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Structure and energy of (1 1 1) low-angle twist boundaries in Al, Cu and Ni

Shuyang Dai [a], Yang Xiang [b,*], David J. Srolovitz [c,d]

[a] Nano Science and Technology Program, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
[b] Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
[c] Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA 19104, USA
[d] Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA 19104, USA

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Abstract

We study the structure and energy of (1 1 1) low-angle twist boundaries in face-centered cubic Al, Cu and Ni, using a generalized Peierls–Nabarro model incorporating the full disregistry vector in the slip plane and the associated stacking fault energy. It is found that dislocation network structures on these 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. We construct a simple model of these networks based upon straight partial dislocation segments. Based on this structural model, we derive an analytical expression for the twist boundary energy as a function of the twist angle θ, intrinsic stacking fault energy and parameters describing the isolated dislocation core. In addition to the θ and $\theta\log\theta$ terms [3] and the θ^2 term [17] in the boundary energy, our new energy expression also includes additional terms in θ that represent the partial dissociation of the dislocation nodes and the effect of the stacking fault energy. The analytical predictions of boundary structure and energy are shown to be in excellent agreement with the Peierls–Nabarro model simulations.

Keywords: Grain boundary structure; Grain boundary energy; Dislocation; Micromechanical modeling; Peierls–Nabarro model

1. Introduction

The structure and properties of grain boundaries of metals have received considerable attention over the past half-century because of their importance for material properties ranging from plastic deformation to fracture to corrosion to phase transformations. While much of the activity in the field has focussed on high-angle grain boundaries with atomic resolution, our understanding of the relationship between grain boundary thermodynamic properties and this level of structural information remains largely specialized and often qualitative in nature [1]. A notable exception has been the structural unit model [2]. The essential difficulty is that while bicrystallography provides constraints on grain boundary structure many of the essential details are contained in the atomic configurations in the core of the boundary itself, and these, in turn, depend on the nature of the atomic bonding. Before the advent of high-resolution transmission electron microscopy and atomistic simulation, our understanding of grain boundaries came largely from simple dislocation models of low-angle boundaries, such as the Read–Shockley model [3]. This approach succeeded because most of the grain boundary was composed of regions of elastically distorted, but otherwise perfect, crystal and most of the grain boundary energy was associated with those elastic fields. These models, however, were incomplete, in that they did not include such effects as stacking faults or include a sophisticated treatment of the dislocation cores. In this paper, we combine the ideas of

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

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generalized stacking fault energy [4] and the Peierls–Nabarro [5,6] model for dislocations with spread cores in a mesoscale simulation of low-angle (1 1 1) twist grain boundaries in face-centered cubic (fcc) metals and, based upon the structural observations, develop a quantitative model for their energetics. While such a model is not readily extendable to high-angle boundaries, it does provide a rigorous structure–thermodynamics linkage that may serve as a model for future studies within other frameworks (e.g. the structural unit model).

It is widely accepted that low-angle grain boundaries can be successfully described in terms of dislocation arrays [1,3,7]. The structures of low-angle grain boundaries have been observed experimentally and via atomistic simulations [1,7,8]. For example, the hexagonal dislocation network structures of low-angle twist boundaries on fcc (1 1 1) planes were observed experimentally in Au [9,10] and Al [11]. Experimental observations of the structures of several low-angle (1 1 1) twist boundaries in Au and boundaries with misorientations close to twins were reported in Ref. [12]. These studies show that the grain boundary dislocation network consists of three sets of dislocations which split into partials, leaving part of the grain boundary nominally perfect crystal and the other containing stacking faults. These studies also found that the partials tended to be straight when the dislocation spacing in the network was small and for metals for which the stacking fault energy was low. These hexagonal dislocation networks and their associated partial dissociations on fcc (1 1 1) planes were also reported from atomistic simulations along with the associated grain boundary energy [13,10]. More recently, there have been similar reports on low-angle grain boundaries in nanoscale particles in Pt [14].

