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Predicting structure and energy of dislocations and grain boundaries

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Abstract

A microscopic phase field (MPF) model is formulated to describe quantitatively the core structure and energy of dislocations using *ab initio* data as input. Based on phase field microelasticity theory implemented in the slip plane using Green's function to describe the long-range elastic interaction, the MPF model is a three-dimensional generalization of the Peierls model. Using the same generalized stacking fault energy as input, the core structure and energy predicted for straight dislocations by the MPF model show complete agreement with those predicted by the Peierls model. The ability of the MPF model to treat dislocations of arbitrary configurations is demonstrated by calculating the structure and energy of a twist grain boundary in aluminum. After discrete lattice sampling a la Nabarro, the grain boundary energy manifests Read–Shockley behavior for low-angle boundaries as well as deep cusps for high-angle special boundaries, indicating a "Peierls torque friction" effect for grain boundaries that has the same physical origin as the Peierls lattice friction for dislocation cores.

Keywords: Core structure; Defect; Aluminum; Peirels model; Phase field method

1. Introduction

Dislocations and grain boundaries (GBs) are fundamental structural defects that dictate the physical and mechanical properties of crystalline solids [1,2]. Defect engineering, where dislocation configurations and grain boundary characters are optimized to achieve specific properties or functionalities, relies on knowledge of the fundamental properties of these defects. Even after decades of research since the discovery of dislocations in the 1930s, predicting their basic properties (e.g. structure, energy and chemistry of a dislocation core) still poses a great challenge [3–13]. While *ab initio* calculations and MD simulations are powerful tools for studying GBs and dislocations, they are limited by the size scale (for example, the low-angle GBs studied in this paper have very large unit cells) and by the complexities of the interactions that they can handle, including chemical composition and timescale. For example, empirical interatomic potentials are typically hard stretched to handle more than two element types. *Ab initio* calculations, while not limited in the element types, are much more limited in size scale, and would also be hard pressed to describe finite-temperature behavior because of timescale limitations.

Because of these limitations, the most widely used methods today in studying dislocations are still based on continuum elasticity. There are two classes of approach to dislocations: the Volterra model [14] and the Peierls model [15] (see also Ref. [16] for a recent review). In the Volterra model, a dislocation is treated as a geometrical line singularity in a linear elastic continuum, so dealing

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with atomic displacements at the very core of the dislocation is avoided. As a result, the size (cut-off radius) and energy associated with a dislocation core are inputs rather than outputs of the model. Discrete dislocation (DD) simulations [17–24], which are mostly based on the Volterra framework, require the definition of the cut-off radius for dislocation cores and the rules for core–core reactions and junction formation. In the Peierls model, on the other hand, a dislocation core is treated by two competing energetic terms: a non-quadratic energy from materials residing in the slipped region, described by the generalized stacking fault (GSF) energy [25–28], which has non-convex parts, and a quadratic elastic energy from materials in the remaining crystal volume. The elastic energy term alone favors an infinitely extended dislocation core, while the inelastic non-convex energy term favors an infinitely contracted core. The interplay of the two yields an equilibrium core structure with a finite size and the associated core energy. The inelastic energy in the Peierls model is a much reduced (1-D [29] or 2-D [25]) section of a general potential energy surface defined in a $3N$-dimensional configurational space (where N is the total number of atoms). In principle, the critical information about core–core interactions required by the DD simulations can be obtained from the Peierls model. The calculation of the elastic energy in the Peierls model, however, employs a dislocation density infinite ribbon to infinite ribbon interaction kernel of $\log r$ type, which limits its applications to straight dislocations.

The phase field model for dislocations [30] employs the Khachaturyan–Shatalov (KS) microelasticity theory [31–33], implemented using the exact 3-D Green function, to describe the long-range elastic interaction. The volume element to volume element interaction kernel of $1/r^3$ type is more general than the previous $\log r$-type interaction kernel. For straight dislocations, these two integrals give exactly the same elastic energy. However, when the symmetry is broken in the dislocation line direction, the $\log r$ kernel no longer works, but the phase field energy functional continues to work as demonstrated [30,34].

However, because of the coarse-grained (10–100b, b as Burgers vector) nature of the method, there has been no rigorous treatment of dislocation cores in these approaches. The incorporation of the GSF energy into the phase field model [34,35] has made it possible to treat dislocation core structures at the sub-Burgers vector resolution, as in the Peierls model, but the predicted core structure by the phase field model [35] still does not converge exactly to the Peierls model. In this paper we formulate a new approach, called the microscopic phase field (MPF) model, taking full advantage of the KS microelasticity theory mentioned above, and show its equivalence to the Peierls model when describing straight dislocations. We then demonstrate the ability of the MPF model to treat more complex dislocation core configurations, such as those seen in GB dislocation networks. Being a 3-D generalization of the Peierls model, the MPF model offers a general quantitative means of predicting the defect size, energy and activation pathway associated with defect nucleation, as well as treating dislocation core–core interactions using *ab initio* electronic structure calculations as input.

In previous phase field dislocation models [30,34,35], the inelastic displacement or strain fields are defined and relaxed in the 3-D space. The local energy density in any volume element is composed of an elastic energy and a crystalline (or GSF) energy. Since, by definition, the crystalline energy reduces to the elastic energy at a small strain value, there is a possible overcounting in the total energy. The Peierls model, on the other hand, does not have this ambiguity since it treats the two energies in separate space: an atomic-layer thin slip plane, where the displacement is inelastic and is treated by a non-convex (the GSF) energy, and the remaining space as a linear elastic body fully described by the quadratic elastic energy. In the present model we formulate a new elasticity expression that, similar to the treatment in the Peierls model, confines the inelastic displacement strictly to the slip plane and resides the elastic energy in the two infinite half spaces. This, together with further removal of the gradient energy term, allows the MPF model to converge to the Peierls model.

The MPF model has a spatial resolution of dislocation core size, similar to the Peierls model. At such a length scale, as discussed earlier, the equilibrium core width is balanced by the elastic energy and the inelastic misfit energy. This is different from the mesoscale phase field dislocation models, where a conventional gradient energy is required to produce a smooth (though artificially wide, mesoscale size) dislocation core. However, a gradient term with distinct physical meaning could still be present at the microscopic scales. For example, a typical gradient form was shown in a continuum transition from a lattice Greens function formulation for Peierls dislocation [36]. Such a form was also found in the transition of a discrete spinodal decomposition model [37] to a continuum one [38] in phase transformation theory. More discussions may be found in Ref. [16].

2. Microscopic phase field dislocation model

In the Peierls model, a dislocation is described by a 1-D spatially continuous distribution of (inelastic) slip displacement traversing a dislocation core. The displacement, mostly local to the core, results in an atomic misfit energy to the crystal, due to local disregistry of atomic positions above and below the slip plane, and a long-range elastic energy. Such a picture can be generalized to a field description of strain field. This results in the basic order parameter in the MPF dislocation model, $\epsilon_{ij}(\mathbf{r})$, defined as an inelastic strain field with reference to a perfect crystal. It is expressed as

$$\epsilon_{ij}(\mathbf{r}) = \sum_{p=1}^{N} \epsilon_{ij}^{p} \eta_p(\mathbf{r}) \tag{1}$$

over all active slip systems, each characterized by a phase field η_p and an associated unit (slip type) strain tensor