On the dislocation properties of $60°$ partial dislocation in silver: core structure and Peierls stress

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Abstract. Two-dimensional modified Peierls-Nabarro dislocation equation concerning the discreteness of crystals is reduced to one-dimensional equation to determined the core structure of partial dislocation in Ag. The generalized stacking fault energy along the Burgers vectors of partial dislocation is a skewed sinusoidal force law, which is related to the intrinsic stacking fault energy and the unstable stacking fault energy. A trial solution appropriate for arbitrary dislocation angle is presented within the variational method. The results show that the half core width increases as the increase of dislocation angle. Moreover, the core width decreases with the increase of the unstable stacking fault energy and the intrinsic stacking fault energy. Peierls stress for $60°$ partial dislocation is in agreement with the experimental results.

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Key words: core structure, partial dislocation, variational method, Peierls stress

1   Introduction

It is widely accepted that extended defects such as dislocations play an important role in defining the mechanical properties of materials [1–5]. In face-centered-cubic (fcc) crystals (such as Ag), the glide dislocations should be dissociated into two Heidenreich-Shockley partial dislocations bounding a stacking fault ribbon among them [6,7]. The dissociation properties make the procedure to determine the mobility of dislocations (Peierls stress) more complex and questionable. Two types of theoretical approaches have been applied to examine the Peierls stress of dissociated dislocations. The first type is based on the direct atomistic simulation using empirical interatomic potentials [8–11]. The second one employs the Peierls stress of single partial dislocation to replace that of the dissociated

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dislocation within the framework of Peierls-Nabarro (P-N) model. The atomistic simulations may not be reliable as the empirical potentials are used. On the other hand, the P-N model provides a conceptual framework for the prediction of the size and mobility of dislocations, namely core structure and Peierls stress [6]. However, a quantitative agreement with experiments has been lacking as the model is essentially a continuum treatment.

Recently, the boundary problem of the half-infinite lattice has been solved by using the lattice Green function method. By virtue of the solution obtained in the boundary problem, a set of dislocation equations have been derived explicitly for the two-dimensional triangular lattice. The dislocation equation only related to displacement of the atoms on the border. Because the displacement field of a dislocation varies slowly in the space, the discrete dislocation equation can be changed into the integro-differential equation, namely the modified P-N dislocation equation [12–14].

In this paper, we focus on the core structure properties and Peierls stress for $60°$ partial dislocation in Ag. We choose to study $60°$ partial dislocation in Ag for two reasons: (i) the intrinsic stacking fault energy ($\gamma_I = 0.021$ Jm^{-2}) is small and dissociation equilibrium distance is large enough so that two partial dislocation should not overlap too much, (ii) the edge dislocation dissociates into two $60°$ partial dislocations and the Peierls stress of single partial dislocation used to replace the dissociated dislocation is more reasonable [15]. In Section 2, the core structure properties of partial dislocation are investigated with the modified P-N equation. Peierls stress for $60°$ partial dislocation in Ag is presented in Section 3. Finally, conclusions are made in Section 4.

2   Core structure of partial dislocations with skewed sinusoidal force law

The 2D modified P-N dislocation equation for straight dislocations that describe the balance of atoms on the border based on the lattice dynamics and the symmetry principle takes the following form [14]

$$-\frac{\beta_e}{2}\frac{d^2u^x}{dx^2} - \frac{K_e}{2\pi}\int_{-\infty}^{+\infty}\frac{dx'}{x'-x}\left(\frac{du^x}{dx}\right)\Big|_{x=x'} = f^x(u^x,u^y), \tag{1}$$

$$-\frac{\beta_s}{2}\frac{d^2u^y}{dx^2} - \frac{K_s}{2\pi}\int_{-\infty}^{+\infty}\frac{dx'}{x'-x}\left(\frac{du^y}{dx}\right)\Big|_{x=x'} = f^y(u^x,u^y), \tag{2}$$

where K_e and K_s are the energy factors of the edge and screw dislocations, u^x and u^y are the edge and screw components of displacements. For the isotropic solid, $K_e = \mu\sigma/(1-\nu)$ and $K_s = \mu\sigma$, with μ being shear modulus and ν Poisson's ratio, σ is the area of the primitive cell of the misfit plane. The coefficients of the second-order derivations β_e and

