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Energy of low angle grain boundaries based on continuum dislocation structure

Luchan Zhang [a], Yejun Gu [b], Yang Xiang [a, *]

[a] Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
[b] Nano Science and Technology Program, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

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ABSTRACT

In this paper, we present a continuum model to compute the energy of low angle grain boundaries for any given degrees of freedom (arbitrary rotation axis, rotation angle and boundary plane orientation) based on a continuum dislocation structure. In our continuum model, we minimize the grain boundary energy associated with the dislocation structure subject to the constraint of Frank's formula for dislocations with all possible Burgers vectors. This constrained minimization problem is solved by the penalty method by which it is turned into an unconstrained minimization problem. The grain boundary dislocation structure is approximated by a network of straight dislocations that predicts the energy and dislocation densities of the grain boundaries. The grain boundary energy based on the calculated dislocation structure is able to incorporate its anisotropic nature. We use our continuum model to systematically study the energy of $<111>$ low angle grain boundaries in fcc Al with any boundary plane orientation and all six possible Burgers vectors. Comparisons with atomistic simulation results show that our continuum model is able to give excellent predictions of the energy and dislocation densities of low angle grain boundaries. We also study the energy of low angle grain boundaries in fcc Al with varying rotation axis while the remaining degrees of freedom are fixed. With modifications, our model can also apply to dislocation structures and energy of heterogeneous interfaces.

1. Introduction

Energetic and dynamic properties of grain boundaries play vital roles in the mechanical and plastic behaviors of polycrystalline materials [1]. These properties of grain boundaries such as grain boundary energy and mobility strongly depend on the structures of grain boundaries, and have attracted considerable research attention for many decades [1–27].

Grain boundary energy and structure are determined by five macroscopic degrees of freedom (DOFs) that include the grain misorientation (three DOFs) and the boundary plane orientation (two DOFs) [1]. Early works focused on the grain boundary energy as a function of misorientation angle. In the classical theory of Read and Shockley [2], the grain boundary energy is $E = E_0\theta(A - \ln\theta)$, where θ is the misorientation angle and parameters E_0 and A depend on the grain boundary orientation. This energy formula was derived based on a dislocation model of grain boundaries with cancellation of the long-range elastic fields. Hasson and Goux [4] measured the energy of tilt boundaries in aluminum using both experimental method and atomistic calculation. Wolf [9,10] invested the structure-energy correlation of grain boundaries of different boundary planes by using molecular dynamics simulations, and described the energy as a function of the misorientation angle. A linear correlation between the energy and the grain boundary volume expansion was observed. There were also studies of grain boundary structure and energy based on coincidence site lattice (CSL) and displacement shift complete (DSC) dislocations or polyhedral/structure unit models [3,5–7].

More systematic examinations of the dependence of the grain boundary energy on all five DOFs have been conducted in recent years. Olmsted et al. [14,16] calculated the energies of a set of 388 distinct grain boundaries by using atomistic simulations, and examined the correlations of the boundary energy with other boundary properties. Especially, they showed that the grain boundary plane orientation is crucial in the determination of boundary energy. Saylor et al. and Holm et al. [12,13,18] experimentally measured the grain boundary character distributions, and

* Corresponding author.
E-mail address: maxiang@ust.hk (Y. Xiang).

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then used the character distributions to reconstruct the grain boundary energies with fixed rotation axes and misorientation angles. They also compared these experimental results of energies with those computed by using molecular dynamics simulations [18]. Assuming the grain boundary energy is a continuous function of the five DOFs, Bulatov et al. [23] constructed a closed-form grain boundary energy function for fcc metals by using a hierarchical interpolation from values of special sets of grain boundaries (low dimensional subsets termed “grofs”).

Low angle grain boundaries can be modelled as arrays of dislocations, and these dislocation structures play crucial roles in determining the energy, dynamics and other properties of the grain boundaries [1,2,28]. As mentioned above, the classical grain boundary energy formula of Read and Shockley [2] was obtained based on the dislocation structure of low angle tilt boundaries in a simple cubic lattice that cancels the long-range elastic fields. Vitek [8] modified the grain boundary energy formula by including the interaction energy of intersecting dislocations in the dislocation structure of twist boundaries. Rittner and Seidman [11] investigated $<110>$ symmetric tilt boundaries in fcc metals with low stacking fault energy by atomistic simulations, and developed a dislocation model of grain boundary dissociation by stacking fault emission. Recently, Dai et al. [21,24] studied the structure and energy of fcc (111) twist grain boundaries using atomic, generalized Peierls-Nabarro and analytical models for all twist angles. They showed that dislocation structures on the twist boundaries can be determined by a single dimensionless parameter with two extreme cases of a hexagonal network of perfect dislocations and triangular network of partial dislocations enclosing stacking faults. Based on these dislocation structures, the twist grain boundary energy was derived as a function of twist angle, including the effects of partial dissociation and the stacking fault energy. A microscopic phase field model was proposed by Shen et al. [25] to describe the structures and energies of twist boundaries. Using discrete lattice sampling, their grain boundary energies agreed with the Read-Shockley model for low angle grain boundaries as well as the deep cusps for high angle special boundaries. Winther et al. [22,27] used discrete dislocation dynamics model to explain the dislocation networks in the deformation-induced grain boundaries aligned with slip planes in Al observed in experiments. They focused on the formation of grain boundaries by dislocation glide. Lim et al. [15,19] showed that the mobility of low angle grain boundaries under applied stress is determined by the constituent dislocation structures and their rearrangements by discrete dislocation dynamics simulations. Wu and Voorhees [20] used the phase field crystal model to simulate the dynamic of a two-dimensional circular grain and observed motion and reaction of the constituent dislocations as the low angle grain shrinks. There are also models in the literature for the dislocation structures of heterogeneous interfaces [29–36] and grain boundaries in hcp crystals [37–39].

