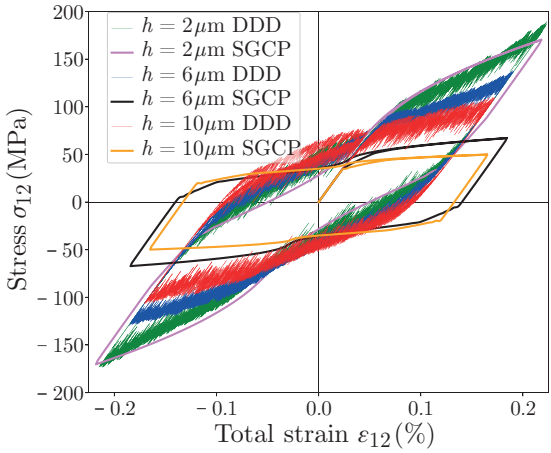

FIGURE 1. Comparison of size effects between DDD and SGCP: h is the geometrical size.

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A coupled chemo-mechanical model for bainitic transformation

THOMAS ANTRETTER

(joint work with Swaroop G. Nagaraja)

Upon cooling carbon steel experiences a phase transformation from its original face-cubic-centered parent phase to the body-cubic-centered product phase bainite. Modeling its evolution requires taking into account various physical phenomena: 1.) carbon diffusion whose velocity depends on the temperature, 2.) carbide precipitation inside the bainite phase if the temperature is low, i.e., in the case of lower bainite, 3.) transformation eigenstrains concomitant to the creation of either a new phase including the formation of carbides, and 4.) accommodation mechanics such as elasticity and crystal plasticity. The literature covers some of the aspects mentioned above, see [1] and [2], but a comprehensive study treating all phenomena in a monolithic way has not been reported so far. In the current work the problem is tackled in a very general variational framework. Starting point is the formulation of the energy storage function that, in addition to strain

energy, contains the contributions due to strain hardening as well as a chemical energy term depending on internal flux variables and gradients thereof. Next, suitable dissipation pseudopotentials have to be proposed that account for dissipation due to plastic slip as well as due to the relevant chemical mechanisms such as diffusion and phase transformation. We arrive at a total continuous-time potential and, after Euler-backward time integration, eventually at a discrete-time potential π^τ whose extremum determines the design variables, where $\boldsymbol{u}$ is the displacment field, γ^α the plastic slip on slip system α, $\gamma^{+\alpha}$ the accumulated plastic slip, $\mathfrak{e}$ the internal flux variables and $\mathfrak{b}$ the internal force variables.

$$\left\{\boldsymbol{u}, \gamma^\alpha, \gamma^{+\alpha}, \mathfrak{e}, \mathfrak{b}\right\} = \operatorname{Arg}\Big\{ \inf_{\boldsymbol{u}\in\mathscr{V}_{\boldsymbol{u}}^\tau} \inf_{\gamma^\alpha} \inf_{\gamma^{+\alpha}} \inf_{\mathfrak{e}\in\mathscr{V}_{\mathfrak{e}}^\tau} \sup_{\mathfrak{b}\in\mathscr{V}_{\mathfrak{b}}^\tau} \pi^\tau \left(\boldsymbol{u}, \gamma^\alpha, \gamma^{+\alpha}, \mathfrak{e}, \mathfrak{b}\right) \Big\}$$

For the chemical contributions to the total energy classical double well potentials are chosen, both for the expressions governing carbon diffusion and for the expressions governing the phase field evolution. The pseudopotential describing the dissipation due to phase evolution as well as due to diffusion also contains a term that accounts for the coupling of these two mechanisms. A crystal plastic yield condition is added to the optimization problem as a side condition multiplied by a Lagrange mulitplier. After numerical implementation of the presented framework using the user-element subroutine functionality of the finite element program of choice the computed field variables can be displayed, as exemplified by Figure 1 showing the carbon distribution trapped inside the bainite sheaf as diffusion velocities are low at the given temperature. The algorithm also provides the evolution of the phase field parameters indicating the phase state (austenite, bainite or precipitate). The coupling of the chemical quantities with the displacment field is demonstrated. As expected, disregarding any plastic accommodation mechanisms would greatly exaggerate the mechanical driving forces of transformation thereby unreasonably speeding up the process of bainite formation. This underlines the importance of taking into account plasticity as it has been done in this work. There are also some noteworthy numerical features: i) the chosen variational formulation results in a symmetric system of equations for the coupled evolution problem [2], ii) the fact that the coupling term between diffusion and phase formation is contained in the dissipation formulation rather than the energy potential leads to a sparse tangent operator, and iii) the plastic slip variables are determined by local iterations at integration points leaving a reduced problem to be solved by global iteration resulting in displacments, order parameters, concentration and chemical potential as nodal variables of the finite element discretization.

The mechanical driving forces mentioned above are mainly due to transformation eigenstrains that are typically significant upon bainite transformation and exhibit a strong anisotropy leading to the characteristic prolate shape of the bainite phase. Determining the deformation gradient accompanying bainitic transformation is not trivial since at any time the bainite sheaf must satisfy a compatibility constraint at the interface with the parent austenite phase. For the particular case of bainite transformation this can only be ensured by additional plasticity in the

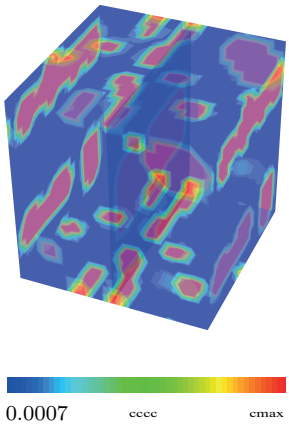

FIGURE 1. Snapshot of the carbon distribution trapped in and around the bainite phase (not shown here).

bainite sheaf. In a follow-up to this work realistic eigenstrains will be implemented computed by a GUI based algorithm developed by Petersmann et al. [3].

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A Cosserat continuum representation of crystal plasticity and recrystallization

ANNA ASK
(joint work with Flavien Ghiglione, Samuel Forest)

The earliest evidence of metalworking—the combined application of force and heat to metals to alter their macroscopic properties—date back to prehistory. Modern experimental techniques have finally allowed the study of the microscopic processes that are activated by the thermomechanical treatment. A significant amount of energy is stored in the crystalline microstructure during viscoplastic deformation due to the production of atomistic defects called dislocations. This energy can be released by processes such as recombination of the dislocations into subgrain boundaries (dynamic recovery) or the nucleation and growth of new, defect-free crystalline grains (static or dynamic recrystallization). The old microstructure

may be entirely replaced after thermomechanical treatment, and the metalworking allows a certain control of the average grain size and crystalline orientation in the new microstructure. While extensively researched, several aspects of this microstructure evolution are still not fully understood or quantified. Questions remain regarding such issues as the exact conditions that favor recovery over recrystallization, or the relationship between the static and dynamic grain boundary properties.

Several approaches have been proposed to model the microstructure evolution that is produced by thermomechanical processing. In this work, a monolithic continuum approach is adopted. The particularity of the proposed framework is that it (i) treats the crystalline orientation as a degree of freedom, (ii) the energy associated with lattice curvature is explicitly taken into account, as well as (iii) the production and annihilation of dislocations in an averaged sense. The main aim is to predict qualitatively the microstructure evolution. This is achieved by combining a crystal plasticity model formulated for a Cosserat continuum and a phase-field method[1]. The Cosserat framework provides the microrotational degrees of freedom which are constrained to follow the crystal orientation of the grains. Unlike a classic crystal plasticity approach, the grain boundaries are diffuse and mobile due to the inclusion of the phase-field dynamics. The phase-field parameter is an order parameter that is sensitive to crystal lattice curvature. Simulations for single crystals and small polycrystals have demonstrated that the proposed approach can predict subgrain boundary formation, dislocation driven grain boundary migration, and possibly grain nucleation [2].

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Size-dependent elastoplasticity relying on Eulerian rates of elastic incompatibilities

Lorenzo Bardella

(joint work with M.B. Rubin)

1. Summary

The notion of elastic incompatibilities considers elastic deformations from one configuration to another. In this contribution elastically anisotropic materials are discussed within the context of a large deformation Eulerian formulation that is free from arbitrary choices of reference and intermediate configurations as well as total and plastic deformation measures. An elastic deformation is defined from an

arbitrary initial configuration that can have a state with elastic incompatibilities. Necessary and sufficient conditions are obtained for additional elastic incompatibilities developing from this initial configuration. Moreover, a second-order Eulerian tensor R_{ij} is proposed, based on the current curl of the rate of plastic deformation tensor, which measures the current rate of elastic incompatibilities related to developing edge and screw dislocations. R_{ij} can in fact be seen as an extension of the elastic counterpart of the rate of the Nye-Kröner dislocation density tensor, as originally defined for small strains and rotations. This allows the study of the size-effect ensuing from a hardening law dependent on R_{ij}. In order to unveil the features of the proposed theory, the torsion of a cylinder is studied under both monotonic and cyclic loading paths.

2. A Lagrangian formulation of total deformation incompatibility

Finite deformation total strains are purely kinematic variables that measure deformation from a specified reference configuration to the current configuration. For example, a material point located by $\mathbf{X}$ in the reference configuration is deformed to its location $\mathbf{x}$ in the current configuration at time t by a one-to-one mapping

$$\mathbf{x} = \mathbf{X}(\mathbf{X}, t)\,, \tag{1}$$

and the associated deformation gradient $\mathbf{F}$ is defined by

$$\mathbf{F} = \partial \mathbf{x}/\partial \mathbf{X}\,.$$

By definition, this mapping and the associated deformation gradient characterize a compatible deformation field from the reference configuration to the present configuration.

One question of compatibility arises when $\mathbf{F}$ is a specified function of $(\mathbf{X}, t)$ and it is not known if an associated compatible deformation field with a mapping of the form (1) exits. Yavari [1] discussed the history of this problem for nonlinear elasticity and generalized the solution for multiply connected regions. Here, attention is confined to simply connected regions for which the necessary and sufficient condition for a compatible mapping (1) to exist is that

$$\oint_C \mathbf{F}\mathrm{d}\mathbf{X} = \int_S \mathrm{Curl}(\mathbf{F})\mathbf{N}\mathrm{d}A = \mathbf{0}$$

for all closed paths C in the body, where Stoke's theorem has been used to convert the line integral to an integral over the enclosed surface. Moreover, Curl( ) is the curl operator with respect to $\mathbf{X}$, $\mathbf{N}$ is the unit normal to the surface S, right-handed relative to the direction of integration on C, and $\mathrm{d}A$ is the reference area element on the surface S. Assuming sufficient continuity, it follows that

$$\mathrm{Curl}(\mathbf{F}) = \mathbf{0}$$

at every point in the body.

3. An Eulerian formulation of elastic deformation for elastoplastic materials

Eckart [2] seems to be the first to propose an Eulerian formulation of constitutive equations for elastically isotropic elastoplastic response of solids. A similar formulation for polymeric liquids was formulated in [3]. These formulations are Eulerian in the sense that they are free from arbitrary specification of reference or intermediate configurations as well as total or plastic deformation measures [4]. An Eulerian formulation of constitutive equations for elastoplastic response of elastically anisotropic materials was developed in [5]. This formulation introduces evolution equations for a right-handed triad $\mathbf{m}_i$ of linearly independent microstructural vectors of the forms

$$\dot{\mathbf{m}}_i = (\mathbf{L} - \mathbf{L}_p)\mathbf{m}_i \,, \tag{2}$$

where $\dot{(\ )}$ denotes the material time derivative, $\mathbf{L}$ is the total velocity gradient, and $\mathbf{L}_p$ is a general second-order tensor characterizing plastic rate, which requires a constitutive equation. The microstructural vectors $\mathbf{m}_i$ characterize elastic deformations and orientation changes of anisotropic directions in the material relative to a zero-stress state. They also determine the Cauchy stress $\mathbf{T}$ in the current state. These microstructural vectors $\mathbf{m}_i$ are internal state variables, as defined by Onat [6], which are assumed to be measurable in the current state.

4. A Lagrangian formulation of elastic incompatibility for elastoplastic materials

The notion of elastic compatibility is Lagrangian in the sense that it requires a definition of elastic deformation between two configurations. Consequently, it is convenient to define the values $\mathbf{M}_i$ of $\mathbf{m}_i$ in the initial configuration at $t = 0$ and the reciprocal vectors $\mathbf{M}^i$ at $t = 0$. Then, the elastic deformation $\mathbf{F}_m$ from this initial configuration to the current configuration at time t is defined by

$$\mathbf{F}_m(t) = \mathbf{m}_s(t) \otimes \mathbf{M}^s \,, \quad \mathbf{F}_m(0) = \mathbf{I} \,,$$

where $\otimes$ denotes the tensor product, the usual summation convention applies to repeated indices, and $\mathbf{I}$ is the identity tensor. This tensor $\mathbf{F}_m$ remains a measure of elastic deformation from the initial configuration even for a general initial configuration in a state with residual stresses. Then, a Nye-Kröner-like tensor $\boldsymbol{\alpha}_e$ [7, 8], which measures elastic incompatibilities from the initial configuration, can be defined by

$$\boldsymbol{\alpha}_e = \mathrm{Curl}(\mathbf{F}_m) \,, \tag{3}$$

where the Curl operator is relative to the initial configuration. If $\boldsymbol{\alpha}_e = \mathbf{0}$ the deformation, as described by $\mathbf{F}_m$ through the evolution of the microstructural vectors $\mathbf{m}_i(t)$, is compatible.

