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An analytical model of interfacial energy based on a lattice-matching interatomic energy

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ABSTRACT

We develop an explicit model for the interfacial energy in crystals that emphasizes the geometric origin of the cusps in the energy profile. We start by formulating a general class of interatomic energies that are reference-configuration-free but explicitly incorporate the lattice geometry of the ground state. In particular, away from the interface the energy is minimized by a perfect lattice. We build these attributes into the energy by locally matching, as best as possible, a perfect lattice to the atomic positions and then quantifying the local energy in terms of the inevitable remaining mismatch, hence the term *lattice-matching* used to describe the resulting interatomic energy. Based on this general energy, we formulate a simpler rigid-lattice model in which the atomic positions on both sides of the interface coincide with perfect, but misoriented, lattices. In addition, we restrict the lattice-matching operation to a binary choice between the perfect lattices on both sides of the interface. Finally, we prove an L^2 – bound on the interatomic energy and use that bound as a basis for comparison with experiment. We specifically consider symmetric tilt grain boundaries (STGB), symmetric twist grain boundaries (STwGB) and asymmetric twist grain boundaries (ATwGB) in face-centered cubic (FCC) and body-centered cubic (BCC) crystals. Two or more materials are considered for each choice of crystal structure and boundary class, with the choice of materials conditioned by the availability of molecular dynamics data. Despite the approximations made, we find very good overall agreement between the predicted interfacial energy structure and that calculated by molecular dynamics. In particular, the positions of the cusps are predicted well, and therefore, although surface reconstruction and faceting are not included in the model, the dominant orientations of the facets are correctly predicted by our geometrical model.

1. Introduction

Interfaces have long been known to be key players in the mechanics of mesoscopic phenomena. Recrystallization (Doherty et al., 1997), microstructure formation in solidification (Watanabe and Tsurekawa, 1999), and microstructure evolution (Demirel et al., 2003) are all examples of phenomena that are significantly influenced by interfacial mechanics. A motivating example of interface-dominated behavior is the manufacture of nanolayered composites by severe plastic

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deformation, in which it has been shown that at high layer density, layer evolution is dominated by interface mechanics (Zheng et al., 2013; Beyerlein et al., 2014). Because of the many instances in which interfaces play a significant role, the understanding and prediction of interfacial behavior has elicited considerable interest. However, interfaces stand out among material defects for their variety and complexity, and attempts to characterize them remain ongoing, with approaches ranging from *ab-initio* quantum-based methods to heuristic geometrical constructions.

The space of interface configurations is large, which hinders efforts to identify one unifying characteristic to which the energy of all interfaces can be linked. Consequently, it becomes necessary to distinguish between—and create models for—different interface types. Interfaces between identical crystal lattices are referred to as homophase or *grain boundaries* (GBs). The simplest non-trivial grain boundaries are *twin boundaries*, which require no displacement of individual atoms in either lattice to maintain registry at the boundary. Twin boundaries have the highest degree of order possible in an interface and have relatively low energy. Many types of high-order boundaries are not twin boundaries, but have a high degree of order and locally minimize the energy. Energy minimizing configurations in the space of interface energy orientations form *energy cusps* near their location in configuration space (Herring, 1954, 1951; Gjostein and Rhines, 1959). Though the interfaces themselves are well-understood, a current challenge is to determine the locations of the cusps, and hence the stability of interfaces in configuration space. The remainder of interface types are *low-order boundaries* due to the large rotation required to obtain them from the nearest high-order boundary, and quantifying their energy can present a challenge for low-order models.

