Dislocation-induced elastic distortion fields in deformed FCC crystals: Discrete dislocation dynamics simulations and experimental measurements

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The statistical characteristics of dislocation-induced elastic distortion fields in deformed FCC crystals are investigated both experimentally and theoretically. Discrete dislocation realizations are generated by the discrete dislocation dynamics method and the induced elastic distortion fields are computed by solving the corresponding boundary value problem. Moreover, sample three-dimensional X-ray measurements for the lattice misorientation are also presented to address the corresponding statistical features and to highlight the possibility to conduct a comparison between experiments and dislocation dynamics simulations.

The current analysis addresses critical issues related to the similarities and differences, in terms of the spatial characteristics, between the elastic strain and lattice rotation fields induced by the same dislocation structure. Moreover, the significance of the elastic strain field contribution to the dislocation density tensor, which is usually considered insignificant during the experimental detection of the dislocation density tensor, is also investigated quantitatively. Finally, we present a preliminary comparison between the elastic distortion fields computed based on discrete dislocation simulations and those measured experimentally through 3D X-ray microscopy.

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Metal-rich Ceramic Phase Stability and Microstructures in Group IV and V Carbides and Nitrides

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Phase stability and phase transformation pathways are critical in determining the morphology of a material's microstructure. For example, in the group V carbides and group IV nitrides, similar metal-rich crystallographic phases are observed between the two systems. Yet the morphology of these phases in the microstructure varies. These microstructures include equiaxed grains of single phases, equiaxed grains with a crisscross pattern of laths, or acicular grains with parallel laths of different phases along the major axis of the grain. In this talk, we investigate the inter-relationship between material microstructure and phase stability in the transition metal carbides and nitrides using experimental characterization of diffusion couples coupled with electronic structure density functional theory (DFT). The combination of these two tools provides unique insight into the interrelationships between equilibrium stability and meta-stability for each specific phase observed in the diffusion couples. Using DFT, the energy of formation for the vacancy ordered rock-salt carbide variants (such as Me_6C_5) and stacking fault variants (such as Me_4C_3 and Me_3C_2) have been investigated. For example, the stability of the Ta_4C_3 or zeta phase has been in question for some time and we now demonstrate that this is because the zeta phase as well as the eta phase (Ta_3C_2) are metastable and likely only exist if the vacancy ordered Me_6C_5 phase cannot form. In addition, the energy of formation for vacancies in the group V carbides reveal why the vacancy ordering Me_6C_5 phase is readily present in some group V carbides and not others. The carbide computational results for the metal rich carbide phases are compared to their equivalent crystallographic structures in the metal-rich nitrides, e.g. Me_4N_3 and Me_3N_2 phases, which have been found to be thermodynamically stable. These computational results provide insights into why certain metal-rich ceramic phases are seen to coarsen within the experimentally observed microstructures. Collectively, the comparison of the computational and experimental findings provides new insight into why specific phases form and its consequences on the morphologies observed within these carbide and nitride microstructures.

Computational multiscale modeling and experimental characterization of martensitic transformations in CoNiAl alloys

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The concept of utilizing ferromagnetic shape memory alloys as embedded sensory particles in aluminum alloys for real time damage detection is discussed. The modeling effort employs molecular dynamics and Monte Carlo atomistic simulations together with finite element modeling at the particle level with developed shape memory alloy constitutive models. The atomistic simulations are performed with a recently developed embedded-atom interatomic potential to study the effect of chemical composition and uniaxial mechanical stresses on the martensitic phase transformation in CoNiAl alloys. The transformation is analogous to the martensitic transformation in Ni-rich NiAl alloys. The martensitic phase has a tetragonal crystal structure and can contain multiple twins arranged in domains of different orientations in a crystal. The predicted martensitic transformations are compared to experimental data obtained from CoNiAl arc-melted buttons of various compositions. Specimens were machined from these buttons, solution-treated and quenched to lock in the shape-memory behavior, and then the martensitic transformation was characterized using differential scanning calorimetry and electron microscopy. The simulation model shows similarities, but also some differences with the experimental data. The temperature and the hysteresis of the transition in the simulation model tend to be higher than the experimental values and are shown to depend strongly on the configurational entropy of the system, which is estimated by using grand-canonical Monte Carlo simulations. The simulation model also indicates a decrease in the transition temperature with increase in the Co concentration, which is in agreement with the experimental data. The technology of embedded sensory particles will serve as the key element in an autonomous structural health monitoring system that will constantly monitor for damage initiation in service, which will enable quick detection of unforeseen damage initiation in real-time and during on-ground inspections.