5. Eulerian rates of elastic incompatibilities for elastoplastic materials

By taking the material derivative of (3) and evaluating the result in the current configuration, it can be shown that Eulerian rates of elastic incompatibility can be defined by

$$R_{ij} = -\mathrm{curl}(\mathbf{L}_p) \cdot (\mathbf{m}'_i \otimes \mathbf{m}'_j)\,, \tag{4}$$

where the curl operator is defined relative to the current configuration, the distortional microstructural vectors $\mathbf{m}'_i$ are defined by

$$\mathbf{m}'_i = J_e^{-1/3}\mathbf{m}_i \quad \text{with} \quad J_e = \mathbf{m}_1 \times \mathbf{m}_2 \cdot \mathbf{m}_3 > 0\,,$$

and $\cdot$ and $\times$ denote, respectively, the inner and vector products. If restricted to small strains and rotations, R_{ij} is the opposite of the rate of the Nye-Kröner dislocation density tensor [7, 8]. Therefore, its off-diagonal and diagonal components, respectively, correspond to edge and screw dislocation density rates.

It is emphasized that the rates R_{ij} are Eulerian as they depend only on the current configuration and rate of deformation. Moreover, they are not pure kinematic measures, being also dependent on the constitutive prescription for $\mathbf{L}_p$. Also, the definition (4) of R_{ij} ensures its invariance under superposed rigid body motion, such as each of its components can be used to introduce size-dependent hardening in the modeling. This approach is an alternative to that followed in [9], which is an Eulerian extension of the higher-order strain gradient plasticity theory of Gurtin [10].

6. The torsion problem

Consider an isotropic cylinder of circular cross-section experiencing cyclic torsional loading governed by the applied twist $\kappa(t)$. The cylindrical polar base vectors $(\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_z)$ are defined relative to the fixed orthonormal triad of vectors $\mathbf{e}_i$ by the expressions

$$\mathbf{e}_r = \cos(\hat{\theta})\mathbf{e}_1 + \sin(\hat{\theta})\mathbf{e}_2\,, \quad \mathbf{e}_\theta = -\sin(\hat{\theta})\mathbf{e}_1 + \cos(\hat{\theta})\mathbf{e}_2\,,$$
$$\mathbf{e}_z = \mathbf{e}_3\,, \qquad\qquad \hat{\theta} = \theta + \kappa z\,.$$

Also, the current location of a material point $\mathbf{x}$ is given by

$$\mathbf{x} = r\mathbf{e}_r + z\mathbf{e}_z\,,$$

such as the total velocity gradient reads

$$\mathbf{L} = z\dot{\kappa}(\mathbf{e}_\theta \otimes \mathbf{e}_r - \mathbf{e}_r \otimes \mathbf{e}_\theta) + r\dot{\kappa}\mathbf{e}_\theta \otimes \mathbf{e}_z\,.$$

This kinematic assumption may for instance be adequate to model severe plastic deformation in higher-pressure torsion [11]. Equilibrium can be satisfied by a radial body force equal to $-\partial T_{rr}/\partial r - (T_{rr} - T_{\theta\theta})/r$. Under these circumstances,

the non-vanishing components of R_{ij} are

$$
\begin{aligned}
R_{11} &= \frac{L_{p\theta z}}{r} m_{1r}^2 \,, \\
R_{22} &= \frac{\partial L_{p\theta z}}{\partial r} m_{2\theta}^2 - \big(\frac{\partial L_{p\theta\theta}}{\partial r} + \frac{L_{p\theta\theta} - L_{prr}}{r}\big) m_{2\theta} m_{2z} \\
&\quad + \frac{\partial L_{pzz}}{\partial r} m_{2\theta} m_{2z} - \big(\frac{\partial L_{pz\theta}}{\partial r} + \frac{L_{pz\theta}}{r}\big) m_{2z}^2 \,, \\
R_{33} &= \frac{\partial L_{p\theta z}}{\partial r} m_{3\theta}^2 - \big(\frac{\partial L_{p\theta\theta}}{\partial r} + \frac{L_{p\theta\theta} - L_{prr}}{r}\big) m_{3\theta} m_{3z} \\
&\quad + \frac{\partial L_{pzz}}{\partial r} m_{3\theta} m_{3z} - \big(\frac{\partial L_{pz\theta}}{\partial r} + \frac{L_{pz\theta}}{r}\big) m_{3z}^2 \,, \\
R_{23} &= \frac{\partial L_{p\theta z}}{\partial r} m_{2\theta} m_{3\theta} - \big(\frac{\partial L_{p\theta\theta}}{\partial r} + \frac{L_{p\theta\theta} - L_{prr}}{r}\big) m_{2\theta} m_{3z} \\
&\quad + \frac{\partial L_{pzz}}{\partial r} m_{2z} m_{3\theta} - \big(\frac{\partial L_{pz\theta}}{\partial r} + \frac{L_{pz\theta}}{r}\big) m_{2z} m_{3z} \,, \\
R_{32} &= \frac{\partial L_{p\theta z}}{\partial r} m_{2\theta} m_{3\theta} - \big(\frac{\partial L_{p\theta\theta}}{\partial r} + \frac{L_{p\theta\theta} - L_{prr}}{r}\big) m_{2z} m_{3\theta} \\
&\quad + \frac{\partial L_{pzz}}{\partial r} m_{2\theta} m_{3z} - \big(\frac{\partial L_{pz\theta}}{\partial r} + \frac{L_{pz\theta}}{r}\big) m_{2z} m_{3z} \,,
\end{aligned}
\tag{5}
$$

where m_{1r}, $m_{2\theta}$, m_{2z}, $m_{3\theta}$, and m_{3z} are the five non-vanishing components of the microstructural vectors $\mathbf{m}_i$. In the framework of small strains and rotations, $L_{prr} = L_{p\theta\theta} = L_{pzz} = 0$, $m_{2z} = m_{3\theta} = 0$, and $R_{23} = R_{32} = 0$ [12].

Given that $\mathbf{L}_p$ depends on $\mathbf{m}_i$, in a complex nonlinear way also involving the plastic spin rate [13], it turns out that the solution of this torsion problem is obtained by integrating five nonlinear differential equations for m_{1r}, $m_{2\theta}$, m_{2z}, $m_{3\theta}$, and m_{3z}, which are functions of r and $\kappa(t)$, to be coupled, in a system, with the evolution equations for the adopted hardening laws. This system of equations automatically satisfies the condition of isochoric total deformation, $J_e = 1$.

This contribution aims at studying the effect on the torsional response of a hardening law dependent on the rates of incompatibilities (5). A similar study has already been carried out in [14] by neglecting finite deformations and the plastic spin. Here, a conventional hardening law is enhanced by adding a dependence on R_{ij} using the smooth transition model proposed in [15, 16]. Among several aspects, this investigation highlights the crucial role of the influence of the material parameter controlling the plastic spin rate, thus confirming and enriching the findings of [12] in the context of higher-order small-strain gradient plasticity.

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Elasto-viscoplastic FFT-based method for mesoscale field dislocation mechanics with defect energy

Stéphane Berbenni
(joint work with Vincent Taupin, Ricardo A. Lebensohn)

A crystal plasticity elasto-viscoplastic FFT (Fast Fourier Transform) formulation with a mesoscale continuum field dislocation mechanics model is presented. The present approach accounts for plastic flow, hardening and densities of geometrically necessary dislocations (GND), in addition to statistically stored dislocations (SSD). Here, the model incorporates a defect energy density that depends on GND densities and an associated internal length scale. This allows to thermodynamically derive internal length scale dependent intra-crystalline backstress (energetic-type hardening) and Peach-Koehler force acting on GND densities. The model considers GND density evolution through a filtered numerical spectral approach [1], which is coupled with stress equilibrium through the elasto-viscoplastic FFT algorithm using Augmented Lagrangian (AL) algorithm. The discrete Fourier transform method together with finite difference schemes [2, 3], is applied to solve both the GND lattice incompatibility problem and the Lippmann-Schwinger equation.

Numerical results are first reported for two-phase channel-type composites with plastic single crystal channels and elastic precipitates for shear loadings. Channel size effects are simulated and analyzed on the overall and local hardening behaviors during monotonous loadings. In addition, the evolutions of GND densities and the role of their associated backstress on size effects are examined during reversible loading. In this case, it is shown that GND density piling-up/unpiling-up can be simulated with this model. Furthermore, it is found that dislocation pile-up is more extended with energetic-type hardening. In a second part, the role of the defect energy internal length scale on polycrystal's hardening is discussed, and compared to those obtained using FFT-based mesoscale field dislocation mechanics without defect energy [4, 5, 6].

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Multiscale modeling of cancellous bone considering mechanical, electric and magnetic effects

Mischa Blaszczyk
(joint work with Verena Stieve, Klaus Hackl)

Osteoporosis is the leading bone disease worldwide. During the course of this disease, cortical bone is replaced by bone marrow, making the bone weaker and more susceptible to fracture. Modeling of bone can improve the understanding of the disease and lead to new early detection tools such as the use of sonography [1]. In addition to the well studied mechanical properties of bone, recent research has laid the groundwork to also include electric and magnetic effects [2, 3].

In this talk, we present a fully coupled multiscale approach considering mechanical, electric and magnetic effects [4, 5, 6]. We use a two-phase material model at the microscale, consisting of the phases cortical bone (modeled as a piezoelectric and insulating solid) and bone marrow (modeled as a viscoelastic and conducting

solid). The material model takes into account the full coupling of Maxwell's equations. To solve the resulting partial differential equations, we resort to the finite element square method (FE^2).

We show simulation results for both scales. To apply the FE^2, we constructed different representative volume elements (RVEs), which differ in volume fractions of cortical bone, simulating different stages of osteoporosis. The numerical results show a drastic reduction of the magnetic field strength resulting from a small mechanical impact for later stages of the disease, which is in conformity with experimental research. Furthermore, we show that the inverse problem - recovering the composition of the bone from the magnetic field strength - can be solved by using Artificial Neural Networks (ANNs).

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Modeling and experimental determination of energetic and dissipative stresses in plastic deformation

Thomas Böhlke
(joint work with Nikola Lalović, Alexander Dyck, Alexander Kauffmann, Martin Heilmaier)

Many phenomenological thermomechanical material models in plasticity of metallic materials use a constant Taylor-Quinney factor to describe the heat release due to deformation induced dissipation. However, this approach often has several shortcomings [1]. In this talk, we will present the derivation of a thermodynamically consistent formulation for the heat source due to plastic deformation in a small deformation setting (cf., [2,3]). The free energy function is determined by specific assumptions on the material behavior motivated by dislocation theory. In order to verify the model experimentally, a combination of mechanical and thermal measurements is performed using infrared thermography during uniaxial tensile tests on Al and Cu specimens. The materials are tested in two conditions, recrystallized and work hardened with low and high initial defect density, respectively. In order to determine and to separate dissipative and energetic parts of the flow stress, an image processing algorithm is applied to reconstruct the heat source due to plastic deformation [4]. Based on the identified heat sources, the dissipative

and energetic parts of the flow stress as well as the Taylor-Quinney coefficient are determined. The results suggest that the proposed thermodynamical model and the experimental method applied can provide valuable insights into a consistent thermomechanical framework of plasticity, since it captures both contributions to flow stress, the energy storage in defects as well as the dissipation due to lattice defect generation and transport.

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Open questions in multiscale mechanics of materials

Laurent Capolungo

Multiscale modeling as an enabler to material design is a vast and rich scientific endeavor. This presentation was dedicated to (1) defining the technological needs for fundamental scientific developments, (2) describing the overall multiscale modeling paradigm and (3) emphasizing some of the epistemic gaps that require more attention to enable phenomenology free constitutive modeling. Grounding our reasoning on the connection between harmonic transition state theory and continuum mechanics, the question of the homogenization of the energy landscape, in the presence of long ranged perturbations induced by line defects, of the homogenization of thermodynamic factors in the presence of disparate defects and of that of attempt frequencies to overcome volumetric defects was present. It was shown in the case of nanolaminate pillars subjected that higher order continuum mechanics approaches can be tailored to emulate the long range field due to complex dislocation pile-up arrangements. Yet, in light of the aforementioned questions related to homogenization, the critical need to establish rigorous mathematical linkages between microstructure configurations, energy barriers, internal stress and entropic contributions to kinetic factors is clear. The author further suggested that a likely

key to unlock such problem could rely on the use of multi-level graphs as fingerprints for microstructure.

Modular Structures and Mechanisms: Place where free-material and topology optimizations meet on a journey from periodic multi-scale to single-scale designs

Martin Doškář

(joint work with Marek Tyburec, Martin Kružík, Jan Zeman)

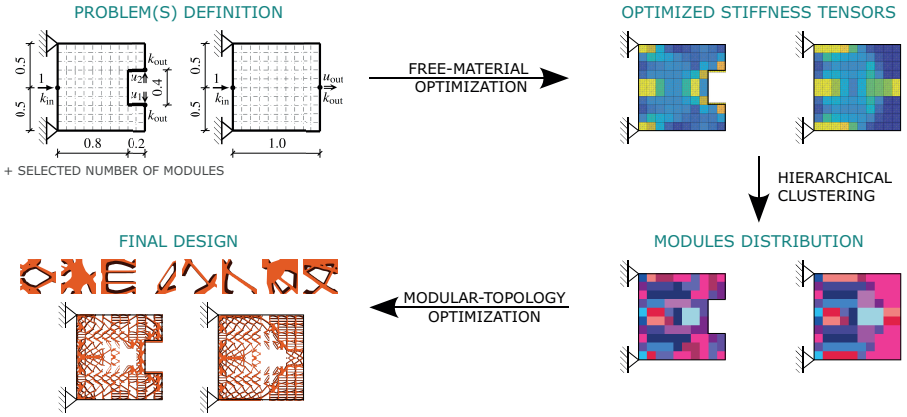

Figure 1. Overview of the proposed optimization scheme illustrating the module design shared for two compliant mechanisms: a force inverter and a gripper.