The experimental measurement of the energy of grain boundaries entails considerable difficulty and there remains a paucity of observational data for validating models of interface energy. Therefore, it is common to resort to atomistic simulations in lieu of experimental data. Density functional theory (DFT) has been used to examine the properties of some grain boundaries and interfaces (Wright and Atlas, 1994; Hartford, 2000). However, the evaluation of general grain boundaries requires consideration of large material samples and is currently prohibitively expensive by DFT. Currently the *de facto* method for garnering grain boundary energy data is molecular dynamics (MD). The typical computational approach is to create two lattices of atoms, bring them together, apply periodic boundary conditions (or other boundary conditions, c.f. Gehlen et al., 1972), and relax to static equilibration. Further, with MD, the interface can be locally relaxed or reconstructed to obtain even lower energy structures at the cusp locations (Kang et al., 2012a). All MD simulations require the use of an empirical interatomic potential. The most commonly used potential in interface calculations is the Embedded Atom Model (EAM) potential (Daw and Baskes, 1984). The literature is rich with MD data on a large subset of the five-dimensional configuration space of interfaces. Data for FCC–FCC (Wolf, 1989a, 1990a,b; Schmidt et al., 1998; Wolf et al., 1992; Merkle and Wolf, 1992; Tschopp and McDowell, 2007a,b), BCC–BCC (Wolf, 1990c, 1989b, 1991), HCP–HCP (Wand and Beyerlein, 2012a, b), and FCC–BCC (Kang et al., 2012b) provide solid benchmarks for model verification.

Considerable effort has also been devoted to devising analytical models of interfacial energy. Theories based on dislocation mechanics can be traced back to the original insights of Taylor (1934), whose treatment of dislocation surfaces led to the celebrated work of Read and Shockley (1950). They considered a generic low-angle tilt boundary between two cubic lattices, and used geometry to determine the corresponding dislocation density. By an appeal to the linear-elastic solution for the stress field of an infinite rows of dislocations, they obtained the classic equation for tilt interface energy as a function of tilt angle, $E = E_0\theta[A - \ln\theta]$. The model has been shown to work well for low angle tilt, and Wolf demonstrated that the model can be adapted to large-angle tilt boundaries to some degree (Wolf, 1989c), although this relationship is generally recognized as strictly empirical (Sutton and Balluffi, 1995). Read and Shockley's contemporary, J.H. van der Merwe, elucidated the elastic field of symmetric tilt grain boundaries using a periodic interplanar potential (van der Merwe, 1950, 1963; Schoeck, 1994). In a similar vein, R. Bullough extended the established theory of Peierls–Nabarro (Schoeck, 1994) for edge dislocations to symmetric tilt boundaries by treating them as arrays of evenly spaced edge dislocations (Bullough et al., 1979). General representations of interfaces as arrays of dislocations were derived by Frank (1950) and Bilby (1954), which can be used to determine networks of geometrically necessary dislocations at dislocation boundaries (Winther et al., 2015). Recent work by van Beers et al. was recently published that uses the Frank–Bilby formalism to connect the atomistic description to a continuum model (van Beers et al., 2015). Despite the insight provided by linear-elastic dislocation models, their ability to predict the cusp structure of interfacial energy for general interfaces is limited owing to the continuum treatment of the crystals.

Another line of inquiry derives from the empirical observation that interfacial energy is largely determined by crystallography. For instance, most face-centered cubic crystals exhibit similar GB anisotropy up to a multiplicative constant (Holm et al., 2010). Several models have been proposed that connect the energy of an interface to a geometrically-determined quantity. Perhaps no geometric object is more commonly encountered in interface theory than the coincident site lattice (CSL). The ratio of the area of the CSL unit cell to the area of the lattice unit cell gives the so-called Σ value of the interface. Because low Σ values correspond, in general, to low energy grain boundaries, the CSL has been proposed as a model for GB energy (Brandon et al., 1964; Brandon, 1966). However the validity of such models has been questioned (Goodhew and Smith, 1980) and, to date, there is no general consensus regarding their reliability for general grain boundaries (Randle, 2001). The *structural unit model* provides an alternative geometric approach (Bishop and Chalmers, 1968, 1971; Weins et al., 1969, 1970; Weins, 1971). The structural unit model is a heuristic method that attempts to characterize interfaces by determining the requisite structures needed for—or resulting from—compatibility between the crystals. The model is helpful in understanding the geometry of unstructured interfaces, but it does not provide a means for predicting GB energy. A similar construction is the *O-lattice* of Bollmann, which provides a geometrical measure of the number of coincident points, or *O-*