Read and Shockley [3] first derived an analytical formula for grain boundary energy as a function of misorientation, θ: $\gamma = E_0\theta(A - \log\theta)$, where E_0 and A are constants. This prediction was based upon the assumption that the grain boundary can be described in terms of sets of straight, parallel dislocations. The constants E_0 and A depend on elastic constants and dislocation core size, respectively. Hokanson and Winchell [15] fitted the energy of twist boundaries, consisting of hexagonal networks of dislocations using the Read–Shockley formula. The energies of these hexagonal networks were calculated numerically and the constants E_0 and A in the formula were fitted. Wang and Vitek [16] reformulated the Read–Shockley formula using the structural unit model of grain boundaries [2] in order to generalize it to higher angles. Vitek [17] showed that the Read–Shockley formula should have an additional term, quadratic in the twist angle θ in order to account for the interaction of intersecting dislocations: $\gamma = E_0\theta(A + B\theta - \log\theta)$. This formula was derived for two sets of dislocations forming a square grid in the twist boundary [17] and was generalized to three sets of straight screw dislocations to approximate the energy of a hexagonal dislocation network in twist boundaries [13].

Lattice dislocations in fcc metals, including the constituent dislocations of low-angle grain boundaries, usually dissociate on (1 1 1) planes into pairs of partials dislocations, separated by planar stacking faults [7]. An early attempt was made by Bullough [18] to estimate the dislocation core width in the regular edge dislocation array of a low-angle tilt boundary as a function of tilt angle, using the Peierls–Nabarro model [5,6] without stacking faults. Taking the stacking fault energy into consideration, Li and Chalmers [19] calculated the equilibrium separation x of partial dislocations in a wall of extended edge dislocations in a low-angle tilt boundary, as a function of tilt angle θ. The relationship $x(\theta)$ was expressed by the solution of nonlinear equations from the force balance due to the interaction between partial dislocations and the effect of the stacking fault. Li and Chalmers obtained an analytical formula for the energy of low-angle tilt boundaries including the effects of dissociation of the constituent dislocation: $\gamma = E_0\theta(A - \log\theta + g(x)) + x\gamma_{sf}/D$, where γ_{sf} is the stacking fault energy, D is the spacing between dislocations in the wall, and $g(x)$ is a function of x describing the interactions of partial dislocations. Ikuhara et al. [20] obtained a similar formula $\gamma = E_0\theta(A - \log\theta) + \alpha\gamma_{sf}$ for low-angle $\langle 0\,0\,0\,1\rangle$ tilt boundaries in alumina bicrystals in which perfect dislocations dissociate into partials separated by stacking faults in the tilt boundary plane, where α denotes the area fraction of the boundary that is faulted.

In low-angle twist grain boundaries in fcc metals, there is ample evidence that dislocation networks are hexagonal, usually with partial dissociation at P_S nodes [7]. The additional complexity associated with dislocation nodes, dislocation dissociation and stacking faults has made it difficult to derive simple, analytical formulae for twist grain boundary energy, such as those of Read–Shockley, Vitek and others. To our knowledge, there are no systematic studies of these network structures in relationship with twist angle and no analytical formulae for the grain boundary energy appropriate to low-angle twist boundaries in fcc metals.

In this paper, we first present a systematic numerical study of the structure and energy of (1 1 1) low-angle twist boundaries in fcc Al, Cu and Ni, using a generalized Peierls–Nabarro model developed by Xiang et al. [21]. This model incorporates the full disregistry vector in the slip plane and the associated stacking fault energy [4], and applies to dislocations of arbitrary shape. Using this approach we determine the equilibrium structure of the twist boundaries, including curved partial dislocations, stacking faults, and faulted and non-faulted nodes, and energy of the twist boundaries. We then construct a simple model of networks of straight partial dislocation segments to describe these dislocation structures that is able to capture the essential features of the generalized Peierls–Nabarro simulation results. Based on this approximate model, we obtain an analytical formula for the energy of these twist boundaries as a function of twist angle θ. In addition to the θ and $\theta\log\theta$ terms obtained by Read and