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Phase field approach to dislocation evolution at large strains: Computational aspects

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ABSTRACT

Computational aspects of the phase field simulations of dislocation nucleation and evolution are addressed. The complete system of equations for the coupled phase field approach to dislocation nucleation and evolution and nonlinear mechanics for large strains is formulated. Analytical solutions for a stationary and propagating single dislocation, dislocation velocity, core energy, and core width are found. Dislocation parameters for nickel are identified based on existing molecular dynamics simulations. In contrast to all previous efforts that are based on the spectral approach, finite element method (FEM) is utilized, which allowed us to treat large strain problems and non-periodic boundary conditions. The single dislocation order parameter profile and the stationary distance between two neighboring dislocations at a semicoherent sharp austenite–martensite interface are in perfect agreement with analytical expressions. The main focus is on proving that the new points of the developed theory can be confirmed in simulations, including possibility of obtaining the desired dislocation height for aligned and inclined dislocations, eliminating spurious stresses, resolving dislocation cores and interaction between cores of different dislocations. Mesh independence of the solutions is demonstrated and the effect of approximating finite element polynomials is analyzed, exhibiting possibility of significant numerical errors when special care is not taken of. Problems of nucleation and evolution of multiple dislocations along the single and multiple slip systems near martensitic lath, and along the sharp austenite –martensite interface, the activity of dislocations with two different orientations in a nanograined material under shear and pressure, and the interaction between two intersecting dislocation systems are studied. Surface-modified partial dislocation was revealed. These problems represent the first step in the future study of interaction of phase transformation and dislocations.

1. Introduction

Dislocational plasticity has been widely studied using continuum theories, see the recent papers Cui et al. (2014); Engels et al. (2012); Fan et al. (2011); Huang et al. (2012); Li et al. (2014); Liu et al. (2011); Öztop et al. (2013); Xiong et al. (2014); Yanilkin et al. (2014). At the nanoscale, phase field theories for dislocations are broadly used for modeling plasticity (Hu and Chen, 2001, 2002; Hu et al., 2004; Hunter et al., 2011, 2010; Jin and Khachaturyan, 2001; Koslowski, 2007; Koslowski et al., 2002; Koslowski and Ortiz, 2004; Kundin et al., 2011; Lei and Koslowski, 2011; Rodney et al., 2003; Shen and Wang, 2004; Vorontsov et al., 2004; Wang et al., 2001a, 2001b, 2001c, 2003, Wang and Li, 2010). Quite sophisticated and physically interesting and important problems are solved, increasing our understanding of plasticity. It is surprising, however, that traditionally in computational mechanics studies on the accuracy and mesh-sensitivity of numerical solutions are almost absent. Thus, it is mentioned in Shen and Wang (2004) that in order to obtain a continuous profile of the order parameter for a dislocation within a core, the grid size should be 0.1 of the interplanar distance. However, such a fine grid has practically never been used in simulations. In Hu et al. (2004) the accuracy of the stress distribution due to a single dislocation and ways to avoid significant oscillations were considered, with a grid size which was 10 times larger than the Burgers vector. Thus, there was no possibility to resolve the dislocation core and stresses were away from the dislocation core, i.e., long-range stresses. In the most practical, larger-scale simulations (Jin and Khachaturyan, 2001; Wang et al., 2001b, 2003), the grid size is even 100 times of the interplanar distance.

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Mesh dependence of the solutions was not studied because it was assumed in Hu et al. (2004); Jin and Khachaturyan (2001); Shen and Wang (2004); Wang et al. (2001b, 2003) that the dislocation height is equal to the mesh size, i.e., the dislocation height is mesh-dependent and non-objective by definition. As it was discussed in Levitas and Javanbakht (2012, 2015), this assumption is made because the dislocation height was not defined by a theory and the system of equations is ill-posed. Traditionally, such formulations are inadmissible in computational mechanics. For similar problems on shear band localization in classical plasticity, a huge literature exists and the problem is regularized using a viscoplastic (e.g., Perzyna (1994)) or (in most cases) a gradient-type regularization (see, e.g., Dietsche et al. (1993); Pamin and De Borst (1995)). This led, in particular, to a significant progress in gradient plasticity. Similar efforts are lacking in the phase field simulations of dislocations as well. As we will show below, dislocations are not localized within a single intergrid band, rather they produce bands with a height of 1 to 10 and more mesh sizes. This can be interpreted as 1 to 10 dislocations in the neighboring parallel planes, but this is unrealistic. Even if the dislocation was localized within one finite element, the interface Σ with the normal $\boldsymbol{n}$ between the dislocation band and the rest of the crystal has theoretically zero width. As we will demonstrate below, this leads to high oscillating internal shear stresses at the interface Σ which have two opposite effects. First, the huge artificial stresses can exceed the critical stress for dislocations and lead to an artificial nucleation of new dislocations. Second, these artificial stresses generate an artificial elastic energy at the interface, which suppresses dislocation motion. Such stresses and a way to suppress them have not been studied yet. Also, there is no description in the literature on how to handle dislocations inclined with respect to the grid.