These recent works employed the discrete dislocation models or atomistic models. Although these models are able to provide detailed information on the dislocation or atomistic structures of individual grain boundaries, continuum model is desired for energetic and dynamics of grain boundaries at larger length scales. For low angle grain boundaries, their energetic and dynamical properties depend strongly on the dislocation structure, for example the grain boundary energy anisotropy [17]. Except for the atomistic calculations by Olmsted et al. [14,16], the available works that explore the dependence of grain boundary energy on all five DOFs by Saylor et al. [13] and Bulatov et al. [23] are mainly based on energy reconstruction or interpolation and do not directly depend on the dislocation microstructure of grain boundaries except for some special grain boundaries. Moreover, although it is well-known that the dislocation structure of a low angle grain boundary should satisfy the Frank's formula [28,40,41], this formula in general is not able to uniquely determine the dislocation structure. For example, there are six possible Burgers vectors in an fcc crystal (neglecting the sign), leading to a total of twelve unknowns (two unknowns of orientation and interdislocation distance for the dislocation distribution of each Burgers vector). While in general the Frank's formula gives at most six linearly independent equations for a planar grain boundary. In the available discrete dislocation dynamics based works on the dislocation structures of low angle grain boundaries [22,27] or heterogeneous interfaces [29–32] (for which a similar equation holds [42]), two or three prescribed Burgers vectors informed by experimental observations or atomistic simulations were adopted. There is no method available in the literature that is able to seek the dislocation structures over dislocations with all possible Burgers vectors, to the best of our knowledge.

In this paper, we present a continuum model to compute the energy of low angle grain boundaries for any given DOFs (arbitrary rotation axis, rotation angle and boundary plane orientation). In our continuum model, we minimize the grain boundary energy associated with the dislocation structure subject to the constraint of Frank's formula with all possible Burgers vectors. This minimization problem is solved by the penalty method. This model is based on the continuum framework for low angle grain boundaries [26], which gives total elastic energy including the long-range energy and local energy of dislocations in terms of dislocation densities on the grain boundary, and the latter is the grain boundary energy when a planar grain boundary is at equilibrium. Our continuum model can be considered a generalization of the classical Read-Shockley model, where a closed-form energy formula was obtained for the special cases of tilt boundaries in a simple cubic lattice for which the Frank's formula is able to determine a unique dislocation structure on a boundary.

We use our continuum model to systematically study the energy of $<111>$ low angle grain boundaries in fcc Al with any boundary plane orientation and all six possible Burgers vectors. Comparisons with results of atomistic simulations show that our continuum model is able to give excellent predictions of the energy and dislocation densities of low angle grain boundaries. We also study the energy of low angle grain boundaries in fcc Al with varying rotation axis while the remaining degrees of freedom are fixed, in which dislocations with all the six Burgers vectors are involved.

Our continuum model is based on the representation of dislocation distributions by the dislocation density potential functions proposed in Ref. [26], which enables the generalization to curved grain boundaries. With modifications, our model can also apply to dislocation structures and energy of heterogeneous interfaces. These generalizations will be explored in the future work.

This paper is organized as follows. In Sec. 2, we present our continuum simulation model. In Sec. 3, we validate our model by applications to the energy of low angle tilt and twist boundaries and compare the results with those available in the literature. In Sec. 4, using the developed continuum simulation model, we systematically study the energy of low angle grain boundaries in fcc Al with $[111]$ rotation axis and any boundary plane orientation. The results are compared with atomistic simulation results. In Sec. 5, we further calculate the energy of low angle grain boundaries in fcc Al with varying rotation axis while the remaining degrees of freedom are fixed. Possible generalizations of the present continuum model are discussed in Sec. 6.

2. The continuum simulation model

In this section, we present a continuum simulation model to compute the energy of low angle grain boundaries based on