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Stress dependence of the dislocation core structure and loop nucleation for face-centered-cubic metals

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ABSTRACT

In face-centered-cubic (fcc) metals, the evolution of Shockley partial dislocations under stress is known to play an important role in plastic deformation. The simulations of the dislocation evolutions, including dislocation dissociation, nucleation and recombination, under applied stress are presented using a phase field dislocation dynamics model that incorporates the γ surface of various fcc metals. As expected, the separation of the leading and trailing partials, termed the equilibrium stacking fault width (SFW), is governed by the details of the γ surface and the external loading conditions. Two important critical stresses, defined as the singular stress and the nucleation stress, are found to determine the stress-dependent evolution mechanism. As a general rule, the SFW increases with the applied stress and diverges when the applied stress exceeds the singular stress. A spontaneous nucleation of partial dislocation loops within the stacking fault (SF) occurs when the applied stress exceeds the nucleation stress. In particular, a new stress-size-dependent nucleation mechanism is observed in the simulations in the case where the singular stress is greater than the nucleation stress for a fcc metal: the nesting loop or nesting dipole can remain in the metastable state without any nucleation even the applied stress is twice as large as the nucleation stress.

1. Introduction

In fcc metals, slip occurs between the close-packed {111} planes and along the ⟨110⟩ direction [1–3]. The dislocation lines and loops in these slip planes will be energetically more favorable for the dissociation state consisting of two Shockley partials bounded with a SF. The SFW is found to be determined by the details of the material γ surface of the slip plane and affected by the external stress conditions [4,5]. In general, the stress dependence of the dislocation core structure and the size of the SF play important roles in a large number of plastic deformation mechanisms, such as twinning, cross-slip, dislocation locking/unlocking, crack tip plasticity, phase transitions and so on [6–8].

The large size of the SF under stress restricts the methods available to investigate this problem. In the last several decades, a number of continuum models have been developed on the basis of the force balances on the dislocation microstructure or the energetically favored state of dislocation dynamics. In summary, they can be classified into two types of models, the Volterra dislocation model and the Peierls-Nabarro type model. In the Volterra model, the equilibrium SFW is determined by the balance of the Peach-Koehler force due to the stress field, the elastic repulsive force between the leading and trailing partial dislocations and the restoring force arising from the SF. Copley and Kear first derived an expression for the SFW as a function of the applied stress and stacking fault energy [9]. Cai et al. derived a concise formula of the ideal separation of two 30° partials [10]. Byun first considered the damping force to the glide of partial dislocations in the force balance equation, researching the angular and stress dependences of the SFW [11]. A critical stress is predicted by the Volterra model for producing the infinite SFW, and it increases with increasing stacking fault energy. In the paper, it is termed the singular stress, τ_∞. However, the Volterra model neglects the effects of the dislocation core and the dislocation curvature on the SFW, and most importantly, the Volterra model constrains the partial dislocations to glide with the unchangeable Burgers vectors under any stress

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condition, which is not consistent with some atomistic simulations [12,13].

To predict the SFW and to investigate the core structures of the partial dislocations under stress, another continuum model for the energetics and dislocation dynamics has been developed based on the concept of the Peierls-Nabarro (PN) model [14–16]. For example, Bulatov and Cai employed the variational Peierls-Nabarro (VPN) model to investigate the stress effects on the SFW for fcc metals. They found that the SFW does increase as the applied stress increases, and moreover, they found that under critical stress, the perfect screw dislocation would split into two perfect 60° dislocations, preempting the 30° partials [17]. This transformation indicates that dislocation nucleation or combination occurs after the perfect dislocation splits into two partials. In this paper, the critical stress to trigger this transformation is defined as the nucleation stress τ_c. Another popular method to investigate the dislocation-SF interaction is the phase field dislocation dynamics (PFDD) model. It is classified as a PN type model because the PFDD model can be viewed as a three-dimensional, coarse-grained PN model [18–21]. The difference is that the PN and VPN models investigate the dislocation dissociation by setting one perfect dislocation in an infinite real space, but the PFDD establishes a dislocation dipole or a dislocation loop in the simulation box to satisfy the periodic boundary condition. Shen and Wang first reproduced the dislocation dissociation process in the PFDD by directly incorporating γ surface data from *ab initio* calculations into the crystalline energy [22]. Hunter et al. employed the PFDD to investigate the dependence of the SFW on the details of the γ surface and found that the equilibrium configurations are not simply proportional to the intrinsic stacking fault energy (ISFE) but related to the ratio between the unstable stacking fault energy (USFE) and the ISFE as well as some other details [23,24]. Beyerlein and Hunter employed the PFDD to investigate the grain size effects on the partial dislocation slip and dislocation loop behavior [25]. Mianroodi and Svendsen introduced an atomistically determined PFDD to model the dislocation dissociation and partial dislocation slip, and they found that external loading can transform a perfect dislocation through a series of core reactions into another 60° perfect dislocation [26]. Soon after, Mianroodi et al. compared the results from their PFDD with molecular statics simulations [27]. In summary, nearly all PFDD works focus on the dislocation dissociation process but not the second transformation, and the relation between the magnitude of the applied stress and the final dislocation energetically favored state is not clear. By identifying the exact physical meaning of the singular stress τ_∞ and the nucleation stress τ_c, the stress dependence of the dislocation evolution is clarified by our work.