Modular design has gained substantial traction due to its capacity to efficiently address manufacturing, reusability, and sustainability while maintaining performance comparable to their traditional non-modular counterparts. However, designing such products poses a challenging task, which involves solving two optimisation problems. First, modules must be optimally distributed within a product-scale domain. Second, the topology of individual modules should be optimized to ensure their seamless cooperation when assembled. Addressing both problems simultaneously is considerably more complex, as it involves an intricate interplay of discrete and continuous nature.

In our previous work on the minimum-compliance design of modular truss structures, we adopted a concurrent approach, combining a metaheuristic method for updating the modular assembly plan with second-order cone programming to generate optimal truss-like module topologies. However, this approach relied on a convex formulation, limiting its applicability. We now introduce a computationally more efficient bi-level sequential strategy that bypasses the need for assembly-level

meta-heuristics and is applicable to continuum structures and mechanisms. In addition, we incorporate manufacturing concerns by means of a three-field approach and continuity constraints.

Our new approach starts by employing free material optimization on a coarse regular discretization. This step yields optimal, element-wise constant stiffness tensors. Subsequently, we partition these stiffness tensors into a predetermined number of clusters, paying careful attention to any underlying symmetries. Interpreting the clustering results within the framework of the Wang tiling formalism produces the assembly plan, where individual codes on module edges reflect similarity among the optimized stiffness tensors. Finally, the topology of individual modules is determined through standard, single-scale topology optimization, utilizing the Solid Isotropic Material with Penalization interpolation scheme and reducing the design space through a mapping that reflects the modular assembly plan.

We demonstrate the efficacy of our strategy through four two-dimensional problems, including the modular minimum-compliance Messerschmitt–Bölkow–Blohm beam, two modular compliant mechanisms (an inverter and a gripper), and a combined modular design of both mechanisms. This showcases the reusability of optimized modules and highlights the seamless transition from a Periodic Unit Cell-based design of material microstructures to traditional single-scale topology optimization. The number of clusters in the partitioning step provides control, opening the door to the rational design of modular metamaterials and mechanisms at the material level. In practical implementation, the combined module designs for the inverter and gripper mechanisms were realised through 3D printing. These physical prototypes underwent rigorous mechanical testing utilizing an in-house testing machine and digital image correlation. These practical trials underscore the potential of the method, revealing a remarkable alignment between the predicted and observed performance.

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Mesoscale Plasticity of Inhomogeneous Alloys: Linking Chemistry and Dislocation Dynamics

Anter El-Azab

This talk is concerned with the impact of composition inhomogeneity on the plastic deformation response of structural alloys. Chemical (composition) inhomogeneity is encountered in many alloy systems of interest and it is caused by thermodynamic and kinetic factors. Examples include but are not limited to spinodal alloys, additive-manufactured alloys, high-entropy alloys, and irradiated structural alloys. The chemical inhomogeneity results in two main effects, coherency stresses at the lattice level and strong spatial dependence of the dislocation properties, especially mobility. In this talk, I will summarize the important physical effects associated with chemical inhomogeneity, present a mathematical, data-driven approach for characterizing the spatial inhomogeneity in irradiated alloys along with a framework of accounting for the chemical inhomogeneity in dislocation dynamics. We will present a reformulation of Cahn's theory of strength of spinodal decomposition and some recent results from full, 3D dislocation dynamics simulations of the mesoscale plasticity of an inhomogeneous ternary alloy. This work is funded by the UD Department f Energy, Office of Fusion Energy Sciences under contract number DE-SC0024585 at Purdue University.

Thermomechanical coupling of phase transformations and constitutive laws to describe microstructural evolution

Wolfgang Flachberger
(joint work with Thomas Antretter)

This work presents a Lagrangian formulation for the coupling of diffusional phase transformations and continuum mechanics using a mixed finite element scheme. The emphasis on the Lagrange formalism is due to its convenience in automated derivation of variational forms to be used with the FEM or other numerical (Galerkin- or Ritz-type) methods. This work follows the principle minimum entropy production [1] while ensuring conservation of energy and conservation of mass of the diffusing species. The diffusion model used is thermodynamically consistent and can also be used to employ the vacancy mechanism of diffusion of substitutional alloys such as derived in [2]. Despite the fact that entropy is loosely associated with "disorder" in a system we want to emphasize that an increase of entropy in a nonequilibrium system can also be accompanied by creation of patterns [3] as depicted in Figure 1.

The approach is used to investigate the impact of mechanical stresses on segregation (Figure 2) and other damage mechanisms observed at the small scales of microelectronic solders. The model is characterized by sharp transitions between phases (sharp interface model) which is in strong contrast to other state-of-the-art methods for describing diffusional phase transformations like the Phase Field Method (PFM). It will however be shown that the presented model can actually

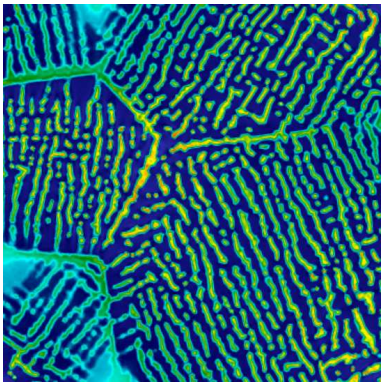

FIGURE 1. Patterns in the concentration emerging from mechanical anisotropy.

be related to the limiting case of having no interface energy and no regularization in the Cahn Hilliard Model. A binary system is studied whose behaviour is described by four differential equations which are solved by an implicit, fully coupled scheme. The diffusion model is used to predict both the phase growth as well as damage relevant phenomena such as trapping of components at grain boundaries and other imperfections. Furthermore, the diffusion is coupled with a constitutive model for the mechanical material behaviour. The coupling is done in both ways considering the influence of diffusion on mechanics via phase-dependent material parameters as well as by considering the influence of stresses and strains on the diffusion. This enables a detailed investigation of the many phenomena that are observed at the small scales of microelectronic solders.

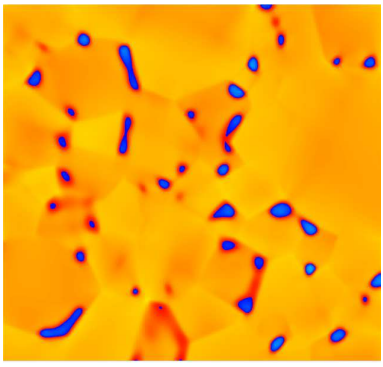

FIGURE 2. Segregation triggered by large pressure gradients at grainboundaries.

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Multiscale analysis of composite structures based on higher-order asymptotic homogenization with boundary layer correction

Samuel Forest

(joint work with Mouad Fergoug, Nicolas Feld, Basile Marchand, Augustin Parret-Fréaud)

Asymptotic homogenization method is often used in multiscale analysis of periodic structures instead of conducting a full field heterogeneous analysis, in order to achieve computational feasibility and efficiency. When completed with a relocalization process, this method may provide relevant estimates to microscale fields within the material. Nevertheless, the construction of a solution near the boundaries remains beyond the capabilities of classical relocalization schemes due to the loss of periodicity in the vicinity of the boundaries. This paper proposes a post-processing scheme in order to conduct the relocalization step within a finite element framework for periodic linear elastic composite materials. It also assesses the boundary layer effect and a new general method, effective for various boundary conditions (Dirichlet, Neumann or mixed), is proposed based on the idea of computing corrective terms as solution of auxiliary problems on the unit-cell. These terms are finally added to the usual fields obtained from the relocalization process to obtain the corrected solution near the boundaries. The efficiency, accuracy and limitation of the proposed approach are studied on various numerical examples [1]. Homogenized models are widely used in multiscale analysis for their computational efficiency, but they often fail to provide sufficient accuracy in regions exhibiting high variations in the so- lution fields. One way to address this limitation is to adaptively couple the homogeneous model with a full field, heterogeneous one in designated zones of interest. Within the framework of finite-element based higher-order asymptotic homogenization [2], this work introduces a modeling error estimator in order to detect regions where refining the material model is necessary. We also analyze the competition between discretization and modeling errors. We finally propose a multiscale enhancement of the classical displacement-based submodeling technique in order to adequately couple the homogeneous and heterogeneous domains. The promise of the proposed methods and the overall associated strategy is illustrated on various numerical examples of elastic fiber-matrix composites [3].

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Phase field based modeling of damage in quasi-brittle polycrystalline microstructures

Jakob Huber

(joint work with Christian Krempazsky and Ewald Werner)

Damage is a process that occurs on several scales. From the separation of atomic bonds over the formation and localization of defects like microvoids and microcracks several mechanisms act conjointly in the damage process. Micromechanical modeling is a way to describe and understand the effects of heterogeneous microstructures on the effective material behavior on the component scale. Effective elastic and plastic material behavior has been successfully predicted by means of micromechanical homogenization [1, 2]. For strongly heterogeneous microstructures the damage process is heavily influence by stress and strain concentrations on the microscale [3].

The modeling of cracks as discontinuities can be divided into discrete and smeared/diffused methods. Major challenges in discrete methods are the necessary remeshing to reduce mesh dependency of crack paths and the need of enriched shape functions near crack tips (see e.g. [4]).

The diffused phase field approach for damage in comparison is a straightforward and universal method that is based on a multi-field solution in which the deformation and damage field variables are coupled in a bidirectional manner [5]. The phase field approach for damage is especially promising for modeling damage on the microscale. Complex crack patterns due to heterogeneous micro stress and strain fields as well as multiple crack initiation sites and coalescence of cracks can be considered without any restrictions. A phase field approach can also depict partial damage in a microstructure which potentially leads to a stress redistribution and should therefore be incorporated in the microdamage simulation. Furthermore, strict discontinuities as modeled in discrete approaches are not necessarily the optimal description of cracks unless one is looking at an ideal crack based on the debonding of atomic layers. On scales larger than the atomic scale one has to deal with a composition of several cracks and pores forming on a smaller scale in the process zone of the crack that is to be modeled. The phase field approach for damage as a diffused method is able to account for such a damage process zone in the vicinity of a crack in a homogenized manner.

In our contribution the promising phase field approach for damage is transferred to polycrystalline microstructures. We compare two different formulations of the surface density which is needed to compute the cumulative surface of microcracks and the associated rate of dissipation. The standard formulation of the surface density is written in terms of the order variable φ, which continuously decreases from 1 to 0 during the damage process

$$a_{\text{surface}} = \frac{1}{2} l_{\text{c}} \left|\nabla\varphi\right|^2 + \frac{1}{2l_{\text{c}}} \left(1-\varphi\right)^2 . \tag{1}$$

Here, the scale parameter l_{c} controls the size of the zone of partial damage accompanying the core of a crack. A modified version proposed in the literature [6] can be formulated by changing the local part to a linear function of the damage state

$$a_{\text{surface}} = \frac{1}{2} l_{\text{c}} \left|\nabla\varphi\right|^2 + \frac{1}{l_{\text{c}}} \left(1-\varphi\right) . \tag{2}$$

The cumulative crack surface is calculated by volume integration of (1) or (2) and multiplication with a material dependent surface energy density.

Figure 1 shows the pattern of microdamage for both formulations at three different stages of the deformation. Stage A shows partial microdamage without microcracks. In stage B a first microcrack appears. It grows further in stage C where it is noticeably influenced in its path by the heterogeneous stress and strain field in the microstructure. The main difference in the patterns of microdamage for the two formulations of the surface energy density is the zone of partial damage. For the standard formulation, partial damage is observed in the entire microstructure, while partial damage is restricted to the vicinity of a microcrack for the modified version. This affects also the path of the microcrack. The compact zone of microdamage allows the crack to develop two approximately symmetric branches in the case of a linear local part of the surface density (2). In the case of a quadratic local part of the surface density (1), there is a favorable direction for the crack growth due to perturbations by the heterogeneous field of partial damage. Therefore, the microcrack tends to be only deflected without branching. For the entire volume element effective energy quantities can be calculated. The predictions of macroscopic failure based on the effective strain energy density and the effective energy release rate are compared. According to the numerical results, the effective strain energy density shows noticeably less uncertainty than the effective energy release rate regarding variations in the morphology of the microstructure. Additionally, the scale parameter leads to a size effect manifesting in the energy release rate which makes the calibration cumbersome. Therefore, the effective energy density is suggested as a more reliable microstructure based criterion for macroscopic damage.

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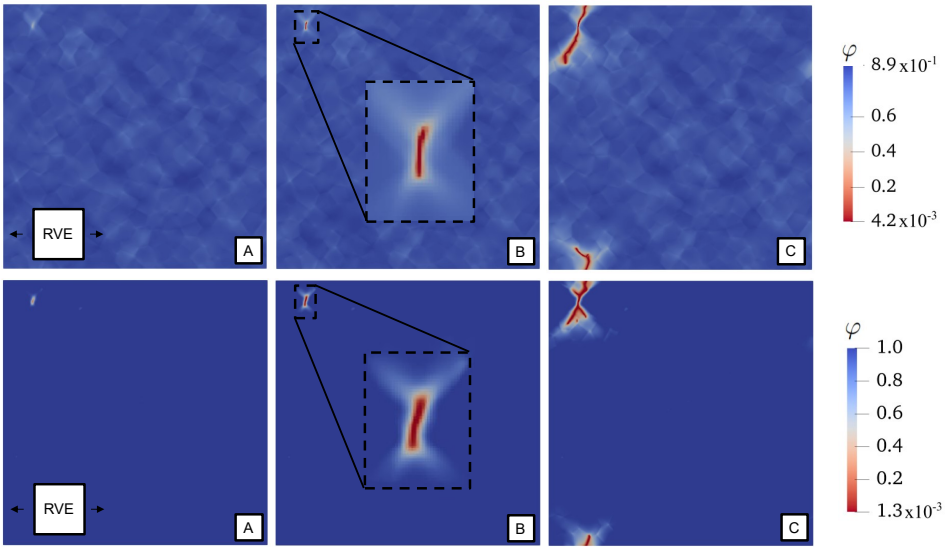

FIGURE 1. Patterns of microdamage with growth of microcracks for standard (top) and modified (bottom) formulation of the surface density. For the standard version (1) partial damage is observed over the whole microstructure. For the modified version (2) partial damage is restricted to the vicinity of a microcrack.

