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The dissociation behavior of dislocation arrays in face centered cubic metals

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ABSTRACT

Dislocations ⟨1 1 0⟩/2 are usually dissociated into two ⟨1 1 2⟩/6 partials with a stacking fault in face centered cubic metals. Their behavior depends strongly on the stacking fault width (SFW) in plastic deformation. However, there is no quantitative study to correlate the SFW with the dislocation configuration when these dislocations are grouped together. In this work, the SFW for different dislocation arrays is analyzed within the framework of the elasticity theory of dislocations and then verified by atomistic simulations. The results demonstrate that the spacing of dislocation arrays has to be taken into account for the SFW variation besides the dislocation character. In addition, the SFW variation with the dislocation spacing seems to be independent to temperature. Our approach can also provide a basis for the accurate estimate of the influence of stacking faults on cross-slip, the competition between slip and twinning during plastic deformations in face centered cubic metals.

1. Introduction

Stacking faults (SFs) are usually formed by the dissociation of perfect dislocations ⟨1 1 0⟩/2 into two Shockley partials ⟨1 1 2⟩/6 in face centered cubic (FCC) metals [1]. They often dominate the behaviors of plastic deformations of these materials to a large extent. For example, dislocations ⟨1 1 0⟩/2 have to glide on the plane {1 1 1} parallel to these SFs because of their restriction. If a dislocation ⟨1 1 0⟩/2 tends to cross slip, its SF have to shrink to a minimum distance on the original glide plane to facilitate its re-dissociation on the new glide plane [2,3]. This process plays an important role in the onset of stage III work-hardening for single crystals and the deformation textures of polycrystals [4]. Besides, SFs significantly impact some more elementary processes, such as synchronous improvement of strength and ductility [5–7], the transition from slip to twinning of the dominant deformation mode in FCC metals including transformation- and twinning-induced plasticity alloys [8], the cracking behaviors of the coherent twin boundary [9] and the formation of various configurations of dislocations including persistent slip bands, labyrinth and cell structures in cyclically deformed FCC metals [10]. In the quantitative study of these phenomena, it is now recognized that the SF width (SFW) is the most important factor that should be taken into account when describing the influence of SFs on the mechanical properties of FCC metals.

Numerous theoretical and experimental attempts [11–17] have been undertaken to analyze the variation of the SFW (termed by d) because of its importance mentioned above. In dissociation of an isolated dislocation ⟨1 1 0⟩/2 without any external loading, the elasticity theory of dislocations successfully predicts that the SFW is simply inversely proportional to the stacking fault energy (SFE denoted by γ_I), and it is also a function of the orientation of a dislocation line. These predictions have been confirmed in the accurate measurement of SFW by the weak-beam technique of transmission electron microscopy (TEM) [4,11,12]. On the other hand, when an isolated dislocation ⟨1 1 0⟩/2 is subjected to an applied loading, the elasticity theory of dislocations demonstrates that the SFW depends on the external loading [13,17]. However Li et al. [16] found that the equilibrium separation of partial dislocations in a wall of extended edge dislocations is a function of the misfit angle of the wall. This means that the dissociation of dislocation arrays or groups is different from that of an isolated dislocation. Unfortunately, this model is concentrated on symmetrical tilt boundaries in which each dislocation has its own glide plane so that it is not valid to the common experimentally observed dislocation arrays in association with cross slip, dislocation multiplications, dislocation pile-ups and so on [18–26]. Because in the latter case all dislocations in each array should glide on a single plane {1 1 1} and it is found that there usually exist two sets of Shockley partial dislocations ⟨1 1 2⟩/6 in each dislocation array, which are formed by the dissociation of a single set of perfect dislocations ⟨1 1 0⟩/2. Therefore, it is meaningful to provide a quantitative description of the SFW variation for dislocation arrays.

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For this purpose, our task is two-fold: (i) to derive an analytical equation to correlate the variation of the SFW d with the dislocation spacing D (the d-D relation or equation hereafter) for different dislocation arrays by applying the elasticity theory of dislocations, and (ii) to perform systematical atomistic simulations to verify the formulae in (i). In (ii), Cu and Ag are selected to conduct atomistic simulations because of their large difference of SFE. At the same time, different empirical potentials of Cu and Ag [27–31] are used to consider the possible influences from the construction of potentials on the simulation results. And the influence of temperature on SFW is also discussed. Finally, the application and generality of the d-D equation for different dislocation types, and its influence on many behaviors of FCC metals during plastic deformations are discussed in detail.