When using a regular grid, the localization of a dislocation band within one intergrid space leads to a small number of points to resolve the dislocation core profile along the slip direction, which results to wrong values for the width and the energy. In addition, a rough discretization leads to creating an artificial athermal threshold Hu et al. (2004), which may arrest dislocations.

Another source of inaccuracy is related to the fact that when the Burgers vector is linearly dependent on the order parameters η (like in Hu and Chen (2001 2002); Hu et al. (2004); Hunter et al. (2011); 2010); Jin and Khachaturyan (2001); Koslowski (2007); Koslowski et al. (2002); Koslowski and Ortiz (2004); Kundin et al. (2011); Lei and Koslowski (2011); Rodney et al. (2003); Shen and Wang (2004); Vorontsov et al. (2004); Wang et al. (2001a, 2001b, 2001c, 2003); Wang and Li (2010)), the thermodynamically equilibrium value of η, and consequently the equilibrium Burgers vector, depend on the stress tensor $\boldsymbol{\sigma}$. This was found in Levitas et al. (2003) analytically and then studied in Hu et al. (2004) numerically. It was demonstrated in Hu et al. (2004) that the stress-dependent Burgers vector changes the stress field of a dislocation and consequently its velocity. Nonlinear dependencies for the Burgers vector, which lead to constant, stress-independent equilibrium Burgers vector have been suggested in Hu et al. (2004); Levitas and Javanbakht (2015); Levitas et al. (2003). However, as it was shown in Levitas and Javanbakht (2015), the nonlinear dependence in Hu et al. (2004) leads to an unrealistic equilibrium stress - order parameter curve, which requires infinite stresses for the lattice instability (theoretical strength). In general, the local equilibrium stress-strain curve and the theoretical shear strength were not analyzed for the previous models, until it was done in Levitas and Javanbakht (2015); Levitas et al. (2003). Note that similar analysis of the local equilibrium stress-strain curve for martensitic phase transformations has been done in Levitas and Preston (2002a, 2002b).

All previous phase field simulations (e.g., in Hu et al. (2004); Jin and Khachaturyan (2001); Koslowski et al. (2002); Koslowski and Ortiz (2004); Shen and Wang (2004); Wang et al. (2001b, 2003)); Wang and Li (2010)) were based on small strain (i.e., < 0.1) theory, which allowed one to use effective spectral methods for the problem solution combined with Khachaturyan–Shatalov microelasticity theory. This also implied periodic boundary conditions. At the same time, local shear strain for n dislocations is huge and is of the order of magnitude of n.

In the papers Levitas and Javanbakht (2012, 2015), the phase field equations for dislocation nucleation and evolution at the nanoscale were derived from thermodynamics laws for large strains and were simplified for small strains as well. The Ginzburg–Landau equations are obtained as the linear kinetic relations between the rate of change of the order parameters and the conjugate thermodynamic driving forces. Several main shortcomings of the previous phase field studies have been resolved. In particular, large strain kinematics is introduced and it is done in a way consistent with phenomenological crystal plasticity. Also, expression for the Helmholtz free energy is advanced in the following directions:

(a) it reproduces the desired, mesh-independent height of dislocation bands for any slip system orientation and prevents dislocation widening;
(b) it excludes the localization of dislocation within a band of a smaller height than the prescribed one but does not produce artificial interface energy;
(c) it penalizes the interaction of different dislocations at the same point;
(d) it allows us to generate desired lattice instability conditions and a stress—order parameter curve, as well as to obtain stress-independent equilibrium Burgers vector and to avoid artificial dissipation during elastic deformation.

Non-periodic boundary conditions for dislocations are introduced, which include the change of the surface energy due to the exit of dislocations from the crystal.

All the above theoretical results make it possible to significantly advance the computational mechanics aspect and the strictness and the accuracy of the simulation of dislocation behavior. This is the main goal of the current paper. The main focus is on proving that the new points of the developed theory can be confirmed in simulations, including the possibility of obtaining the desired dislocation height for aligned and inclined dislocations, eliminating spurious stresses, resolving dislocation cores and the interaction between cores of different dislocations.

First, analytical solutions for a stationary and propagating single dislocation, dislocation velocity, core energy, and core width are found. Dislocation parameters for nickel are identified based on the results of molecular dynamics simulations in Lee et al. (2011). They also include the effect of the gradient term along the dislocation height. In contrast to all previous efforts that utilize the spectral approach, FEM is applied, which allowed us to treat large strain problems and non-periodic boundary conditions. In particular, free external surface is considered, for which the boundary condition looks different than for phase transformations. The single dislocation order parameter profile and the stationary distance between two neighboring dislocations at a semicoherent sharp austenite–martensite interface are in perfect agreement with analytical expressions. Note that the last problem has a shear strain equal to 3, i.e., the large strain formulation is tested to some extend as well. For a system of multiple parallel dislocations, it is shown that one can indeed obtain an objective solution with the prescribed dislocation height and eliminate artificial stresses at the boundary between the dislocation band and the rest of the crystal or between different dislocation bands. For non-optimal meshes and types of finite elements, solutions may differ significantly from the objective (correct) ones, with different numbers of dislocations, averaged stresses, and huge spurious oscillating stresses between the dislocation band and the rest of the crystal or between different dislocation bands. For models without the prescribed dislocation height, the solution is strongly mesh-dependent, with