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Strain gradient plasticity modeling: current progress and open questions

Mohamed Jebahi

(joint work with Yaovi Armand Amouzou-Adoun, Samuel Forest, Marc Fivel)

Strain gradient plasticity emerges as a highly promising framework for elucidating the size-dependent behavior of materials at small scales, ranging from a few hundreds of nanometers to a few tens of micrometers [1, 2]. The leading edge of this research has seen the development of an advanced strain gradient plasticity model specifically designed for single crystals. This model employs a multi-kinematic decomposition strategy to decompose the plastic slip gradients into recoverable and unrecoverable components [3]. Within this framework, the defect energy density is articulated through a combination of quadratic and less-than-quadratic functions, providing a robust basis for capturing complex material behaviors. To evaluate the effectiveness of this model, it was applied to simulate the shear response of a slender two-dimensional plate having an infinite length in x-direction and a small width w in y-direction. For simplicity, only two slip systems are considered in this plate, with the top and bottom edges assumed to be fully passivated (zero plastic slips at these edges). Comparative analysis with discrete dislocation dynamics (DDD) simulations [4], serving as the benchmark for this study, reveals the model capabilities to qualitatively reproduce key size-dependent characteristics observed by DDD. By manipulating specific model parameters, the scaling exponent factor r in the scaling relationship (w^{-r}) can easily be adjusted within the interval [1.0, 2.0], demonstrating the model flexibility in representing size effects over a range from linear to quadratic scaling. However, a notable limitation of the model is that it cannot mimic scaling relationships with exponents less than 1, which are generally predicted by DDD and observed in several small-scale experimental investigations. This limitation underscores a significant challenge and opens a critical avenue for further research within the domain of strain gradient plasticity. It raises pivotal questions about the capabilities of existing strain gradient plasticity models to fully encapsulate the nuances of size effects. As such, this area remains ripe for innovation, inviting advancements that can bridge persisting gaps and provide a more comprehensive understanding of material behaviors at small scales.

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Exploration of structure-property linkages and inverse design of materials by active learning

Markus Kästner

(joint work with Alexander Raßloff, Paul Seibert, Karl A. Kalina)

Being able to design, e.g., the microstructure of a material to achieve a desired behavior is a key enabler for innovation. To achieve this goal, knowledge about the influence of the local material structure on the mechanical properties of the material, e.g. measured in terms of stiffness, strength or ductility, must be acquired. Ideally, experiments and simulation results are combined to build structure-property linkages. The key challenge is then to invert this knowledge to find a material structure for a desired set of material properties. This process is known as inverse design. While surely inverse design is challenging, even the forward prediction of SP linkages using multiscale simulations of complex microstructures is still a demanding task. The difficulties lie in (i) describing the features of the local material structure, (ii) reconstructing plausible 3D statistically representative volume elements (SVEs), e. g., from 2D slices like microscopy images, (iii) modeling the complex and non-linear effective constitutive response and (iv) using it in an efficient multiscale scheme.

In this contribution, we present recently developed methods that aim at addressing these issues and it is shown how to integrate them in an efficient workflow. Descriptors are employed to characterize complex microstructures. Examples of such descriptors are volume fraction, generalized spatial n-point correlations or Gram matrices of pre-trained convolutional neural networks. Corresponding SVEs are generated using differentiable microstructure characterization and reconstruction (DMCR). An advantage of DMCR over similarly efficient reconstruction algorithms is that it allows to prescribe generic high-dimensional microstructure descriptors as long as they are differentiable. The reconstructed structures are then used for numerical simulation and effective properties are obtained from homogenization techniques. Together with the descriptors of the local material structure, SP linkages are set up.

As engineering data, including the SP linkages, are generally costly to generate, inverse design has to cope with scarce data. We therefore employ a Bayesian optimization approach and it is shown that significantly less data are needed in comparison to classical sampling procedures and alternative inverse design methods which is due to the iterative data augmentation. The approach is demonstrated for spinodoid metamaterials. In future work, the active learning augmentation loop could be applied to a broader range of materials.

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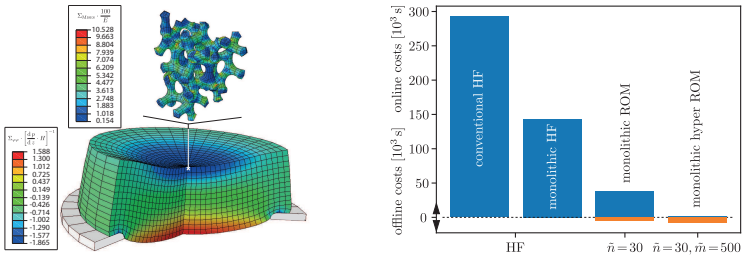
Computational Homogenization in Nonlinear Material Modeling: Accuracy – Efficiency – Flexibility

Björn Kiefer

(joint work with Martin Abendroth, Geralf Hütter, Nils Lange, Alexander Malik, Vincent von Oertzen)

This contribution reflects on recent work in our group regarding computational homogenization approaches. A more general discussion, and corresponding literature references, of similar developments in the scientific community can be found in the publications cited below. In a two-scale setting, the main goal of numerical homogenization in solid mechanics is to predict effective behavior of a material or structure on the macroscopic scale, while directly taking into account microstructural information. This can also be accomplished by semi-analytical micromechanics techniques, but computational homogenization approaches offer a much broader range of applicability, e.g., regarding complexity of the microstructure, or in accounting for physical and geometrical nonlinearities as well as multiphysical phenomena. When different methods are compared in the literature, the discussion typically centers on computational efficiency. More precisely, this usually means a comparison of *online* simulation costs to achieve a certain level of accuracy, while *offline* efforts, to train a neural network prior to the actual analysis of the problem, for instance, are seldom quantified. We believe that a fair comparison should also include several other criteria, such as flexibility towards adaptation, effort of implementation, information sought, or even required hardware. The method of choice will therefore generally depend on the context in which it is to be employed, and the fastest method might not necessarily be the most suitable.

The FE^2 method has the advantage of enabling high-fidelity (HF) computational analyses of inhomogeneous physical fields on both scales. This inherently comes at the price of very high computational effort. However, by means of a monolithic solution approach as well as reduced-order modeling (ROM) and hyper-integration techniques, numerical speed-up factors of up to three orders of magnitude were recently achieved, see [1, 2]. This has significantly increased the competitiveness of the FE^2 method and enabled its application to much larger nonlinear problems. Figure 1 shows an example of a complex two-scale problem and the comparison of on- and offline computational costs for different variants of the method. As an alternative approach to modeling such foam-like structures, a hybrid methodology was recently presented in [3]. It builds on the format of a classical non-associative plasticity formulation, but incorporates feed-forward



(a) Two-scale simulation of a flow-through filter with a Weaire-Phelan-type microstructure.

(b) Computational effort (online and offline costs) relative to high fidelity FE analysis on both scales.

FIGURE 1. Application example of the monolithic FE^2 method employing reduced-order modeling and hyper integration, see [2]. A finite strain, hypo-elastic creep problem with a total of ≈ 52 million degrees of freedom is considered.

neural networks (NN) to allow accurate descriptions of complex yield surfaces and plastic flow potentials. Such a technique is much more efficient in the FEA of large foam structures and simultaneously very general with respect to the nature of the macroscopic behavior it can capture. Its downside is the immense effort necessary to generate sufficiently rich virtual data sets for the training of the NN, which also have to be regenerated each time a new microstructural topology is considered. The monolithic hyper ROM FE^2 method also requires off-line effort in certain training steps, but its share of the total computational time is much lower, e.g., about 3% in the example of Figure 1. In consequence, the hybrid method will generally be more suitable if many macroscale computations with the identical microstructure are to be carried out. The FE^2 method, on the other hand, has advantages if FEA with many different, or even evolving, microstructures is of main interest, and perhaps detailed knowledge of microscopic fields is required. Our computationally most efficient tool for the macroscopic analysis of inelastic foam structures was recently presented in [4]. It relies entirely on analytical expressions for the central functions of associative/nonassociative plasticity, whose parameters are identified by means of nonlinear optimization. This calibration procedure is similar to the NN training in the hybrid approach, albeit with much lower requirements regarding the size and diversity of the data base generated by microscale RVE simulations. The computational efficiency in this case comes at the cost of flexibility regarding the range of possible macroscale behavior and gives no insight into stress- or strain concentrations within the microstructure.

Finally, first ideas for a much more general theoretical treatment of homogenization in space and time, based on the notion of weighted averaging operators, were proposed in [5]. Even though phase-field modeling was considered as the particular area of application therein, these fundamental concepts very generally

apply to scale transitions in solid mechanics, including those lacking clear separation of the considered scales, which is a key requirement for the computational homogenization techniques discussed above.

A much more detailed quantitative comparison of the discussed approaches and their algorithmic implementations based on representative numerical examples will be given in a forthcoming journal paper currently in preparation.

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Rate-independent systems with non-convexities: Examples, solution concepts, (time-) discretization schemes

Dorothee Knees

Many mechanical models can be interpreted as rate-independent systems. Classical examples are models from plasticity, phase-field fracture or damage models that are based on Griffith's criterion and many others. In a variational setting one can characterize them by prescribing an energy (functional) and a dissipation (pseudo-) potential. If the energy is not convex or if the dissipation potential not only depends on the velocity/rate at which states change but also on the state, then solutions to such systems might be discontinuous in time even if the applied loads depend smoothly on the time variable. In the last 25 years, several solution concepts were developed that allow for discontinuous solutions and introduce jump conditions for the discontinuities, see [13] for an overview.

A simple example showing that a continuous solution might not exist is a friction problem for a gliding mass point pulled via an elastic spring, [10]. It is assumed that the friction coefficient depends on the position of the mass. Neglecting inertia terms the problem can be formulated as follows: Let $z : [0,T] \to \mathbb{R}$ denote the position of the mass at time t and let $\ell(t) - z(t)$ be the elongation of the spring at time t. The elastic energy stored in the spring is given by $\mathcal{E}(\ell, z) = \frac{a}{2}(\ell - z)^2$ with $a > 0$ denoting Hooke's constant. For modeling the friction we assume that the normal force between the mass and the surface is constant but the friction coefficient $\mu : \mathbb{R} \to [0, \infty)$ depends on the position of the mass. In terms of the dissipation potential $\mathcal{R}(z, v) = \mu(z)|v|$ and the energy functional $\mathcal{E}$ the evolution

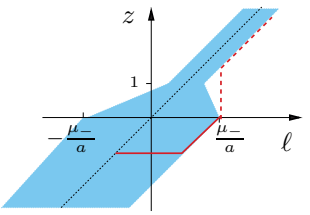

FIGURE 1. Blue: Set $\mathcal{S}$; Red: Solution trajectory.

problem reads as follows: Given an initial position z_0 and a function $\ell : [0,T] \to \mathbb{R}$ find $z : [0,T] \to \mathbb{R}$ satisfying $z(0) = z_0$ and

$$0 \in \partial_v \mathcal{R}(z(t), \dot{z}(t)) + \mathrm{D}_z \mathcal{E}(\ell(t), z(t))\,. \tag{1}$$

Observe that this evolution inclusion in particular implies that along solutions we necessarily have $-\mathrm{D}_z\mathcal{E}(\ell(t), z(t)) \in [-\mu(z(t)), \mu(z(t))]$. In particular, the trajectories $t \mapsto (\ell(t), z(t))$ lie in the set $\mathcal{S} := \{(\ell, z) \in \mathbb{R}^2\,;\, z - \ell \in [-\frac{\mu(z)}{a}, \frac{\mu(z)}{a}]\}$. Let now $\mu_- > \mu_+ > 0$ and $\mu(z) = \mu_-$ for $z \le 0$, $\mu(z) = \mu_+$ for $z > 1$ and linearly interpolated in between. Figure 1 shows the set $\mathcal{S}$ for the case $\mu_- - \mu_+ > a$. Assume now that $z_0 < 0$ and $\ell(t) = t + z_0$. There exists a (unique) Lipschitz continuous solution to (1) until t_* with $\ell(t_*) = \frac{\mu_-}{a}$ but it is not possible to extend this solution in a continuous way beyond this point.

This phenomenon is intrinsic to rate-independent systems when the dissipation potential depends on the state (as in our example) or when the energy functional is not convex. We refer to [5, 9] for an example with a non-convex energy involving a crack propagation problem based on the Griffith fracture criterion.

Several solution concepts were developed allowing for discontinuous solutions and introducing different jump criteria. The most popular ones are the concept of Global Energetic Solutions [14] and the concept of Balanced Viscosity Solutions, [2, 11]. The first one is derived from a time-incremental global minimization scheme while the latter solution class is based on a vanishing viscosity analysis.