2. Theoretical consideration

In this section, the isotropic elasticity theory of dislocations is employed to derive the d-D relation. Fig. 1(a) sketches an array of perfect dislocations with the Burgers vector $\boldsymbol{b} = [1\ \bar{1}\ 0]/2$ on a single glide plane. It represents a typical dislocation array gliding on a single plane observed in the experiments [18–26]. We assume that these dislocations in Fig. 1(a) can be placed into a coordinate system {$\boldsymbol{xyz}$}, where $\boldsymbol{x}$ is parallel to $\boldsymbol{b}$ ($\boldsymbol{x}\|\boldsymbol{b}$), and $\boldsymbol{z}$ is parallel to the normal of their glide plane (1 1 1). The dislocation line direction $\boldsymbol{l}$ is restricted to the $\boldsymbol{x}$-$\boldsymbol{y}$ glide plane, and it makes an angle θ with $\boldsymbol{x}$. The angle θ is restricted in the range from 0 to 90°, because it suffices to model the change from screw to edge dislocations (imagining $\boldsymbol{b}$ is fixed along $\boldsymbol{x}$). This coordinate system {$\boldsymbol{xyz}$} will be also selected for the atomistic simulations in the next section.

According to the isotropic elasticity theory of dislocations [1], the stress tensor $\sum^{s}$ arising from a single dislocation $\boldsymbol{b}$ at the origin in Fig. 1(a) has two non-zero components:

$$\sigma^{s}_{xz} = \frac{G(x\sin\theta + y\cos\theta)}{2\pi\left[(x\sin\theta + y\cos\theta)^2 + z^2\right]}\left[b_s\cos\theta + \frac{b_e\sin\theta}{1-\nu}\frac{(x\sin\theta + y\cos\theta)^2 - z^2}{(x\sin\theta + y\cos\theta)^2 + z^2}\right] \tag{1}$$

$$\sigma^{s}_{yz} = -\frac{G(x\sin\theta + y\cos\theta)}{2\pi\left[(x\sin\theta + y\cos\theta)^2 + z^2\right]}\left[b_s\sin\theta - \frac{b_e\cos\theta}{1-\nu}\frac{(x\sin\theta + y\cos\theta)^2 - z^2}{(x\sin\theta + y\cos\theta)^2 + z^2}\right] \tag{2}$$

Correspondingly, the stress tensor $\sum^{a}$ of the dislocation array in Fig. 1(a) can be derived by superposing the stresses of each dislocation in Eqs. (1) and (2) on the basis of Refs. [1,32,33] and its non-zero components are:

$$\sigma^{a}_{xz} = \frac{G\sin(X\sin\theta + Y\cos\theta)}{2DA}\left(b_s\cos\theta + \frac{b_e\sin\theta}{1-\nu}\frac{A - Z\sinh Z}{A}\right) \tag{3}$$

$$\sigma^{a}_{yz} = -\frac{G\sin(X\sin\theta + Y\cos\theta)}{2DA}\left(b_s\sin\theta - \frac{b_e\cos\theta}{1-\nu}\frac{A - Z\sinh Z}{A}\right) \tag{4}$$

Note that all the stresses in the above equations are expressed in {$\boldsymbol{xyz}$} and $A = \cosh Z - \cos(X\sin\theta + Y\cos\theta)$, $X = 2\pi x/D$, $Y = 2\pi y/D$, $Z = 2\pi z/D$. In this work, G, b, ν denote the shear modulus, the length of the Burgers vector $\boldsymbol{b}$, and the Poisson's ratio, respectively.

