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Electronic-structure study of an edge dislocation in Aluminum and the role of macroscopic deformations on its energetics

Mrinal Iyer, Balachandran Radhakrishnan, Vikram Gavini *

Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, USA

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ABSTRACT

We employed a real-space formulation of orbital-free density functional theory using finite-element basis to study the defect-core and energetics of an edge dislocation in Aluminum. Our study shows that the core-size of a perfect edge dislocation is around ten times the magnitude of the Burgers vector. This finding is contrary to the widely accepted notion that continuum descriptions of dislocation energetics are accurate beyond ~1–3 Burgers vector from the dislocation line. Consistent with prior electronic-structure studies, we find that the perfect edge dislocation dissociates into two Shockley partials with a partial separation distance of 12.8 Å. Interestingly, our study revealed a significant influence of macroscopic deformations on the core-energy of Shockley partials. We show that this dependence of the core-energy on macroscopic deformations results in an additional force on dislocations, beyond the Peach–Koehler force, that is proportional to strain gradients. Further, we demonstrate that this force from core-effects can be significant and can play an important role in governing the dislocation behavior in regions of inhomogeneous deformations.

1. Introduction

Dislocations are line defects in crystalline materials which play an important role in governing the deformation and failure mechanisms in solids. The energetics of dislocations and their interactions with other defects—solute atoms, precipitates, grain boundaries, surfaces and interfaces—significantly influence the mechanical properties of crystalline materials (cf. e.g. Hirth and Lothe, 1968; Meyers et al., 2006; Uchic et al., 2004; Trinkle and Woodward, 2005; Zhu et al., 2007; Gavini et al., 2007b; Leyson et al., 2010). For instance, the kinetic barriers to dislocation motion—dislocation glide and climb—and their dependence on crystallographic planes and directions govern ductility and creep in metals (Bulatov et al., 1995; Duesbery and Vitek, 1998; Lu et al., 2000; Kabir et al., 2010). Interaction of dislocations with vacancies, solute atoms and precipitates results in solid–solution strengthening/softening, precipitate hardening and aging in metals (Pollock and Argon, 1992; Lu and Kaxiras, 2002; Trinkle and Woodward, 2005; Yasi et al., 2010; Leyson et al., 2010). Further, dislocation interactions with grain boundaries and surfaces are responsible for the observed strengthening mechanisms like the Hall–Petch effect (Hansen, 2004), and enhanced yield strength in surface dominated nanostructures (Uchic et al., 2004; Greer and Nix, 2006).

The behavior of dislocations (nucleation, kinetics, evolution) in crystalline materials is governed by physics on multiple

* Corresponding author.
E-mail address: vikramg@umich.edu (V. Gavini).

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length-scales. In particular, a dislocation produces elastic fields that are long-ranged, and through these elastic fields interacts with other defects and external loads at macroscopic scales. On the other hand, the quantum-mechanical and atomistic scale interactions play an important role in governing the nucleation and kinetics of these defects. While atomistic scale interactions can significantly influence the behavior of dislocations, these are localized to a region around the dislocation line referred to as the dislocation-core. Thus, the energy of a dislocation is composed of the stored elastic energy ($E_{elastic}$), associated with the elastic fields outside the dislocation-core, and a core-energy (E_{core}) associated with quantum-mechanical and atomistic scale interactions inside the dislocation-core. Continuum theories based on elastic formulations have been widely used to study deformation and failure mechanisms mediated through dislocations (cf. e.g. Rice, 1992; Fleck et al., 1994; Nix and Gao, 1998; Ghoniem et al., 2000; Arsenlis and Parks, 2002), where the energetics of dislocations are solely determined by the elastic energy and the core-energy is often assumed to be an inconsequential constant. In order to overcome the inability of continuum theories to describe the dislocation-core, explicit atomistic calculations based on empirical interatomic potentials have also been employed to study deformation mechanisms mediated by dislocations (cf. e.g. Tadmor et al., 1996; Kelchner et al., 1998; Gumbsch and Gao, 1999; Li et al., 2002; Marian et al., 2004a,b), and have provided many useful insights. However, interatomic potentials, whose parameters are often fit to bulk properties, may not accurately describe the defect-core which is governed by the electronic-structure (cf. e.g. Gumbsch and Daw, 1991; Ismail-Beigi and Arias, 2000; Woodward et al., 2008).

