A continuum framework for the treatment of mechano-chemically driven phase transformations with a group/sub-group character

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We consider the continuum formulation and numerical solution of mechano-chemically driven phase transformation problems that are characterized by a free energy function that is non- convex with respect to strain and composition. The non-convexity demands that at least the first gradients of strain and composition be included in the formulation to ensure mathematical well-posedness, and physically consistent solutions. The corresponding chemical problem was famously treated by Cahn and Hilliard in 1958, while Toupin followed with the nonlinear elasticity problem in 1962. The coupled, nonlinear, initial and boundary value problem has not been solved to our knowledge, mainly because of the smoothness requirement imposed by the higher-order partial differential equation of nonlinear strain gradient elasticity. Here, we draw upon interpolation functions with a spline basis to surmount this difficulty, and also extend them to the Cahn-Hilliard description of the chemical problem. The mathematical formulation is variationally derived, and its numerical implementation is made possible by a weak treatment of higher-order boundary conditions. The use of algorithmic differentiation also makes the exact linearization tractable.

Combined Atomistic/Continuum Modeling of Strain Localization in Metallic Glass

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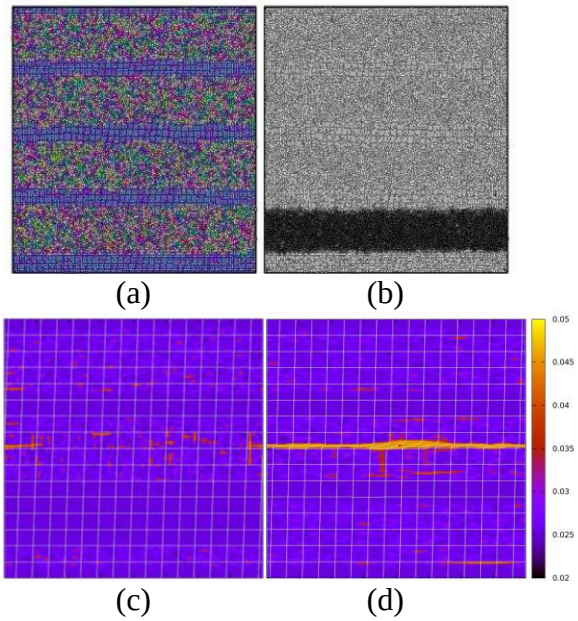
The modeling of metallic glass mechanical response, including the prediction of failure, requires the establishment of numerically tractable continuum descriptions of viscoplasticity that incorporate relevant atomistic mechanisms and can be parameterized to metallic glass microstructure. Here we deploy the shear transformation zone (STZ) theory [1] to make quantitative predictions of deformation and failure processes in amorphous solids. This is done in the context of a thermodynamic theory wherein the local disorder is quantified in terms of an effective temperature. [2] Molecular dynamics (MD) simulation is used to parameterize the model. A highly optimized fully Eulerian implementation of the STZ theory is implemented [3] to investigate monolithic metallic glasses and metallic glass crystal composite materials subjected to very large strains, such as those that arise in failure processes such as strain localization. We then perform cross-comparisons between continuum theory and MD predictions using structural parameters that can be independently measured in MD. The onset of failure depends sensitively on the coarse-grained stochastic field that represents the structural inhomogeneity, the details of which determine the mechanical response as well as the onset of instabilities. The properties of this stochastic field are further studied to provide insights into the structure of amorphous solids.



In these images from 3D MD simulations and 2D continuum simulations crystalline layers have been inserted between amorphous regions to create a lamellar composite. In (a) the atoms in MD are colored by potential energy, while in (b) the atoms are light or dark depending on the local shear strain. In (c) and (d) the local values of the effective temperature in the continuum simulation are shown.

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Strain Functionals for Characterizing Atomistic and Other Geometries

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The development of a set of strain tensor functionals that are suitable for characterizing arbitrarily ordered atomistic structures is described. The approach starts by transforming the discrete atomic coordinates to a continuous and differentiable density function,[1] here using Gaussian smoothing envelopes. The local geometries are then characterized in terms of a Taylor series expansion about each atomic center. From the properties of the Gaussian function, the n-th order derivatives can be directly related to the n-th order moments of the neighboring atom positions. This is similar to an approach used by Zimmerman et al [2], except that the neighborhoods are smooth rather than discrete. The current approach is similar to the Second Order Maximum Entropy (SOME) method, developed by Cyron et al [3] for interpolation in a mesh-free continuum code, where Gaussian functions are used to develop a least-biased definition of a neighborhood. The Cartesian moments can be transformed to solid harmonic functions (also called 3D Zernike functions), which retain radial information compared to other previous analyses based on spherical harmonic functions. Those functions can be further recast in terms of Rotationally Invariant Functions (RIF) that cleanly isolate different types of shape distortions (strains) and orientation factors. Similar RIF descriptions have been previously used for pattern recognition and image processing [4,5]. When fully coupled with the SOME approach, the mapping here would become a unitary basis transformation so that the derived shape factors can be quantitatively related to strains.

