

# Comparison of 3D phase field and Peierls-Nabarro modeling of dislocation dissociation, glide and twinning in fcc systems

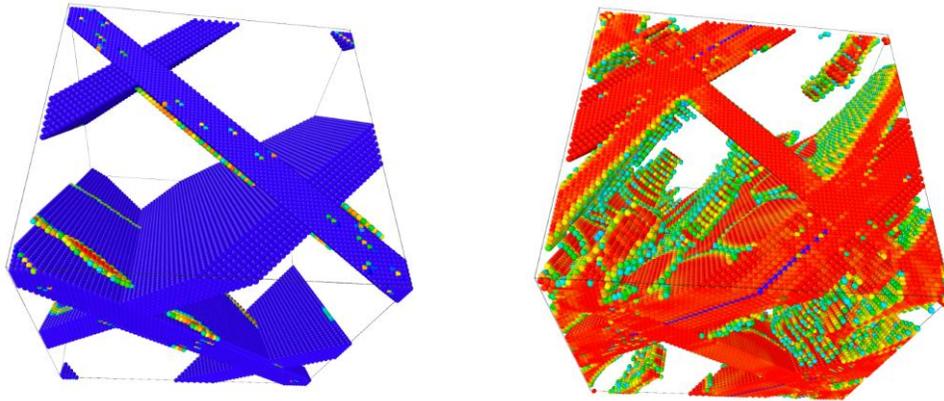
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The purpose of this work is the development and comparison of two approaches to the modeling of dislocation dissociation, glide and twinning in fcc systems. The first of these is a phase-field (PF) approach (e.g., [1-2]), while the second is a dynamic generalization of existing static Peierls-Nabarro (PN) models (e.g., [3]). In contrast to [1,2], the current PF approach [4] is based on two phase-fields per glide plane. This is analogous to and consistent with the current PN model based on two disregistry fields per glide plane [5]. In both cases, the corresponding free energy model accounts in particular for the stacking fault (SF) energy of the material determined via *ab initio* means.

Considering periodic systems and employing Fourier methods, both models are applied in a comparative fashion. As an example application of the phase field approach, consider the loading of Al and Cu and corresponding microstructure development in Figure 1.



**Figure 1.** Phase field modeling of dislocation-based deformation in Al (left) and Cu (right) during uniaxial compression. Blue: ideal glide; red: SF/twin; green: dislocation line.

As shown, in case of Cu (right), loading results in the formation of multiple SF layers and twinning. On the other hand, in Al (left), the deformation is governed almost solely by ideal dislocation glide. Analogous results from the PN model and additional examples will be discussed.

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[2] A. Hunter et al., *Mod. Mat. Sci. Eng.* 21, 025015 (2013).

[3] Y. Xiang et al., *Acta Mat.* 56, 1447 (2008).

[4] J. Mianroodi, B. Svendsen, submitted (2014).

[5] J. Mianroodi, B. Svendsen, in preparation (2014).

## Defect Nucleation in Crystals

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Transition state theory is of interest because it allows the prediction of rate and temperature effects upon defect initiation in crystals. More importantly, it is valid for arbitrary loading rates, in particular loading rates achievable in the laboratory and suffers from none of the limitations in this regard inherent in molecular dynamics simulations. We describe here a recently-developed transition state theory model for the initiation of crystal defects. This model makes use of a previous model for zero-temperature defect initiation in combination with multi-dimensional harmonic transition state theory. Harmonic transition state theory requires an accurate determination of the saddle point activation energy. The present model presents a relatively simple means of determining this quantity that does not require an *a priori* assumption as to the nature of the nucleated defect. Moreover various other quantities required by transition state theory are calculated in a rather natural fashion. We apply the model to several examples of defect initiation. The first is that of triaxial stretching of an fcc crystal, for which the relevant defect is spherical cavitation. The other, considerably more complicated, example is that of nanoindentation on the (001) surface of a gold crystal. Here the initial defect is a dislocation that nucleates at five atomic planes beneath the indenter. In both cases, excellent agreement is observed between the model predictions and the results of independent molecular dynamics simulations over a range of loading rates. The predictions of the model may also be compared to available experimental data, and we comment upon efforts in this direction.

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## **Atomistic Modeling at Experimental Strain Rates: Plasticity in Amorphous Solids**

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We present a new computational approach that couples a recently developed potential energy surface exploration technique with mechanical deformation to study the deformation of atomistic systems at strain rates that are much slower, i.e. experimentally-relevant, as compared to classical molecular dynamics simulations. Examples of the new insights into the plasticity of amorphous solids that are obtained using this new approach will be given, with a particular emphasis on how the shear transformation zone characteristics, which are the amorphous analog to dislocations in crystalline solids, undergo a transition that is strain-rate and temperature-dependent, and how surface effects impact the shear transformation zone characteristics.