In the following we focus on balanced viscosity solutions for phase field fracture and damage models and discuss different time-discretization strategies to approximate such solutions. To simplify the presentation we stay in the two-dimensional setting and consider the model by Ambrosio and Tortorelli.

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with a Lipschitz boundary characterizing the physical body that is assumed to be linearly elastic and that may undergo damage if the applied loadings are large enough. Let $u : [0,T] \times \Omega \to \mathbb{R}^2$ denote the displacement field and $z : [0,T] \times \Omega \to \mathbb{R}$ the scalar damage variable. Here, $z(t,x) = 1$ means no damage at all while $z(t,x) = 0$ indicates maximum damage in the material point x at time t. For simplicity we assume homogeneous Dirichlet boundary conditions for the displacement field u, hence the state space for u is chosen as $\mathcal{U} := H^1_0(\Omega; \mathbb{R}^2)$. Given time dependent loads $\ell : [0,T] \to \mathcal{U}^*$ the energy

functional $\mathcal{E} : [0,T] \times \mathcal{U} \times \mathcal{Z} \to \mathbb{R}$ is given by

$$\mathcal{E}(t,u,z) = \int_\Omega \tfrac{g(z)}{2}\mathbb{C}e(u) : e(u) + H(z) + \frac{1}{2}|\nabla z|^2 \,\mathrm{d}x - \langle \ell(t), u\rangle.$$

Here, $e(u) = \mathrm{sym}(\nabla u)$ is the linearised strain tensor, $\mathbb{C}$ the (material dependent) elasticity tensor and g, H are quadratic and convex functions with $g(0) > 0$ and $g'(0) = 0$. For $\mu > 0$ the dissipation potential is given by

$$\mathcal{R}(v) = \int_\Omega \mu|v| + \chi_{(-\infty,0]}(v)\,\mathrm{d}x\,.$$

Here, χ_K is the characteristic function associated with the set K and takes values in $\{0,\infty\}$. Given ℓ and $z_0 \in \mathcal{Z} := H^1(\Omega)$ the task is to find displacements $u : [0,T] \to \mathcal{U}$ and the damage field $z : [0,T] \to \mathcal{Z}$ satisfying $z(0) = z_0$ and

$$0 = \mathrm{D}_u\mathcal{E}(t,u(t),z(t))\,, \tag{2}$$

$$0 \in \partial\mathcal{R}(\dot z(t)) + \mathrm{D}_z\mathcal{E}(t,u(t),z(t))\,. \tag{3}$$

The first equation is the static balance of linear momentum while the second encodes the evolution law for the damage variable. The existence of global energetic solutions to (2)–(3) was proved in [3, 12, 16] (also with more general assumptions on $\mathcal{E}$), while the existence of balanced viscosity solutions was established in the papers [7, 8]. Adapted to our notation we have the following theorem (see [7] for precise assumptions) stating the existence of a parametrized balanced viscosity solution

Theorem 1. *There exist functions $\hat t : [0,S] \to [0,T]$, $\hat z : [0,S] \to \mathcal{Z}$ (both Lipschitz continuous) and functions $\hat u : [0,S] \to \mathcal{U}$ and $\lambda : [0,S] \to [0,\infty)$ with $\hat z(0) = z_0$, $\hat t(0) = 0$, $\hat t(S) = T$ and such that for almost all $s \in [0,S]$ the normalization and complementarity conditions*

$$\hat t'(s) \geq 0,\ \hat t'(s) + \|\hat z'(s)\|_{\mathcal{Z}} \leq 1,\ \lambda(s)\hat t'(s) = 0\,,$$

and the balance and evolution laws hold:

$$0 = \mathrm{D}_u\mathcal{E}(\hat t(s),\hat u(s),\hat z(s))\,, \qquad 0 \in \partial\mathcal{R}(\hat z'(s)) + \lambda(s)\hat z'(s) + \mathrm{D}_z\mathcal{E}(\hat t(s),\hat u(s),\hat z(s))\,.$$

The proof starts from a time-discrete and viscously regularized version of (2)–(3) and shows the convergence of (subsequences of) discrete solutions to balanced viscosity solutions provided that the time step size and the viscosity parameter vanish in a suitable relation. This approach could also serve as a starting point for numerical procedures. However, as observed in [9], in practice it is difficult to choose the time-step size and the viscosity parameter in a way such that discrete solutions show the correct behavior when it comes to jump discontinuities.

A different discretization approach was introduced and analyzed in [2] for a finite dimensional setting, extended in [4] to an infinite dimensional model class and in [1] to phase field damage models. The idea is to consider trajectories of solutions in a parametrized framework as in Theorem 1 and to discretize with respect to the parameter s. This automatically enforces some time-adaptivity close to points, where the solutions have a jump (with respect to the physical time).

The scheme reads as follows: Fix a locality parameter $\rho > 0$ and a norm $\|\cdot\|_{\mathcal{V}}$ with $\mathcal{V} = L^\alpha(\Omega)$ and α large enough (depending on regularity properties). Given (t_k, u_k, z_k) determine the values $(t_{k+1}, u_{k+1}, z_{k+1})$ as follows

(1) Constrained minimization: Determine (u_{k+1}, z_{k+1}) with

$$u_{k+1} = \operatorname{argmin}\{\mathcal{E}(t_k, v, z_{k+1})\,;\, v \in \mathcal{U}\}$$
$$z_{k+1} = \operatorname{argmin}\{\mathcal{E}(t_k, u_{k+1}, \zeta) + \mathcal{R}(\zeta - z_k)\,;\, \zeta \in \mathcal{Z},\, \|\zeta - z_k\|_{\mathcal{V}} \le \rho\}$$

(2) Time update: $t_{k+1} := t_k + \rho - \|z_{k+1} - z_k\|_{\mathcal{V}}$.

(3) Repeat until $t_{k+1} = T$.

In [1, 15], we combined this idea with an alternate minimization scheme to solve the minimization problems. It is shown in [1] that discrete solutions generated with this scheme for $\rho \to 0$ converge to $\mathcal{V}$-parametrized balanced viscosity solutions. The numerical experiments show that this scheme also is reasonable from a numerical point of view.

In practice, for approximating solutions to models of Ambrosio-Tortorelli type, pure alternate minimization schemes (staggered schemes) are frequently used. In [15] we present an example with a separately quadratic and separately convex energy (but not convex as a whole) and of a similar structure as in the Ambrosio-Tortorelli case, where pure alternate minimization in the limit neither generates global energetic solutions nor balanced viscosity solutions. Hence, a physical/mechanical interpretation of solutions generated with a pure alternate minimization scheme is not entirely clear, see also the analysis in [6].

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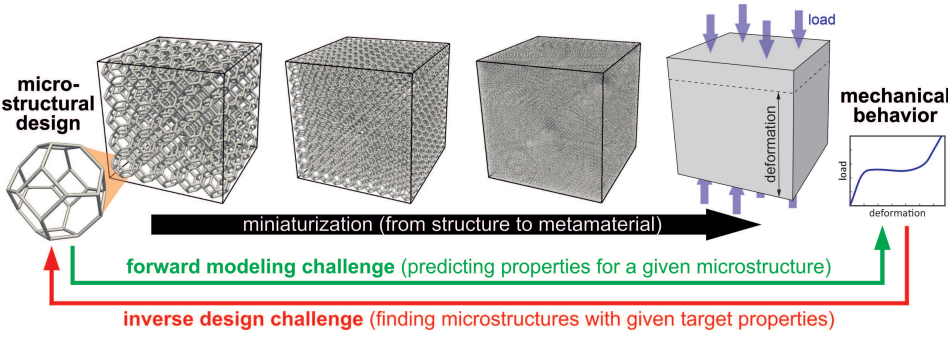
Multiscale Design of Architected Materials

Dennis M. Kochmann
(joint work with Jan-Hendrik Bastek, Siddhant Kumar, Li Zheng)

Advances in additive manufacturing have enabled the fabrication of architected materials (often referred to as *metamaterials*) with the aim of creating novel materials with as-designed, optimized, peculiar, extreme, or generally beneficial properties. Among the mechanical properties of interest are, e.g., high specific stiffness, strength, fracture toughness, but also energy absorption or the guidance of mechanical linear and nonlinear stress waves. Designing such structures with target properties requires theoretical-computational approaches for their inverse design, answering the question: *given target properties, what multiscale design realizes those?* By 'multiscale design' we refer to the optimization process on (at least) two scales: while the macroscopic optimization problem aims for an optimal geometric shape that beneficially distributes the mass of the body for a given loading scenario, the microscopic inverse design problem aims to additionally identify microstructural designs on a smaller scale. Altogether this admits not only optimizing a macroscopic objects (as in classical topology optimization), but it moreover optimizes the local mechanical properties of that structure (by tuning its architecture on a smaller scale).



Classical approaches to enable such multiscale design include, e.g., two-scale topology optimziation of beam lattices [1], in which the architecture on the smaller scale selects unit cells with optimal local homogenized mechanical properties, while the macroscale optimization routine (enabled by finite elements) yields optimal shapes – altogether resulting in a spatially graded beam network with, e.g., maximum stiffness for a given load case. Besides beam-based designs, an analogous two-scale topology optimization approach was used for spinodal-type architectures representated by Gaussian random fields [2, 3]. Since the microscale architecture in both cases (beam lattices and spinodoids) is not isotropic, the obtained optimized structures can beneficially surpasse classical SIMP-based topology optimization. Going beyond quasistatics, multiscale design can also tackle dynamic material properties such as wave guidance in graded 2D beam networks. A recent approach used ray tracing [4] combined with an adjoint-based optimization scheme to predict spatially variant beam lattices that were tuned to, e.g., redirect waves, focus diverse waves at a point, or to split waves based on frequency [5].

In recent years, tools of machine learning (ML) have offered new opportunities for the design of architected materials. For example, the combination of neural networks for the forward prediction of effective material properties (such as the homogenized effective stiffness of periodic beam unit cells) and for the inverse prediction of structures with target properties have proven to be a powerful *tandem neural network* strategy to accelerate both property prediction and inverse design [6]. Trained on a large dataset of beam unit cells with their associated pre-computed, homogenized 3D anisotropic elastic stiffness properties, the neural networks were able to accurately predict beam lattices with target anisotropic stiffness for applications, e.g., in bone implants whose properties mimic that of natural bone [6]. Moreover, the use of variational autoencoders allowed to interpolate between beam unit cells and to optimize their effective properties, interestingly predicting structures with properties far outside the limites of all structures contained in the training set [7]. Finally, video diffusion models have recently been shown to impressively predict cellular structures (accounting for an elastoplastic base material as well as frictional contact between parts of the structure) with an as-designed nonlinear stress-strain response in compression [8]. Inspired by ML-generated videos, this video diffusion approach yields not only optimal structures with as-designed stress-strain behavior, but it also provides videos of the full-field displacement and stress distribution inside the compressed structures (thus bypassing costly finite element calculations, which were required only for the training set generation).

Such ML-based approaches are generally beneficial when the underlying architecture can be described by a small set of microstructural descriptors and when the target response (such as the elasticity tensor or the stress-strain curve) can be described by a small set of parameters. It is to be expected that the emerging ML-based tools for the inverse design of architected materials is only the beginning, and more powerful and versatile tools are yet to come.

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Computational homogenization of metamaterials including solid-fluid interaction

Varvara Kouznetsova

(joint work with Renan Liupekevicius, Hans van Dommelen, Marc Geers)

This talk will first present a brief overview of dynamic metamaterials, that possess architected substructure specifically designed to manipulate elastic/acoustic waves. The microstructure of dynamic metamaterials is designed to provoke interaction between propagating mechanical waves and fine scale mechanisms, leading to emerging phenomena, such as band gaps, i.e. frequency ranges in which waves do not propagate or highly attenuated, negative refraction index etc. The underlying physical mechanisms used in the design of dynamic metamaterials make use of either Bragg scattering phenomenon, e.g. in Phononic Crystals (PC), or localized microstructural resonances, which is the underlying principle of Locally Resonant Acoustic Metamaterials (LRAM); a combination of these two distinct physical mechanisms has also been proposed. This talk will specifically focus on LRAM type of metamaterials. A few selected examples of potential applications of LRAM metamaterials will be shown, e.g. filtering of forced vibration frequencies in a metamaterial plate [1], wave filtering by positive/negative refraction [2] and negative reflection from an LRAM metasurface [3].

Next, the need for computational methodologies able to describe the behaviour of finite size metamaterial structures subjected to non-trivial (boundary) constraints and excitations will be addressed. To this, aim a computational homogenization framework is proposed. Departing from the previously developed computational homogenization approach for solid LRAMs [4, 5], this contribution

specifically focusses on air saturated poroelastic metamaterials with localized resonances [6]. At the unit cell scale, the linear elastic structural domain and the fluid domain are modelled explicitly using the respective balance equations and the fluid-structure interaction conditions at the interfaces. At the macroscale a mixture approach is adopted. The micro- and macroscale problems are coupled through an extended version of the Hill-Mandel principle, leading to a variationally consistent averaging scheme of the microscale fields. The effective macroscopic constitutive relations are obtained by replacing the microscale problem with a reduced-order model. The reduced micro-scale model is obtained by projecting the fully-resolved micro-scale model on the longwave basis and the local resonance basis, yielding the closed-form expressions for the homogenized material properties. The resulting macroscopic model is an enriched porous continuum with internal variables that represent the microscale local resonance dynamics at the macroscale. The Biot model is recovered from the homogenized model as a special case. Numerical examples demonstrate the framework's validity in modeling wave transmission through a porous layer, Figure 1.