The partial dislocation arrays $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ in Fig. 1(b) come from the dissociation of the dislocation array $\boldsymbol{b}$ in Fig. 1(a). It is noted that a translation occurs in the $\boldsymbol{x}$-$\boldsymbol{y}$ plane associated with the dislocation dissociation for each partial pair relative to their original position before dissociation. This translation can be involved when applying Eqs. (1)–(4) to the partial dislocations $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ by a simple coordinate transformation, e.g. $\Sigma^{s}_{\boldsymbol{b}_1}$ and $\Sigma^{a}_{\boldsymbol{b}_1}$ (or $\Sigma^{s}_{\boldsymbol{b}_2}$ and $\Sigma^{a}_{\boldsymbol{b}_2}$) represent the stress tensors of an isolated dislocation and a dislocation array with the Burgers vector $\boldsymbol{b}_1$ (or $\boldsymbol{b}_2$) by replacing x by $x \pm d\sin\theta/2$ and y by $y \pm d\cos\theta/2$. In this case, the two partials $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ nearest to the origin are selected to establish the d-D relation. The stress tensor of these two partial dislocation arrays excluding the selected two partials $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ nearest to the origin can be easily derived as:

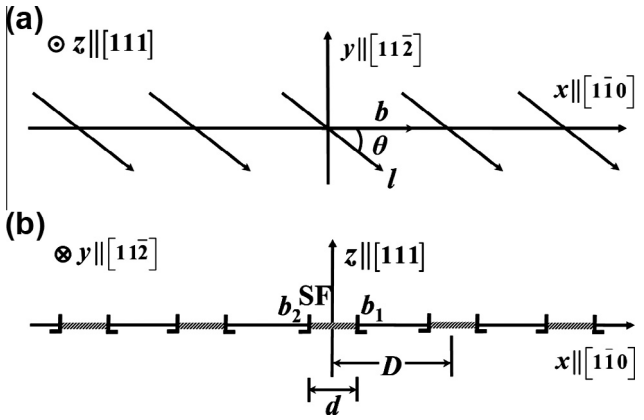

Fig. 1. (a) An array of perfect dislocations with the Burgers vector $\boldsymbol{b}$. Their glide plane is parallel to the $\boldsymbol{x}$-$\boldsymbol{y}$ plane, in which the dislocation line direction $\boldsymbol{l}$ makes an angle θ with $\boldsymbol{x}$. (b) Each perfect dislocation in (a) dissociates into two Shockley partials $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$. Only five dislocations are sketched for clarity. In (b), $\theta = 90°$ is selected as an example. See parameters in the text.

$$\Sigma^{r} = \Sigma^{r}_{\boldsymbol{b}_1} + \Sigma^{r}_{\boldsymbol{b}_2} \tag{5}$$

where

$$\Sigma^{r}_{\boldsymbol{b}_1} = \Sigma^{a}_{\boldsymbol{b}_1} - \Sigma^{s}_{\boldsymbol{b}_1} \tag{6}$$

$$\Sigma^{r}_{\boldsymbol{b}_2} = \Sigma^{a}_{\boldsymbol{b}_2} - \Sigma^{s}_{\boldsymbol{b}_2} \tag{7}$$

Here the stress tensor $\Sigma^{r}_{\boldsymbol{b}_1}$ (or $\Sigma^{r}_{\boldsymbol{b}_2}$) denotes the stress tensor of the partial dislocation $\boldsymbol{b}_1$ (or $\boldsymbol{b}_2$) without the one nearest to the origin in Fig. 1(b). Besides the stress in Eq. (5), the interaction and SF

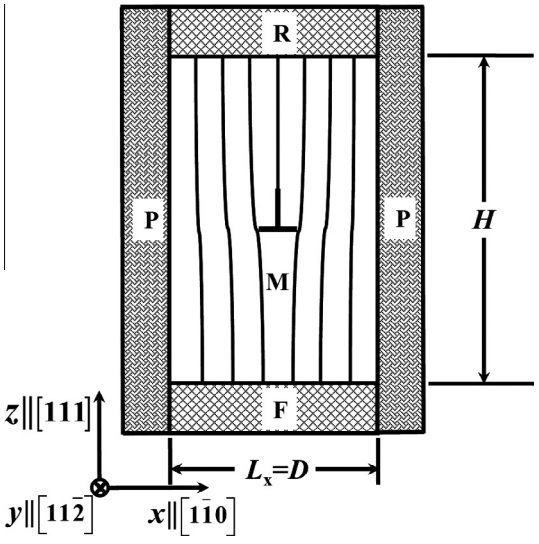

Fig. 2. Schematic presentation of simulated crystallite with M: region of mobile atoms, P: regions where periodic boundaries are applied, F: lower fixed block and R: upper rigid mobile block. See other parameters in the text.