# **Spectral finite-element based methodology for large scale electronic-structure calculations using density functional theory**

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Material defects are ubiquitous. They occur in very small concentrations, yet have profound influence on macroscopic properties of materials. The development of a mathematical model which accurately describes such defects presents a unique challenge since such a model must incorporate physics at multiple length scales. This involves resolving the defect core at quantum mechanical scale as well as the long range elastic fields away from the defect. One of the most popular electronic structure theories which can be used to achieve the above goal is Kohn-Sham density functional theory (DFT). However, the complexity of these calculations restricts the computations to sample sizes of the order of a few hundred atoms. To extend the DFT calculations to realistic sample sizes that can accurately capture the long ranged fields generated by defects, an efficient approach that can seamlessly bridge quantum mechanical and continuum scales using single physics (DFT) is highly desirable. The development of real-space electronic structure calculations using a finite-element discretization of DFT is an important step in the above direction. The ability to handle complex geometries, arbitrary boundary conditions and more importantly the coarse-graining nature of basis sets makes finite-elements highly desirable especially in problems involving defects.

Following this line of thought, we first develop an efficient real-space approach to perform electronic structure calculations using an adaptive higher-order spectral finite-element discretization. The key ideas involved are to use an a-priori mesh adaption technique and subsequently employ Chebyshev acceleration strategies in conjunction with special quadrature rules to reduce the computational cost in solving the DFT problem. Our studies show that staggering computational savings of the order of 1000-fold can be realized by using sixth-order finite-element discretization, in comparison to linear finite-elements and compares favorably with other widely used basis-sets. Next, we address the problem of computational complexity involved in solving the DFT problem which scales cubically with number of atoms in the system. To this end, we formulate a sub-quadratic scaling subspace projection technique to conduct large-scale electronic structure calculations using DFT. The proposed methodology takes advantage of the representation of Kohn-Sham Hamiltonian in Lowden orthonormalized finite-element basis constructed using spectral finite-elements in conjunction with Gauss-Lobatto-Legendre quadrature rules. Further, the proposed approach treats both metallic and insulating systems on the same footing by projecting the Kohn-Sham Hamiltonian in a non-orthogonal localized basis constructed from the Chebyshev filtered subspace. We further demonstrate the scaling, efficiency and accuracy of the proposed algorithm on full three dimensional systems involving metallic aluminium nano-clusters up to 3430 atoms and insulating alkane chains up to 8000 atoms using pseudopotential calculations. We also demonstrate the proposed algorithm on all-electron calculations up to 5000 electrons.

# Enabling strain hardening modeling via efficient time-integrators in dislocation dynamics simulations

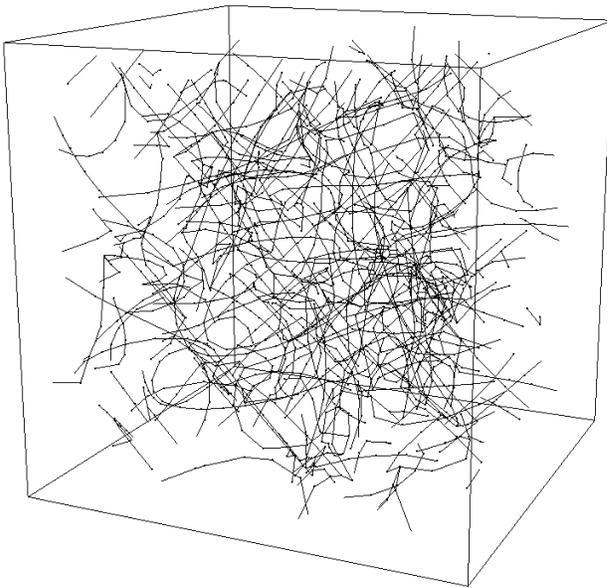
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Dislocation dynamics (DD) provides a systematic framework for the simulation of metal plasticity and strain hardening. DD models follow the motion of a network of dislocation lines discretized into segments and connected by a set of nodes, which are the degrees of freedom of the system [1] (see figure 1). In order for DD simulations to provide insight into the strain hardening process, they must be able to reach plastic strains on the order of experimental values (>10%). Despite the development of massively parallel algorithms and codes, this level of plastic strain has been out of reach thus far.

A major cause of this computational gap is inefficient time integration. In order to remove this limitation, we have developed advanced time integration algorithms for 3D DD simulations [2]. We show that DD simulations contain unstable modes, which force explicit time-integrators to take very small time steps, while implicit time-integrators offer much better performance. Unfortunately, there also exist unstable and highly non-linear modes that require a very small time step even when an implicit integrator is used. A significant speed-up is then achieved by the sub-cycling algorithm, in which nodes involved in the unstable and non-linear modes are time-integrated with small time steps while the remaining nodes are integrated with larger time steps. The performance of these advanced algorithms in large-scale DD simulations is evaluated.