Section 2 gives the formulation of the PFDD in the context of geometric linearity and static loading. The relation between the gradient energy parameter and the size of the dislocation core is clarified. In Section 3, the generalized stacking fault energy (GSFE) used in the PFDD is derived from the misfit energy format from the literature, in which the ISFE is controlled by a dimensionless parameter. The PFDD predicts the equilibrium SFW in good agreement with the results from the Volterra and VPN models. In Section 4, the stress dependence of the dislocation transformation as a perfect screw dislocation dipole and a dislocation loop is produced in the simulations. The conclusions follow in Section 5.

The notation rules of continuum mechanics are used [19,28]. Vectors and higher-order tensors are written in bold font; scalars and components of vectors and tensors are written in italic font. The rule of tensor calculation follows the Einstein summation convention, e.g., the dot product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is $\mathbf{a}\cdot\mathbf{b} = a_i b_i$. The outer product of two vectors is $\mathbf{a}\otimes\mathbf{b} = a_i b_j \mathbf{e_i}\otimes\mathbf{e_j}$. The colon denotes summation over two sets of indices: $\mathbf{A} : \mathbf{B} = A_{ij}B_{ij}$. Let $\operatorname{sym}\mathbf{A} := (\mathbf{A} + \mathbf{A}^{\mathrm{T}})/2$ represent the symmetric part of $\mathbf{A}$. Additional notation will be introduced as needed.

2. Phase field theory of dislocation dynamics

A brief description of the PFDD incorporating the dislocation structure of fcc metals is presented here. The PFDD is restricted to isothermal conditions and quasi-static loading for investigating the stress dependence on the dislocation core structure. A more detailed discussion of the PFDD can be found in Refs. [21,22,26,27,29]. Let $\mathbf{u}$ be the displacement, $\mathbf{H} = \nabla\mathbf{u}$ the distortion field, $\operatorname{sym}\mathbf{E}$ the strain field, and $\phi = (\phi_1, \ldots, \phi_n)$ the phase fields. Following the notation of Mianroodi et al. [27], the total free energy of the dislocation system is written as a sum of three contributions, i.e.,

$$\psi(\mathbf{E}, \phi, \nabla\phi) = \psi_{\mathrm{ela}}(\mathbf{E}, \phi) + \psi_{\mathrm{sfe}}(\phi) + \psi_{\mathrm{grad}}(\nabla\phi) \tag{1}$$

where

$$\psi_{\mathrm{ela}}(\mathbf{E}, \phi) = \frac{1}{2}(\mathbf{E} - \mathbf{E}_{\mathrm{R}}(\phi)) : \mathbf{C}_{\mathbf{E}} : (\mathbf{E} - \mathbf{E}_{\mathrm{R}}(\phi))$$

$$\psi_{\mathrm{sfe}}(\phi) = \psi|_{\mathrm{hom}}(\mathbf{E}_{\mathrm{R}}(\phi), \phi)$$

$$\psi_{\mathrm{grad}}(\nabla\phi) = \xi\sum_{\alpha}\left[\left(\mathbf{n}^{(\alpha)}\times\nabla\right)\phi_\alpha\right]^2$$

The first term of the above equation is the elastic energy, where $\mathbf{E}_{\mathrm{R}} = \operatorname{sym}\mathbf{H}_{\mathrm{R}}$ is the residual strain; the distortion field is $\mathbf{H}_{\mathrm{R}}(\phi) = \sum\phi_a\mathbf{H}_a$, $\mathbf{H}_a = \mathbf{b}_a\otimes\mathbf{n}_a/d_a$; $\mathbf{b}_a$ is the Burgers vector; $\mathbf{n}_a$ is the unit normal of the slip plane; and d_a is the interplanar space of the two adjacent slip planes. The second term is the GSFE, also called the crystalline energy or misfit energy, which is commonly given with reference to the material γ surface. The third term is the gradient energy, which is useful to increase the dislocation core width artificially to increase the numerical stability. The parameter ξ is associated with the dislocation core width. It is worth noting that Mianroodi and Svendsen rewrite the gradient term to fit the data from the atomistic simulations [26]. Here, the gradient form of Wang et al. is used in our model [30,31], and the precise magnitude relation between the gradient parameter ξ and the dislocation core size is clarified later.

The elastic balance equilibrium is built on the PFDD as usual by the quasi-static mechanical equilibrium:

$$\nabla\cdot\mathbf{T} = 0 \tag{2}$$

with linear elastic stress,

$$\mathbf{T} = \frac{\partial\psi}{\partial\mathbf{E}} = \mathbf{C}_{\mathbf{E}} : (\mathbf{E} - \mathbf{E}_{\mathrm{R}}) \tag{3}$$

where $\mathbf{C}_{\mathbf{E}}$ is Young's modulus, a fourth order tensor.

The evolution of the phase fields is governed by the time-dependent Ginzburg-Landau equation,

$$\frac{\partial\phi_a}{\partial t} = -m_0\frac{\delta\psi}{\delta\phi_a} = m_0\left(\nabla\cdot\frac{\partial\psi}{\partial\nabla\phi_a} - \frac{\partial\psi}{\partial\phi_a}\right) \tag{4}$$

where m_0 is the mobility constant. Eq. (2) is subject to stress-based boundary conditions solved in Fourier space using the Fast Fourier Transformation, and Eq. (4) is subject to the no-flux periodic boundary solved in real space using the finite difference method.

To determine relation between the gradient parameter and the dislocation core width, the one-dimensional (1-D) PFDD and the