Examples of using these RIF basis functions to classify the deformation geometries observed in Molecular Dynamics (MD) simulations of Cu and Ta under strong compression will be shown. The expansions are carried out to fourth order, which is what is required to distinguish between crystal structures. The resulting functionals allow different types of defect structures and deformations to be readily identified, along with the pathways of the deformation processes. The analysis can then be extended to vector quantities (velocities, forces) so that the analogous momentum and stress functions functionals can be defined, leading to a thermodynamically consistent coarse-graining procedure.[1] It can also be extended to tensors, such as the crystal orientation matrices used in finite element simulations of polycrystalline materials. The gradients and higher order derivatives of these functions can then used to identify and characterize the grain boundaries and higher order junctions.

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In-situ Neutron Measurement and Modeling of Martensitic Phase Transformation

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A martensitic phase transformation model is proposed and implemented in a polycrystal plasticity code to describe mechanical response of transformation induced plasticity (TRIP) steel. The transformed martensite domains are introduced as new grains and included in the homogenized effective medium. The stress induced by the martensitic phase transformation strain is accounted for. The phase transformation model is implemented into the framework of an elastic-visco-plastic self-consistent (EVPSC) model for polycrystalline materials. The new model is evaluated by comparing simulations of mechanical response, volume fraction evolution, texture evolution, and internal stress evolution to in-situ neutron diffraction measurements of an austenitic stainless steel.

Smart use of Density Functional Theory calculations to drive Newtonian dynamics

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We present a method for adaptively creating and sampling a database of density functional calculations in order to simulate large, complex atomistic systems at finite temperatures. The database consists of configurational/cluster-to-force maps and has a metric property via the Kabsch algorithm which we exploit in structuring the database for efficiency and accuracy. Details of the formulation including the correlation between local configuration size and force accuracy, will be discussed, as well as a number of practical applications of the method.

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Structural phase transformations in solids - Atomistic insight on mechanisms and interface properties

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Atomistic modelling of the dynamics of phase transformations is a particularly challenging task. If the mechanism of the phase transformation is governed by so-called rare events then the time scale of interest will reach far beyond the capabilities of regular molecular dynamics simulations.

The atomistic rearrangements during solid-solid phase transformations in bulk systems involve massive structural changes including concerted multi-atom processes. The interface between two structurally different phases leads to a complex energy landscape that needs to be explored during the dynamical evolution of the interface. Here, we employ an adaptive kinetic Monte Carlo approach to investigate such processes at the interface between cubic and topologically close-packed phases in transition metals. In particular we investigate the transformation between BCC and A15 in molybdenum. During the dynamical simulations a finite, disordered interface region evolves to compensate the structural mismatch between the two crystal phases. This disordered interface region makes the identification of a single transformation mechanism difficult. Still, from our simulations we extract a layer transformation time which we relate to an effective barrier for the transformation mechanism and discuss the corresponding atomistic processes that we find along the transformation path.

Three-dimensional iso-geometric solutions to Toupin's gradient elasticity theory at finite strains and its application to study of dislocation cores and defects

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We present, to the best of our knowledge, the first complete three-dimensional solutions to a broad range of boundary value problems for a general theory of finite strain gradient elasticity. We have chosen for our work, Toupin's theory [Arch. Rat. Mech. Anal., 11(1), 385-414, 1962]– one of the more general formulations of strain gradient elasticity. Our framework has three crucial ingredients: The first is iso-geometric analysis [Hughes et al., Comp. Meth. App. Mech. Engrg., 194(39-41], 4135-4195, 2005), which we have adopted for its straightforward and robust representation of C1-continuity. The second is a weak treatment of the higher-order Dirichlet boundary conditions in the formulation, which control the development of strain gradients in the solution. The third ingredient is algorithmic (automatic) differentiation, which eliminates the need for linearization "by hand" of the rather complicated geometric and material nonlinearities in gradient elasticity at finite strains. We present a number of numerical solutions to demonstrate that the framework is applicable to arbitrary boundary value problems in three dimensions. We discuss size effects, the role of higher-order boundary conditions, and perhaps most importantly, the application of the framework to resolve elastic fields around crack tips and dislocation cores.

A concurrent atomistic-continuum study of sequential slip-transfer reactions for dislocation pile-ups at grain boundaries

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Grain boundaries (GBs) play an important role in determining bulk mechanical properties of polycrystals such as strength, ductility, and resistance to fatigue and fracture [1]. In particular, slip transfer reactions with GBs are complex; dislocations can be reflected, absorbed or desorbed at the interface, and/or transmitted directly, in addition to the possibility of shear-induced GB migration. However, modeling of interface impingement of dislocation pile-ups at grain boundaries has been well beyond the reach of most modeling techniques that seek to resolve atomic level structure during interface reactions due to the accompanying long range stress fields of the pileup, combined with other 3D features of interface structure and mixed dislocation character. In this work, concurrent atomistic-continuum (CAC) simulations [2] are performed to study sequential edge or screw dislocation impingement from a given pile-up on a coherent twin boundary, a $\Sigma 3$ (112) incoherent twin boundary, and a $\Sigma 11$ symmetric tilt grain boundary in Cu and Al. Results elucidate the role of specific GB structures and dislocation character in interface absorption-desorption reactions, including evolution of the structure of the interface in the process.

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