**Figure 1:** A snapshot of a typical DD simulation of an FCC metal subjected to uniaxial loading.

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## **A numerical and computational framework for hierarchical multi-scale simulations on large scale computers**

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Over the last few decades, multi-scale modeling (MSM) has become a dominant paradigm in materials modeling and simulation. The practical impact of MSM depends, to a great extent, on the ability to utilize modern computing platforms. However, since there are no general numerical and computational frameworks for MSM the vast majority of multi-scale material models are developed on a case-by-case basis. Therefore, we seek to formulate an adaptive numerical and computational framework for MSM on large scale computers. We do not plan to develop a specific method for MSM simulations, but instead, aim to develop a broad and flexible numerical framework for designing and developing such simulations. Our focus is primarily on new scalable numerical algorithms applicable in a wide range of MSM applications. These algorithms fall mostly into the the three areas: i) scalable data transfer between parallel applications, ii) adaptive strategies for MSM, and iii) data analytics for MSM. We present a formulation of our numerical and computational MSM framework. Subsequently, we describe development of a new two-scale multi-scale model of composites utilizing our framework.

## Acceleration of microscale polycrystal plasticity models using GPUs

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We present a framework for accelerating the computation of microscale polycrystal plasticity models using GPUs, for use with black-box commercial Finite Element (FE) software.

There is growing recognition within the mechanics community of the need to incorporate microstructure evolution into macroscale engineering simulations. However, many microscale models are computationally prohibitive for macroscale finite element simulations of thermo-mechanical forming processes, and other engineering applications.

We have previously demonstrated that Taylor-type plasticity models can be used to accurately predict the microscale texture evolution of cubic materials, and that this model is amenable to a computational speed-up exceeding 100x when using a spectral representation. We presently demonstrate that such computations are ideally suited to GPUs affording additional orders-of-magnitude speed-up, and we devise a scalable computational framework highly suitable for parallelized implementations.

In the present work, we have developed an implementation of the Spectral Taylor model on GPUs using nVidia's CUDA Fortran, constituting a standalone computational application/service. We have also developed a simple, light-weight C-scheduler using Unix sockets to pass data to and from the app, and show how this can be trivially called from within the commercial finite element package Abaqus. As a case study, we have fit the model's plasticity parameters to experimental tension/compression data for a cubic polycrystalline metal, whose initial texture has been characterized via EBSD, and we show results from a macroscale simulation computed on a desktop workstation utilizing single- and dual-GPUs. Further, we show results from a distributed architecture computation, demonstrating how the same implementation can utilize non-local GPUs across a network with absolutely no modifications.

In addition to the accelerated computation of the microscale texture evolution, we emphasize the ability of the method to utilize non-local computational resources; further, we assert that the implementation is sufficiently abstract so as to be compatible with virtually any FEA package that permits user-defined material models, e.g. Sandia National Lab's SIERRA framework, with only trivial modifications.

## 3D phase field modeling for nanowire growth by vapor-liquid-solid mechanism

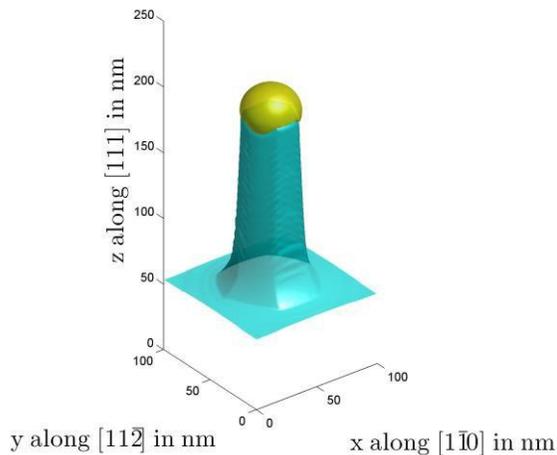
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Nanowire (NW) has promising applications in many fields such as integrated circuits, solar cells or solar cells, for its special electronic and optical properties [1]. Vapor-liquid-solid (VLS) process is a widely used NW growth method; however, many fundamental questions including the nucleation failure and growths kinking are still not fully understood. The answers to these questions are important for better control of the NW orientation, yield and quality required for industry applications. Therefore, a 3D computational model studying VLS mechanism that can both capture the realistic NW morphology and reach the experimental time scale is critically needed.



**Figure 1:** simulation snapshot shows the NW growth along [111] orientation.

We developed a 3D multi-phase field model for VLS NW growth [2]. The model captures the equilibrium catalyst droplet shape on the substrate prior to NW growth. For the NW growth process, the model captures the NW tapering and sidewall facets in good agreement with experimental observations. The model predicts the steady-state NW growth velocity is a linear function of the vapor chemical potential and the inverse of catalyst diameter, providing a confirmation of the Gibbs-Thomson effect in nanowire growth [3]. The model is applied to study the instability of the catalyst droplet on top of the NW, which is important for understanding the onset of growth kinking.

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