Electronic-structure calculations using plane-wave implementations of density functional theory (DFT) have been employed to study the dislocation core-structure in a wide range of crystalline materials (cf. e.g. Ismail-Beigi and Arias, 2000; Blase et al., 2000; Frederiksen and Jacobsen, 2003; Woodward et al., 2008; Clouet et al., 2009) and the energetics of dislocation–solute interactions in metals with different crystallographic symmetries (Trinkle and Woodward, 2005; Yasi et al., 2010). As the displacement fields produced by isolated dislocations are not compatible with periodic boundary conditions, these calculations have either been restricted to artificial dipole and quadrapole configurations of dislocations or free-surfaces have been introduced to contain isolated dislocations. Recent efforts have also focused on the development of flexible boundary conditions by extending the lattice Green's function method to electronic-structure calculations (Trinkle, 2008). Flexible boundary conditions accurately account for the long-ranged elastic fields of an isolated dislocation (Woodward et al., 2008), however, the electronic-structure in these studies is computed by introducing free surfaces to accommodate the restrictive periodic boundary conditions associated with plane-wave based DFT implementations. While these aforementioned studies have provided useful insights into the dislocation core-structure, a direct quantification of the dislocation core-energy solely from electronic-structure calculations and its role in governing dislocation behavior has remained elusive thus far. We note that some prior *ab initio* studies using a dipole or quadrapole configuration of dislocations (cf. e.g. Blase et al., 2000; Li et al., 2004; Clouet et al., 2009) have attempted to indirectly compute the core-energy of an isolated dislocation by subtracting from the total energy the elastic interaction energy between dislocations in the simulation cell and their periodic images. This approach assumes that the spacing between dislocations is large enough that the dislocation-cores do not overlap. However, these prior studies have been conducted on computational cells containing a few hundred atoms, which, as demonstrated in this work, are much smaller than the core-size of an isolated perfect edge dislocation in Aluminum.

In this work, we conduct large-scale electronic-structure calculations using orbital-free density functional theory to study an edge dislocation in Aluminum. In our study, we use the WGC kinetic energy functional (Wang et al., 1999) which has been shown to be in good agreement with Kohn–Sham DFT for a wide range of material properties in Aluminum (Wang et al., 1999; Carling and Carter, 2003; Ho et al., 2007; Shin et al., 2009). We employ a local real-space formulation of orbital-free density functional theory (Gavini et al., 2007c; Radhakrishnan and Gavini, 2010), where the extended interactions are reformulated as local variational problems. This real-space formulation of orbital-free density functional theory is used in conjunction with the finite-element basis that enables the consideration of complex geometries and general boundary conditions, which is crucial in resolving the aforementioned limitations of plane-wave basis in the study of energetics of isolated dislocations.

We begin our study by computing the size of the dislocation-core for a perfect edge dislocation in Aluminum. To this end, we consider a perfect edge dislocation with the atomic positions given by isotropic elasticity theory. For these fixed atomic positions, we identify the region where the perturbations in the electronic-structure arising from the defect-core are significant and have a non-trivial contribution to the dislocation energy. This allows us to unambiguously identify the dislocation-core from the viewpoint of energetics. Our study suggests that the dislocation core-size of a perfect edge dislocation is about $10|\mathbf{b}|$, where $\mathbf{b}$ denotes the Burgers vector. This estimate is much larger than conventional estimates based on displacement fields, which suggest a dislocation core-size of $1–3|\mathbf{b}|$ (Hirth and Lothe, 1968; Peierls, 1940; Banerjee et al., 2007; Weinberger and Cai, 2008), and underscores the long-ranged nature of the perturbations in electronic fields arising from defects. We note that a similar long-ranged nature of the electronic fields was observed in recent studies on point defects (Gavini et al., 2007a; Radhakrishnan and Gavini, 2010; Gavini and Liu, 2011). As a next step in our study, we allow for atomic relaxations, and the perfect edge dislocation dissociates into Shockley partials with a partial separation distance of 12.8 Å. The dislocation energy per unit length of the relaxed Shockley partials in the simulation domain corresponding to the identified core-size, which denotes the dislocation core-energy, is computed to be 0.4 eV/Å.

We next study the role of macroscopic deformations on the dislocation core-energy and core-structure. In particular, we considered a wide range of macroscopic deformations including: (i) equi-triaxial strains representing volumetric deformations; (ii) uniaxial strains along the Burgers vector, normal to the slip plane, and along the dislocation line; (iii) equi-