Finally, the proposed framework is specialized and demonstrated for acoustic labyrinthine metamaterials, consisting of a fluid (air) domain coiled by rigid solid walls, exhibiting localized resonance in the fluid phase [7].

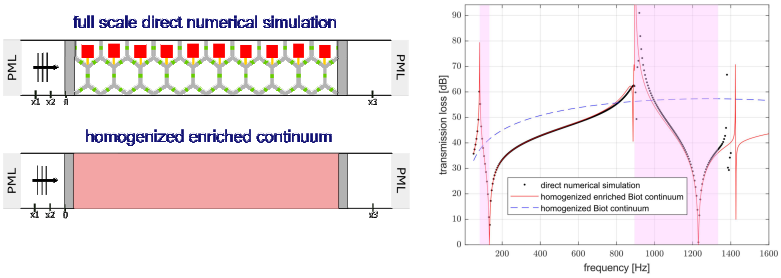

FIGURE 1. Transmission through an acoustic metamaterial layer, computed using the fully resolved direct numerical simulation and the proposed homogenization approach.

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Multi-scale modelling of plasticity and damage in dual-phase steels

Varvara Kouznetsova
(joint work with Lei Liu, Francesco Maresca, Johan Hoefnagels, Tijmen Vermeij, Marc Geers)

Damage initiation in many multi-phase materials can be attributed to a peculiar deformation mode, where one of the phases deforms anisotropically by forming serrated, jagged interface impinging on another (approximately isotropic) phase. This locally induces large strain concentrations at the fine scale in the near-interface second phase, where nano-voids can form and grow, leading to damage and crack formation. Examples include twins impinging on a grain boundary [1], crystalline-amorphous interface [2] or martensite-ferrite interface in advanced multi-phase steels, where martensite islands typically deform by sliding on the retained austenite films [3].

This contribution presented multi-scale modelling framework to predict the damage initiation and propagation at such interfaces using the dual-phase steel (DP) microstructure as an example. Two scales are considered: the DP steel mesoscale consisting of multiple lath martensite (M) islands embedded in a ferrite (F) matrix, and the microscale M/F interfacial zone unit cell resolving the martensite substructure. Based on the emerging microscopic damage initiation pattern associated with the substructure boundary sliding, an effective M/F interface damage indicator is determined from the microstructural response, along with the effective sliding of the martensite island. Relating these two effective quantities leads to an effective interface damage indicator model in terms of the mesoscopic kinematics [4]. The proposed multi-scale modelling framework is next used to predict the damage initiation locations in an experimentally characterized DP steel microstructure. At the majority of the considered M/F interface locations the damage indicator predicted by the model qualitative correlates very well with the experimental observations [5].

Finally, an model for the interface damage propagation has been developed. In addition to the classical cohesive interface deformation mechanism, the anisotropic deformation of one phase, when favourably oriented, induces a distinct interface opening mechanism. The proposed computational homogenization framework captures these two microscopic mechanisms, i.e. jagged damage and cohesive opening.

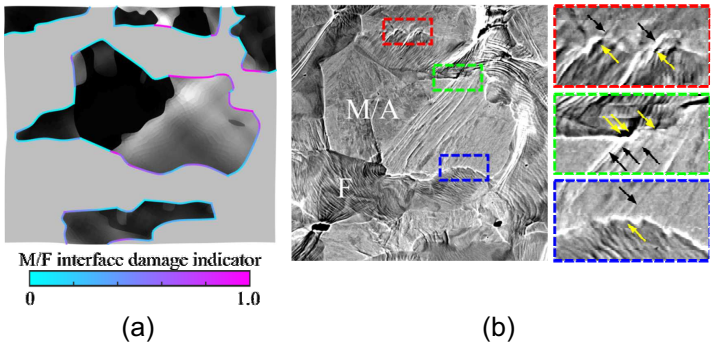

FIGURE 1. Martensite-Ferrite interface damage initiation in a dual-phase steel (a) predicted by the developed multi-scale framework and (b) identified experimentally.

The mesostructure, comprising multiple anisotropic particles in an isotropic matrix, is modelled with interfaces represented by enriched cohesive zones. The microscopic interfacial zone unit cell resolves the laminated structure of the anisotropic phase, defining the effective interface separation and internal kinematic quantities associated with the jagged and cohesive deformation mechanisms. The generalized Hill-Mandel condition yields tractions work-conjugated to these internal kinematic quantities, leading to a mesoscale enriched cohesive law identified through representative microscopic unit cell simulations. Computational examples demonstrate the importance of the jagged deformation mechanism on the interface damage development, but also on the strain partitioning among the phases. The proposed microphysics-based effective interface model provides a valuable tool for understanding and predicting interface damage in complex materials.

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Nonlocal hyperelasticity: Analysis of variational models involving finite-horizon fractional gradients

Carolin Kreisbeck
(joint work with Javier Cueto and Hidde Schönberger)

Peridynamics, which was initiated in the early 2000s in a seminal work by Silling and has attracted increased attention since (see, e.g. [3] and the references therein), is a nonlocal formulation of continuum mechanics that models material behavior based on the interactions between individual points. Unlike conventional mechanics, it is a derivative-free approach that naturally accommodates discontinuities like cracks and fractures, making it well-suited for modeling failure in complex materials. While bond-based peridynamics models are rather limited in the material properties they can describe, the generalization to state-based peridynamics, where one considers the combined effect of bonds in a neighborhood of each point, offers more flexibilty.

In this context, Bellido, Cueto & Mora-Corral in [1, 2] recently proposed a model of nonlocal hyperelasticity, where the energy functionals are integral functionals depending on nonlocal gradients, instead of usual deformation gradients as in the classical theory; precisely,

$$\mathcal{E}(u) = \int_\Omega f(x, D^s_\delta u)\,dx \qquad \text{for } u \in H^{s,p,\delta}_0(\Omega;\mathbb{R}^m), \tag{1}$$

with $\Omega \subset \mathbb{R}^n$ a bounded Lipschitz domain, $p \in (1,\infty)$, and $f : \Omega \times \mathbb{R}^{m\times n} \to \mathbb{R}$ a Carathéodory function with p-growth and p-coercivity. The operators D^s_δ are derived from the Riesz fractional gradient D^s (see e.g. [6, 4, 7]) with fractional parameter $s \in (0,1)$; with its natural invariance and homogeneity properties, the latter is a concept of fractional derivative well-suited for applications. The gradients D^s_δ combine these features with the benefits of a finite range of interaction, called horizon $\delta > 0$, which is particularly relevant for models on bounded domains. For smooth functions $\varphi \in C^\infty_c(\mathbb{R}^n;\mathbb{R}^m)$, the finite-horizon gradient D^s_δ is given by

$$D^s_\delta\varphi(x) = c_{n,s,\delta}\int_{\mathbb{R}^n} \frac{\varphi(y)-\varphi(x)}{|y-x|^{n+s}} \otimes \frac{y-x}{|y-x|} w_\delta(y-x)\,dy$$

with a non-negative smooth cut-off function w_δ compactly supported in the ball $B_\delta(0) \subset \mathbb{R}^n$ and normalizing constant $c_{n,s,\delta} > 0$. Via duality, this definition can be extended to weak derivatives, and the associated function spaces are defined analogously to classical Sobolev spaces. After prescribing volumetric boundary conditions by requiring zero values in a collar of thickness δ round the boundary of the domain, one obtains the function space $H^{s,p,\delta}_0(\Omega;\mathbb{R}^m)$, for which relevant technical tools such as Poincaré inequalities and compact embeddings [1, 5] are available. Besides, we mention a lemma about strong convergence in the collar region. It follows as a consequence of a nonlocal Leibniz rule and states that any weakly converging sequence in $H^{s,p,\delta}_0(\Omega;\mathbb{R}^m)$ converges strongly in L^p in any compact set contained in $\Omega \setminus \Omega_{-\delta}$ with $\Omega_{-\delta} := \{x \in \Omega : \operatorname{dist}(x,\partial\Omega) > \delta\}$.

The overall goal of the featured work [5] is to contribute to the development of an existence theory and asymptotic analysis for variational problems involving nonlocal gradients, both of which are substantial for putting nonlocal hyperelasticity on a solid mathematical footing. Based on the direct method, we address the following aspects: Characterization of weak lower semicontinuity of $\mathcal{E}$, variational convergence for parameter-dependent families of nonlocal integral functionals, including relaxation and homogenization, and localization as the fractional parameter tends to 1.

To provide some more detail, we start by pointing out that quasiconvexity, the natural convexity notion in the classical calculus of variations, turns out to characterize weak lower semicontinuity also in the nonlocal setting.

Theorem 1 [5, Theorem 5]**.** *The functional $\mathcal{E}$ is (sequentially) weakly lower semicontinuous if and only if $f(x,\cdot)$ is quasiconvex for a.e. $x \in \Omega_{-\delta}$.*

As a consequence of a general Γ-convergence statement (see [5, Theorem 6]), one can infer nonlocal analogs of classical relaxation and homogenization results. These allow to capture the effective behavior of materials with microstructure formation and periodic small-scale heterogeneities, respectively.

Theorem 2 [5, Corollary 3 and 4]**.** *(i) The relaxation $\mathcal{E}^{\mathrm{rlx}}$ of the functional $\mathcal{E}$, that is, its weak lower semicontinuous envelope, is given by*

$$\mathcal{E}^{\mathrm{rlx}}(u) = \int_{\Omega_{-\delta}} f^{\mathrm{qc}}(x, D^s_\delta u)\,dx + \int_{\Omega\setminus\Omega_{-\delta}} f(x, D^s_\delta u)\,dx$$

for $u \in H^{s,p,\delta}_0(\Omega;\mathbb{R}^m)$, where f^{qc} is the quasiconvexification of f.

(ii) Suppose $\mathcal{E}_\varepsilon$ for $\varepsilon > 0$ is given as in (1) with a density $f_\varepsilon := f(\frac{\cdot}{\varepsilon},\cdot)$ and $f : \mathbb{R}^n \times \mathbb{R}^{m\times n} \to \mathbb{R}$ $(0,1)^n$-periodic in the first variable. Then,

$$\mathcal{E}^{\mathrm{hom}}(u) = \Gamma(L^p)\text{-}\lim_{\varepsilon\to 0} \mathcal{E}_\varepsilon(u) = \int_{\Omega_{-\delta}} f^{\mathrm{hom}}(D^s_\delta u)\,dx + \int_{\Omega\setminus\Omega_{-\delta}} \overline{f}(D^s_\delta u)\,dx$$

for $u \in H^{s,p,\delta}_0(\Omega;\mathbb{R}^m)$, where f^{hom} denotes the homogenized integrand determined via the classical multicell formula, and $\overline{f}$ is obtained by taking the average of f in the first variable.

Note that the integral contributions over $\Omega_{-\delta}$ in the previous theorem feature precisely the same integrands as in the corresponding (by now) standard local theories. The reason for this parallel is rooted in the translation method explained below. On the other hand, the behavior in the boundary layer is due to the strong convergence in the collar.

Finally, as a consistency check for the newly proposed model, we establish a rigorous link with its classical counterpart by studying the limiting behavior as the fractional index s tends to 1. The nonlocal gradient D^s_δ localizes to the classical one and the same can be confirmed for the associated variational problems.

Theorem 3 [5, Theorem 7]**.** *Let $\mathcal{E}_s$ for $s \in (0,1)$ be as in (1) with f quasiconvex in its second variable. Then, the family $(\mathcal{E}_s)_s$ is equi-coercive and Γ-converges with*

respect to L^p-convergence as $s \to 1$ to a limit functional that is determined (up to a constant) by

$$\mathcal{E}_1(u) = \int_{\Omega_{-\delta}} f(x, \nabla u)\, dx \quad \text{for } u \in W_0^{1,p}(\Omega_{-\delta}; \mathbb{R}^m).$$

Our analysis and the proofs of Theorems 1-3 rely significantly on one key technical ingredient, namely, suitable translation operators that facilitate switching between the nonlocal and classical gradients. Precisely, it holds for $\varphi \in C_c^\infty(\mathbb{R}^n; \mathbb{R}^m)$ that

$$D_\delta^s \varphi = \nabla(Q_\delta^s * \varphi) \qquad \text{and} \qquad \nabla\varphi = D_\delta^s(\mathcal{P}_\delta^s \varphi),$$

where Q_δ^s is a compactly supported integrable kernel function, and $\mathcal{P}_\delta^s$ is the inverse of the convolution with Q_δ^s, see [1, 5]. A generalization of these identities to functions in (nonlocal) Sobolev spaces (see [5, Theorem 2]) gives rise to a useful method for transferring well-established results on local problems to the nonlocal setting, with applicability also beyond the problems discussed here.

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Optimal Korn-Maxwell-Sobolev inequalities

Peter Lewintan

(joint work with Franz Gmeineder, Patrizio Neff, Stefan Müller, Jean Van Schaftingen)

We present a complete picture of coercive Korn-type inequalities for generalised incompatible fields, and optimally extend and unify several previously known inequalities that are crucial to the existence theory for a variety of models in continuum mechanics. More precisely, we classify completely the interplay between a space dimension $n \in \mathbb{N}$, an integrability $p \geq 1$, an algebraic part map $\mathscr{A} : V \to \widetilde{V}$ and a linear homogeneous k-th order differential operator $\mathbb{B} = \sum_{|\alpha|=k} \mathbb{B}_\alpha \partial^\alpha$ with

linear $\mathbb{B}_\alpha : V \to W$, whereby V, $\widetilde{V}$ and W denote finite dimensional spaces, such that

$$\|P\|_{\mathfrak{X}_{k,p}(\mathbb{R}^n)} \leq c\left(\|\mathscr{A}[P]\|_{\mathfrak{X}_{k,p}(\mathbb{R}^n)} + \|\mathbb{B}P\|_{\mathrm{L}^p(\mathbb{R}^n)}\right) \qquad \forall\, P \in \mathrm{C}_c^\infty(\mathbb{R}^n; V),$$

with a constant $c = c(n, p, \mathscr{A}, \mathbb{B}) > 0$ and function spaces $\mathfrak{X}_{k,p}(\mathbb{R}^n)$ chosen in such a way that this inequality scales suitably.