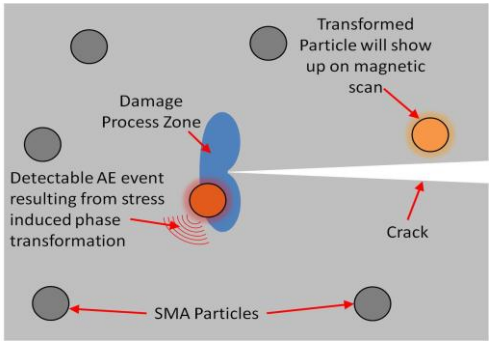

Figure 1: Embedded sensory particles, which undergo a detectable phase transformation in the presence of a crack.

Stagnation of microstructure features in simulated grain growth

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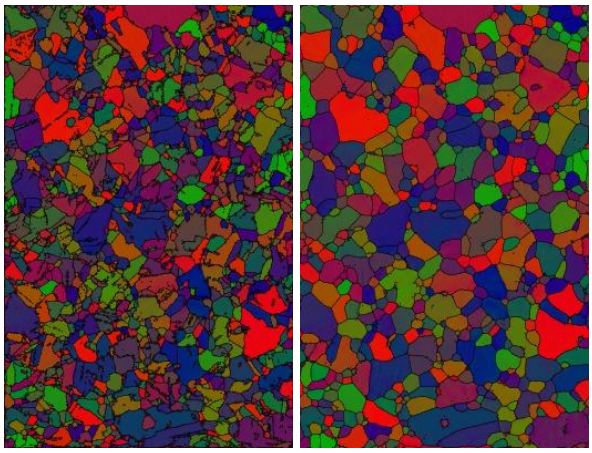
The mechanical properties of polycrystalline materials depend on microstructure properties such as grain size, texture, grain boundary character distribution (GBCD) as well as higher order correlations in the topological networks [1]. Coarsening of these microstructures through thermal treatment can vary depending on the anisotropy of the material and the network of special and random boundaries. Owing to the properties of the material being directly related to the microstructure, it is important that simulation methods agree with experimental results on a statistical and phenomenological level.

A new approach to the traditional 2D Potts model will be introduced which is combined with a grain boundary energy function [2] to study anisotropic grain growth systems. This method relieves several problems inherent with meshed simulations. We apply this approach to experimentally obtained 2D EBSD data and synchrotron-generated 3D HEDM data as inputs. Comparison of microstructure energy evolution is performed and stability of microstructure features (boundaries, triple junctions) between experiment and simulation performed. This type of validation allows us to analyze the dynamics of boundaries and triple junctions of purely simulated microstructures. Chains of triple junctions that promote growth (and those that hinder it) will be studied. These results can help to guide experimental efforts in searching for salient features in measured microstructures and reliably predict its evolution.



(a) (b)

Figure 1: Simulated annealing (b) of a grain boundary engineered Cu specimen obtained experimentally via EBSD (a)

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Massively Parallel Cellular Automata Algorithms for the Simulation of Primary Recrystallization

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Primary recrystallization is a softening mechanism used during industrial annealing in order to regain formability after forming operations and to tailor the final properties of metallic materials. Microstructural evolution along this process is basically determined by grain boundary motion and its interaction with various microstructural defects such as dislocations and particles. This interaction however, occurs atomistically in a complex manner. Owing to this complexity, the development of cost-efficient and sustainable annealing treatments can particularly benefit from 3D computer modelling.

In this regard, classical mesoscopic modelling approaches, such as cellular automata, are advantageous because they combine accurate spatial representation of microstructural features with real-time scaling, enabling a direct comparison with experimental data. Nevertheless, the limitation of cellular automata models is their computational efficiency. In this contribution, two fundamentally different 3D cellular automata models for recrystallization are presented and contrasted. These models were designed and optimized for their execution in parallel computing architectures.

The first model is based on a classical 3D domain decomposition scheme to evolve accurately and efficiently large microstructures. As expected from such approach, this model is computationally constrained by sub-domain communication. To overcome this limitation in the second approach, large simulations domains are partitioned and executed as separate entities, whose evolution is corrected statistically by the introduction of impingement on a local level. Experimental findings in an Al-Fe-Si alloy were used to test the accuracy of the models.

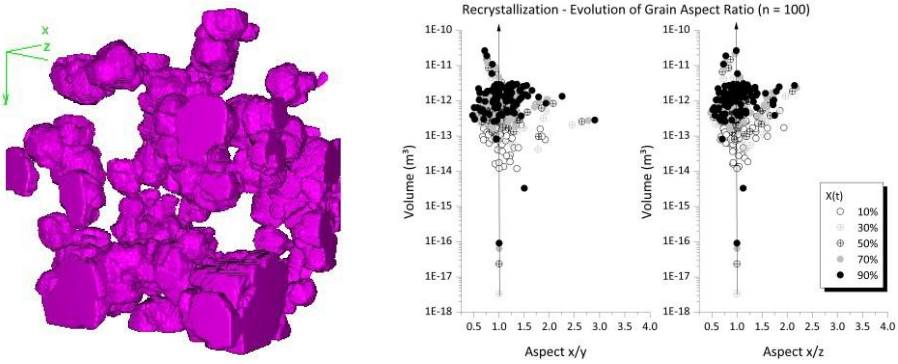

Figure 1: Visualization of the recrystallization front after 20% volume transformation (to the left) and statistics of grain volume and shape at advanced stages of growth (to the right).

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Validating Phase Field Models using Microstructural Experimental Data

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The phase field method has emerged as a powerful tool to model microstructure evolution due to its flexibility. In particular, Idaho National Laboratory's MOOSE framework is making it simpler to conduct 3D multiphysics phase field simulations of the coevolution of microstructure and properties. However, as phase field simulations are more widely used to provide insight on material behavior, it becomes increasingly important to validate these models against experimental data. While some validation can be obtained using homogenized information about the microstructure, such as an average grain size or phase concentration, the most valuable comparisons come from 2D and 3D microstructural characterization across time. New experimental techniques, including nondestructive 3D characterization and in situ microscopy, are providing exciting opportunities for phase field model validation. However, best practices for such validation are still being determined. In this presentation, we will discuss work currently underway at Idaho National Laboratory to directly compare 3D phase field simulation results to data obtained using state-of-the-art experimental techniques. These efforts include attempts to directly reconstruct experimental microstructures as simulation initial conditions and directly compare to the experimental evolution as well as comparisons between similar microstructures.

Understanding deformation mechanisms of a dense hydrous magnesium silicate (Phase A)

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Water plays important roles within the upper mantle of the Earth. It promotes partial melting and magma formation, phase transformation kinetics, and affects the mantle dynamics. Dense hydrous magnesium silicates (DHMS), such as Phase A [$Mg_7Si_2O_8(OH)_6$], are good candidates for water reservoirs in the mantle. Because of Phase A's stability at relatively low pressures and high water contents (>11 wt%), it is the first product of the breakdown of antigorite, which makes it particularly interesting as a possible carrier of water in subduction zones. The importance of these hydrous phases is not restricted to water storage. Indeed, at greater depths, the knowledge of the rheological properties of hydrous phases is also important for a better understanding of the dynamics of subduction.

First, Mussi *et al.* [1] have performed an experimental study of the deformation mechanisms of Phase A at 673°K and 973°K at 11 GPa. They have observed dislocation activity in basal, prismatic and pyramidal planes, with dissociation of dislocations in the basal and pyramidal planes. To complete these studies, we modelled dislocation core structures in this mineral. In this study, we focus on the core structures of dislocations with $\frac{1}{3}[2\bar{1}\bar{1}0]$, $\frac{1}{3}[01\bar{1}0]$ and [0001] Burgers vectors. We have first investigated the structural and elastic properties of Phase A at high pressure based on first-principles calculations (or DFT). To understand how the structure of Phase A can be sheared, generalized stacking fault energies (or γ-surfaces) are calculated for the basal and prismatic planes, obtained with accurate DFT calculations. We found several energy minima in the basal plane and in both types of prismatic planes, suggesting possible dislocation dissociations in these planes. The core structures of screw and edge dislocations have been calculated using the Peierls-Nabarro-Galerkin method [2] involving γ-surfaces as an input. These calculations confirm the dissociation of dislocations for all Burgers vectors. Finally, we apply simple shear on our model to obtain the Peierls stress in each plane, in order to determine the easiest slip systems for this mineral.

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Recent progresses on the characterization of crystal plasticity behavior of nuclear structural materials

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The FP7 PERFORM60 European project [1,2] aims at developing and validating multi-scale models to predict the behavior of reactor pressure vessel steels (tempered bainitic steel) and of in-core materials (made of austenitic steels) for which crystal plasticity laws are to be validated. Crystal plasticity finite element calculations are conducted to reproduce the kinematic fields (displacement and strain) observed at the surface of polycrystalline aggregates during in-situ SEM tensile experiments [3,4]. The observed differences between calculations and experiments are used to optimize crystal plasticity law parameters using a finite element updating procedure, or to compare without parameter optimization different constitutive laws with commonly used parameters validated using only the material effective (macroscopic) behavior. Some recent key results include the introduction of a specific cost function used for the identification of crystal plasticity parameters, a study of the well-posedness of the identification inverse problem depending on the considered set of unknown constitutive parameters, the investigation of strain gradient plasticity effects in the microstructural deformation of austenitic steel aggregates, and the assessment of temperature variation on the reactor pressure vessel steel response in term of crystal plasticity mechanisms and strain distributions.

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