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Natural fluctuations in slip-dominated mechanics: Stochastic solver for crystal plasticity simulations

Jaime Marian

The deformation of crystalline materials by dislocation motion takes place in discrete amounts determined by the Burgers vector. Dislocations may move individually or in bundles, potentially giving rise to intermittent slip. This confers plastic deformation a certain degree of variability that can be interpreted as being caused by stochastic fluctuations in dislocation behavior. However, crystal plasticity (CP) models are almost always formulated in a continuum sense, assuming that fluctuations average out over large material volumes and/or cancel out due to multi-slip contributions. Nevertheless, plastic fluctuations are known to be important in confined volumes at or below the micron scale, at high temperatures, and under low strain rate/stress deformation conditions. Here, we present a stochastic solver for CP models based on the residence-time algorithm that naturally captures plastic fluctuations by sampling among the set of active slip systems in the crystal. The method solves the evolution equations of explicit CP formulations, which are recast as stochastic ordinary differential equations and integrated discretely in time. The stochastic CP model is numerically stable by design and naturally breaks the symmetry of plastic slip by sampling among the active plastic shear rates with the correct probability. This can lead to phenomena such as intermittent slip or plastic localization without adding external symmetry-breaking operations to the model. To demonstrate its capabilities, the method is applied to body-centered cubic tungsten single crystals under a variety of temperatures, loading orientations, and imposed strain rates.

Concepts in Linking Nonequilibrium Statistical Mechanics of Thermally Activated Dislocation Ensembles to Internal State Variable Theory

David McDowell

This work lends new insight into the interpretation of internal state variable (ISV) theory and fundamentals of the behavior of thermally activated dislocation ensembles. We formally define physical concepts undergirding ISV theory such as configurational subsystems (e.g., individual grains or phases), constrained local equilibrium, and thermally activated dislocation reactions in the context of crystal plasticity and then implement these concepts within a nonequilibrium statistical thermodynamics framework. The primal importance of the Gibbs free energy barrier to dislocation reactions within each subsystem is emphasized since the enthalpy barriers are affected by local constraint and resulting long-range and short-range athermal internal stresses acting within subsystems. On this basis, thermal and configurational intrinsic entropy change are formally introduced at each step in the same way as in first principles methods based on probability of pending dislocation reactions. We distinguish equilibrium thermodynamics up to the saddle point of reactions, for which change of both configurational and thermal entropy applies, from post-saddle point extended glide of dislocations, which couples with the thermal bath via dispersive phonon dynamics. We introduce the concept of "degree-of-correlation" of thermally activated dislocation processes both within each subsystem and across the overall ensemble of subsystems, based on the ratio of the weighted average enthalpy barrier to the maximum (rate-limiting) enthalpy barrier, and argue that nonequilibrium trajectories progressively trend towards correlated behavior of the ensemble by virtue of internal stress redistribution among subsystems that are favorable and unfavorable to reactions. The degree-of-correlation is a many-body concept involving populations of dislocations within and among various configurational subsystems. The maximal intrinsic entropy production heuristic is considered in light of the concept of progressive increase in the degree-of-correlation of enthalpy barriers within and among subsystems. It is suggested that this framework may be useful as a scaffold for application of machine learning to use disparate information from atomistic and discrete dislocation dynamics simulations to inform likely estimates of reduced order ISV models.

Computations with heterologous continua: Mesoscale phase field model for high T solid mechanics

Sinisa Mesarovic

The mechanisms of sintering and creep are based on diffusion of atoms: through the bulk of crystals, through interfaces between the grains, and, through surfaces (grain-gas interfaces), and their subsequent deposition on the surface. The process is driven by surface energy of internal surfaces and it may be aided by applied macroscopic stress, and even by plastic deformation. To study the mechanisms on

the mesoscale, a computational phase field model for moving interfaces is indicated, which should include stress and concentration driven diffusion through bulk and surfaces, as well as the growth of new lattice. In the early stages of sintering, the gas flows out of the domain, while in the later stages, when pores cease to percolate, the gas is compressed in closed pores.

Modeling of solids with diffusion requires formulation of lattice continuum, whereby the material is represented by lattice sites (as opposed to the traditional mass continuum where the material is identified with mass). With gas represented by mass continuum, we are faced with the problem of formulating the phase field model which encompasses heterologous continua.

Specifically, the unique continuous velocity/displacement fields that characterize the phase field formulation must undergo rapid transitions at (diffuse) interfaces. These transitions account for lattice growth rates of grains which are diffusion-controlled and defined relative to the lattice velocity. We present preliminary computational results and theoretical analysis.

A few outstanding problems in the theory of composites

Graeme Milton

This talk presented three outstanding problems in the theory of composites. The first concerned extremal materials in linear elasticity. In three dimensions the non-trivial ones can be classed as unimode, bimode, trimode, quadramode, and pentamode, according to the number of independent easy modes of deformation, or equivalently according to the number of very small eigenvalues of the elasticity tensor [8]. (The prefixes come from those of polygons) The simplest pentamodes have a diamond like structure with each bond being replaced by a double cone, so that four conical tips meet at each node. Balance of forces means that the tension in one double cone determines the tension in the three other double cones that meet it at the node, and by induction the stress in the material. Like rubber they can be stiff to hydrostatic compression, yet very compliant to shearing. Unlike rubber, pentamodes can be structured so that the stiff mode is not hydrostatic but rather a linear combination of a hydrostatic and a shear loading. This allows them to be useful for guiding stress. Applications of pentamodes include cloaking [14, 15] and using them for seismic isolators [16]. Both isotropic and anisotropic pentamodes have been studied numerically, physically constructed, and studied experimentally: see, for example, [3, 4, 17, 5, 2, 18, 13, 7]. The bicycle company Specialized uses what are essentially pentamodes in some of its bicycle seats that are manufactured by the 3-d printing company Carbon. By superimposing pentamodes, distorting the structures to avoid clashes, if necessary, one can obtain any extremal material. However, this construction is rather unsatisfactory when one considers finite, rather than infinitesimal, deformations as then the pentamode substructures will collide, or interact with each other if the intervening space is filled with an extremely compliant material rather than void. So one question is whether one can get all possible materials that in addition to being extremal

still function under finite deformation? One can, for example, get quadramode materials by adding additional double cone links between nodes in a pentamode structure, but it is doubtful whether one can get all quadramode materials in this way.

A second problem concerns three or two dimensional composites of an elastic materials with void (or for technical reasons it may just be extremely compliant rather than being truly void). Confining attention to isotropic composites the effective (bulk, shear) moduli are confined to a rectangle in the (bulk, shear) plane given by the well-known Hashin-Shtrikman bounds [1]. One question is weather one can improve these bounds, or alternatively identify microostructure attaining the Hashin-Shtrikman shear modulus bound, but not the Hashin-Shtrikman bulk modulus bound. Microstructures have been identified that attain the Hashin-Shtrikman bulk modulus bound, but which have arbitrarily small shear modulus bound [11]. However these microstructures get ripped apart under any finite shearing deformation. So the question is then whether one can obtain bounds and optimal microstrucure for finite shears, rather than just infinitesimal ones. Similar questions can be asked for anisotropic composites [11].

A final question concerned deformations of periodic arrangements, in two or three dimensions, of rods linked by hinges. The Guest-Hutchington modes are revealed by looking for periodic infinitesimal deformations. However, deformations need not be macroscopically affine: see, for example, [9, 10]. So the problem is to identify the deformations that are not macroscopically affine. Can they be obtained from the periodic deformations in the limit as the size of their unit cell, relative to the size of the unit cell of the underlying periodic rod-hinge structure approaches infinity?

Of course there are many more open questions, some of which are discussed in the paper [12]. One of them has been solved by Christian Kern, who, much to my surprise, found that hierarchical laminate materials could reproduce the change of sign of the Hall coefficient found in interlocking ring structures [6].

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Extensions of the Cahn-Hilliard equation to temperature dependent settings

Anja Schlömerkemper

The Cahn-Hilliard equation is an equation of mathematical physics that models the dynamics of binary media. This talk is a presentation of the main ideas of the article [1]. We derive and di extensions of the Cahn-Hilliard equation. The derivation of the models is based on a combination of methods from non-equilibrium thermodynamics and an energetic variational approach. Furthermore, we use approach to derive models available in the literature. For a comparison of the various models see [1]. The standard double-well potential in Cahn-Hilliard is replaced by a temperature dependent variant that allows a transition from double-well to single-well potentials as temperature increases. Moreover, tickness of the diffuse interface is allowed to vary with temperature. That is, the starting point is a free energy of the form

$$\psi(\phi, \nabla\phi, \theta) = \frac{\tilde{\epsilon}(\theta)}{2}|\nabla\phi|^2 + \frac{1}{\tilde{\epsilon}(\theta)}\Big(W(\phi) + c(\theta)\phi^2\Big) - g(\theta),$$

where ϕ denotes the phase field function and θ the temperature. We focus on two different assumptions on the transport property of the temperature. In a first model we assume that the temperature is transported along the trajectory of the

flow map of the effective vel of the microscopic particles. In a second model we assume that the temperature is fixed on a background and is thus independent of the flow map. By assuming in addition suitable dissipation potentials, wain two models that satisfy the first and second law of thermodynamics. We address the question of which model is to be considered more appropriate from a mathematical perspective. We investigate well-posedness of the systems, which might be used as a selection criterion. Whhe first model causes difficulties due to a singularity of the phase field parameter, the second model is proven to have unique classical solution. To this end, we work on the whole space and consider smaitial data in Besov spaces. Then, by a fixed-point argument and use of the Littlewood-Paley decomposition, we prove existence of classical solutions for small times.

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Essential boundary conditions in FFT-based computational micromechanics

Matti Schneider
(joint work with Lennart Risthaus)

Computational homogenization methods based on the Fast Fourier Transform (FFT) have been established in recent years as powerful computational approaches to handle materials with heterogeneous microstructure represented on a discrete (voxel) grid.

In its original formulation, the method imposes periodic boundary conditions on the displacement fluctuation. There is a number of situations, however, where other boundary conditions like essential, i.e., clamping, boundary conditions would be more favorable, i.e., for non-periodic microstructures, e.g., coming from micro-CT, or when actual micro-experiments are simulated. Unfortunately, the approach which is successful for thermal conductivity, i.e., using the discrete sine transform, does not work, essentially due to the mixing of sine and cosine terms appearing for the shear terms. Workarounds in the literature impose essential boundary conditions via Lagrange multipliers, which is possible, but comes at the expense of a deteriorated numerical performance.

In the talk, we introduce a trick which permits to impose essential boundary conditions in FFT-based computational micromechanics in such a way that the entire solver technolology established in the periodic setting becomes available in the case at hand, as well. We demonstrate the potential of the novel piece of technology by dedicated computational experiments.

A data-based derivation of internal stress for the coarse-graining in dislocation-based plasticity

Katrin Schulz

The plasticity properties of metal, such as strength and ductility, are governed by the movement and the interaction of dislocations. Therefore, for small scale simulations, incorporating the knowledge regarding dislocation dynamics becomes more important due to the existence of size effect and micro level heterogeneity. Among the pioneer works, a key component capturing the microscopic characteristics is the back stress conjugated with the defect energy potential [1]. The defect energy potential is often assumed to be of a quadratic form and derived based on thermodynamic consistency. The resulting back stress will be of the second order gradient of plastic strain, and shows good capability for simulating material behaviour at smaller scales. However, until now, the exact formulation of the defect energy potential and the back stress term as well as the connection to the dislocation characteristics stay unclear.

In this presentation, we thus introduce a framework for the derivation of the back stress term based on the statistical analysis of data from discrete dislocation dynamic simulations. By investigating the dislocation structure formation within the coarse graining benchmark systems under various combinations of numerical and microstructure conditions, e.g. element size, initial dislocation density, and the gradient of geometrically necessary dislocations, the heterogeneous dislocation structures formation within an element is identified. The resulting structure can be further predicted by the collected data base statistically or by a machine learning approach. We derive the near field correction stress within a coarse-grained system according to the uneven stress field induced by the heterogeneous dislocation structure formation. The derivation is assumed to be a mechanism-based explanation applicable to the back stress within gradient plasticity theory.

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Elastic interactions in Object kinetic Monte Carlo for defect evolution: Hydrogen and radiation defect migration

Javier Segurado

(joint work with Rodrigo Santos-Güemes, Gonzalo Álvarez, Christophe Ortiz)

Object Kinetic Monte Carlo (OkMC) allows to study evolution of defects as well as solute atoms in materials without the severe time and size limitations of atomistic approaches. In OkMC migration takes place by overcoming an energy barrier. In the presence of an elastic field this barrier is modified, and the defects jump with probabilities biased by the spatially dependent elastic fields. This work will present first an FFT based approach to introduce the elastic fields caused by any type of

dislocation, point defects, solute atoms and second phases in OkMC simulations [1]. The elastic fields of mobile and immobile dislocation lines are pre-computed using Field Dislocation Mechanics with a non-singular core description solved using a FFT approach. During the OkMC simulation, for each possible defect jump, the elastic energy contribution is computed multiplying the external stress with the defect strain field moved to the position of interest by the shift theorem. The model will be applied to study the migration of prismatic loops and self-interstitials in iron, accounting for their mutual interaction and the presence of other immobile dislocations. The second part of the talk will propose a method to use non-regular grids in the computation of the elastic fields produced by dislocation and other defects [2]. This method allows to concentrate several Fourier points near dislocation lines to accurately represent their core and inelastic strain.

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A new look at twin branching in shape memory alloys: a 1D continuum model and energy dissipation effects

Stanisław Stupkiewicz

(joint work with Seyedshoja Amini, Mohsen Rezaee-Hajidehi)

Twin branching is a commonly observed phenomenon in martensitic transformations in shape memory alloys. Competition between interfacial and elastic strain energy contributions leads to the refinement of twin laminates close to the macroscopic interface between twinned martensite and austenite. The corresponding scaling laws have been widely studied starting from the work of Kohn and Müller [1]. In a discrete setting, Seiner et al. [2] developed an explicit, low-energy construction of the branched microstructure that is able to realistically predict the twin spacing and the number of branching generations.

In this work, we develop a 1D continuum model of twin branching. The free energy of the branched microstructure comprises the interfacial and elastic strain energy contributions, the latter calibrated using the respective upper-bound estimate derived by Seiner et al. [2]. The total free energy is then minimized, and the corresponding Euler-Lagrange equation is solved numerically using the finite element method. The results show a good agreement with the model of Seiner et al. [2] in the entire range of physically relevant parameters. Importantly, our continuum framework admits incorporation of energy dissipation. The effect of rate-dependent and rate-independent dissipation on the evolution of the branched microstructure can thus be studied.

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Different peridynamic approaches to wave propagation and dynamic fracture

Kerstin Weinberg

In the sense of a non-local continuum formulation, peridynamics describes the interactions between material points. In its original version it refers to only one spring-like stiffness parameter and, thus, the standard bond-based peridynamic model is not consistent with classical linear elasticity. Several extensions have been introduced since. In this contribution, we present different current peridynamic material formulations and study their ability to model motion, wave propagation and dynamic fracture.

In general, the position of a material point inside a body $\mathcal{B}_0$ is described in a reference placement as $\mathbf{X}$ and in its current position as

$$\mathbf{x} = \mathbf{X} + \mathbf{u} \tag{1}$$

with the displacement $\mathbf{u}(\mathbf{X})$. In peridynamics, material points interact with other points inside of their a *neighborhood* $\mathcal{H}$, which is defined as the set of points inside a sphere with the radius $\delta \in \mathbb{R}^+$, also named the *horizon*. The interaction of the point $\mathbf{X}$ with its neighbor $\mathbf{X}'$ is called *bond*. The evaluation of the bond interactions for all $\mathbf{X} \in \mathcal{B}_0$ results in the peridynamic integro-differential equation of motion, cf. [1, 2].

$$\rho_0\, \ddot{\mathbf{u}}(\mathbf{X},t) = \int_{\mathcal{H}_0} \mathbf{f}(\mathbf{X}, \mathbf{\Delta X}, t)\mathrm{d}V' + \mathbf{b_0}^{\mathrm{ext}}(\mathbf{X},t) \qquad \forall \mathbf{X} \in \mathcal{B}_0\ ,\ t \geq 0\ . \tag{2}$$

For numerical simulation, the continuum is typically point-wise discretized, which, together with the underlying non-local continuum mechanics formulation, makes it ideally suited for dynamic fracture simulation. An important implication is the correct treatment of elastic waves, such as pressure and stress waves inside a body. This motivated us to investigate and compare the elastic wave propagation behavior of a bond-based peridynamic, a continuum-kinematics-based peridynamic, and a non-ordinary state-based peridynamic formulation [3, 4].

As illustrated in Figure 1, we found significant differences in the ability of the different peridynamic formulations to reproduce a material's wave speed. Using the example of a longitudinal pressure wave inside an elastic bar, we show that the different formulations approach the the classical solutions to a different extent.

All simulations are performed with our Julia package `Peridynamics.jl` [5].

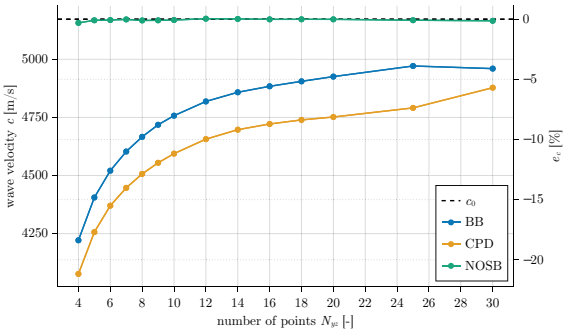

FIGURE 1. Wave propagation velocity c, calculated with different discretizations from 6400 up to 2700000 material points

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Waves in materials with heterogeneous microstructures

CHRISTIAN WIENERS

Materials with periodic microstructures are well studied in the literature:

- The effective equations for static and quasi-static elasticity can be computed efficiently with the FE^2 approach (see [6] for an efficient implementation also for quasi-static plasticity with damage).
- The limit equation for compressional waves in a layered medium is explicitly known (also for stochastic material parameters, see [5]).
- The two-scale limit of the linear Maxwell model is the Debey model with convolution in time [7]. Therefore, the technique of periodic unfolding is adapted to the Symmetric Friedrichs System

$$L_\delta \mathbf{u} = M_\delta \partial_t \mathbf{u} + D_\delta \mathbf{u} + A\mathbf{u}\,, \qquad \mathbf{u} = (\mathbf{E}, \mathbf{H})^\top$$

with periodic symmetric matrices M_δ, D_δ, and $A\mathbf{u} = (-\operatorname{curl}\mathbf{H}, \operatorname{curl}\mathbf{E})^\top$ (see [2, 1] for the comprehensive analysis).

Here we show that the two-scale analysis can be generalized to weak solutions of general symmetric Friedrichs systems and that this approach also applies to viscoelastic solids. The homogenization limit for the corresponding first-order system for velocity and stress $(\mathbf{v}, \boldsymbol{\sigma})^\top$ with $A(\mathbf{v}, \boldsymbol{\sigma})^\top = (\operatorname{div}\boldsymbol{\sigma}, \nabla^{\mathrm{sym}}\mathbf{v})^\top$ also yields a convolution in time. A special case are Generalized Standard Linear Solids [4], where the convolution kernel is approximated by memory variables.

For the evaluation of the effective model we use the formulation for weak solutions of first-order systems summarized in [3] based on the LL^* method which yields a uniform bound for the solution in L_2 for $\delta \in (0, \delta_0)$, so that a weak limit for $\delta \longrightarrow 0$ exists.

Finally we indicate that also for general microstructures which are not necessarily periodic an adaption of the FE^2 in form of a Petrov-Galerkin system can be derived to approximate the effective solution on a coarse mesh with suitable test functions which are defined backward in time and can be approximated on a fine mesh.

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Concurrent Atomistic-Continuum Simulation of the Plastic Flow in Heterogeneous Alloys

Liming Xiong

In this talk, we present a concurrent atomistic-continuum (CAC) methodology and its applications in modeling the dislocation-mediated plastic flow in heterogeneous alloys. As a multiscale simulation tool built upon a formulation that unifies the atomistic and continuum description of materials, one main unique feature of CAC is to retain the microscale dislocation slip, the atomic-scale dif- fusion

and kink dynamics on the dislocation line, as well as the nanoscale grain boundary (GB) structure evolution all within one model. The applicability of CAC is demonstrated through: (i) modeling the dislocation loop nucleation and growth from atomistic to microscale; (ii) characterizing the core structure/stress heterogeneity induced by atomic-level diffusion along a micrometer-long dislo- cation line; (iii) quantifying the stress concentration induced by the slip-GB reaction and its contribution to the subsequent structure changes, such as GB structure reconfiguration, phase transformation, dislocation transmission and so on. The limitations of the single-scale methods in modeling these material defor- mation behaviors are highlighted. The extension of CAC to a finite-temperature CAC through phonon density states-based algorithm are discussed.

Outcome: Providing the community with an alternative vehicle to bridge atom- istic with continuum by formulating the local stress-/GB-state based metrics of slip transfer that can be informed into higher scale models, such as dislocation dynamics (DD) or crystal plasticity finite element (CPFE); for simulating the plastic flow in heterogeneous alloys under deformation.

Open Questions: How to consolidate the CAC simulation results into the constitutive rules or slip transfer metrics that can be used in computer software at the engineering scale?

Universal Deformations in Nonlinear Elasticity and Anelasticity

Arash Yavari

For a given class of materials, universal deformations are those deformations that can be maintained in the absence of body forces and by applying only boundary tractions. Universal deformations play a crucial role in nonlinear elasticity: i) They have had an important organizational role in the semi-inverse solutions in nonlinear elasticity (and anelasticity), and ii) they offer guidance for designing experiments for determining the constitutive relations of a specific material. Their systematic study was initiated in the 1950s by Jerry Ericksen [2, 1] for homogeneous compressible and incompressible isotropic solids.

First, universal deformations for homogeneous transversely isotropic, orthotropic, and monoclinic solids are discussed [3]. In this case, there are no general solutions unless universal material preferred directions are also specified. It is shown that for compressible transversely isotropic, orthotropic, and monoclinic solids universal deformations are homogeneous and that the material preferred directions are uniform. Next, for incompressible transversely isotropic, orthotropic, and monoclinic solids we derive the corresponding universality constraints. These are constraints that are imposed by equilibrium equations and the arbitrariness of the energy function. We show that these constraints include those of incompressible isotropic solids. Hence, we consider the known universal deformations for each of the six known families of universal deformations for isotropic solids and find the corresponding universal material preferred directions for transversely

isotropic, orthotropic, and monoclinic solids. We next extend Ericksen's analysis of universal deformations to inhomogeneous compressible and incompressible isotropic and anisotropic solids [4, 5]. We show that a necessary condition for the known universal deformations of homogeneous isotropic solids to be universal for inhomogeneous solids is that inhomogeneities respect the symmetries of the deformations. Symmetries of a deformation are encoded in the symmetries of its pulled-back metric (or its right Cauchy-Green strain). We show that this necessary condition is sufficient as well for all the known families of universal deformations except for Family 5. Finally we consider both compressible and incompressible inhomogeneous transversely isotropic, orthotropic, and monoclinic solids. We show that the universality constraints for inhomogeneous anisotropic solids include those of the corresponding inhomogeneous isotropic and homogeneous anisotropic solids. For compressible solids, universal deformations are homogeneous and the material preferred directions are uniform. For each of the three classes of anisotropic solids we find the corresponding universal inhomogeneities–those inhomogeneities (position dependence of the energy function) that are consistent with the universality constraints. For incompressible anisotropic solids we find the universal inhomogeneities for each of the six known families of universal deformations.

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Geometry of needle-like microstructures in martensites

Barbara Zwicknagl

(joint work with Sergio Conti, Nora Lüthen, Martin Lenz, Martin Rumpf, and Jan Verhülsdonk)

In this talk, we discuss recent analytical and numerical results obtained in [1, 2, 3, 4] on special martensitic microstructures as they have been observed experimentally in a variety of materials, such as shape-memory materials including NiAl-alloys or YBCO materials (see e.g. [7]). These needle-like patterns are essentially two-dimensional laminated structures where one variant occurs in a needle-type shape that thins out close to a macrointerface. Such structures can be observed at length scales from nano- to milimeters.

Our aim is to understand the geometry of these needle-type structures, in particular the tapering length scale and the bending angle.

We follow the variational approach to model pattern formation in martensites in the framework of the phenomenological theory of martensite (see [5]). We focus on a cell of periodicity of the laminated structure and characterize optimal needle-structures as solutions to a shape-optimization problem, minimizing the elastic energy in the transition layer around the macrointerface. For that, we consider both, geometrically nonlinear and geometrically linear elasticity. It has been observed in several numerical studies in the literature before (see e.g. [2, 4] for an overview of some references) that models based on linearized elasticity are often not able to reproduce the experimentally observed patterns, while on the other hand geometrically linear models have proven to be sufficient to predict the bending of the needle from its (measured) tapering length (see e.g. [6] and the references therein).

Our findings support these observations and underline in particular that geometrically nonlinear elasticity is necessary to determine the length scale of the needle tapering. Precisely, we study numerically and analytically the infimal energy in terms of three problem parameters, namely the order parameter δ related to the eigenstrains of the martensitic variants, the tapering length ℓ of the needle, which determines the size of the transition layer, and the volume fractions of the two variants in the laminated structure. It turns out that in the geometrically linearized setting, the minimal energy in the transition layer decays as ℓ^{-1} as the tapering length of the needle ℓ tends to infinity. This shows that the optimal tapering length scale in the geometrically linearized setting is $+\infty$, which does not reflect experimental finding. In contrast, in the geometrically nonlinear setting, the optimal tapering length behaves as δ^{-1}, i.e., it is inversely proportional to the order parameter. This is shown numerically in [2, 3] and made analytically rigorous in terms of scaling laws for the infimal energies in [1, Theorems 3.1 and 4.1]. A main ingredient in the quantitative numerical comparison of the nonlinear and the linearized setting are problem-adapted elastic free energy densities (see [3, 4] and the references therein).

We also consider more complex interfaces where needle-type structures of different orientation meet. Experimental findings often show certain long-range effects. More precisely, needle tips seem to influence the shapes of the other laminate in front of them (see e.g. [7]). Our numerical results in [3] indicate that such transparency effects can also be explained as a result of elastic energy minimization.

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