β_s relate with the acoustic phonon velocity and the lattice geometry structure

$$\beta_e = \frac{3}{4}\Omega\mu\left(\frac{2-2\nu}{1-2\nu} - \tan^2\theta\cos^2\phi\right), \tag{3}$$

$$\beta_s = \frac{3}{4}\Omega\mu(1-\tan^2\theta\sin^2\phi), \tag{4}$$

where θ and ϕ are the orientation angles of the relative position of a pair of neighbor atoms in the intrinsic frame with the axes given by the polarization directions, and $\theta = \pi/4$ and $\phi = \pi/6$ for fcc crystals, Ω is the volume of the primitive cell. By comparing with the generalized 2D P-N equation in P-N model, there are two extra second-order derivations that represent the discreteness effect of crystal in the new equation. While β_e and β_s are taken to be zero, namely the discreteness effect is neglected, the generalized 2D P-N equation can be obtained [16].

In order to obtain the core structure of partial dislocations, the dislocation equation for partial dislocation or for the mixed dislocation should be deduced. As we know, the dislocation equation in lattice theory is the equilibrium equation of atoms on the border. The force subjected by atoms along the Burger vector of partial dislocation can be obtained easily, and that can be balanced by the restoring force resulted from the generalized stacking fault energy curve along the Burgers vector. The dislocation equation for partial dislocation can be written as

$$-\frac{\beta_b}{2}\frac{d^2u}{dx^2} - \frac{K_b}{2\pi}\int_{-\infty}^{+\infty}\frac{dx'}{x'-x}\left(\frac{du}{dx}\right)\Big|_{x=x'} = f(u), \tag{5}$$

where β_b and K_b can be represented as

$$\beta_b = \beta_e\sin^2\varphi + \beta_s\cos^2\varphi, \tag{6}$$

$$K_b = K_e\sin^2\varphi + K_s\cos^2\varphi, \tag{7}$$

and u and $f(u)$ are the displacement and the restoring force of atoms on the border along Burgers vector of partial dislocation, and φ is the dislocation angle of partial dislocation the included angle between dislocation line and Burgers vector of partial dislocation . For the isotropic solid,

$$K_b = \mu\sigma\left((1-\nu)^{-1}\sin^2\varphi + \cos^2\varphi\right).$$

While β_b is taken to be zero, Eq. (5) is the same as the equation deduced by Joós et al. in continuum theory that has been extensively used [17–20]. Eq. (5) for partial dislocations is only related to the dislocation angle of the partial dislocation based on the assumption that the direction of the displacement u is always along the direction of the Burgers vector b according to purely geometrical considerations. We can express the assumption by [21,22]

$$\frac{u^x}{u^y} = \tan\varphi.$$

The restoring force $f(u)$ is defined as the gradient of the so-called generalized stacking fault energy $\gamma(u)$ along the Burgers vector of partial dislocation

$$f(u) = -\frac{\partial \gamma(u)}{\partial u}.$$

The generalized stacking fault energy curve can be represented by the following Fourier series

$$\gamma(u) = \gamma_0 + \gamma_1 \cos(\pi u/b) + \gamma_2 \cos(2\pi u/b) + \cdots \tag{8}$$

While the relative displacement between two half-infinite crystal is 0, the stacking fault energy is given by $\gamma(u)|_{u=0} = 0$ which refers to a perfect crystal. The intrinsic stacking fault energy γ_I is resulted from displacement b along the Burgers vector of partial dislocations, i.e. an intrinsic stacking fault is formed in the fcc crystal. Therefore, the following mathematical relations can be obtained

$$\gamma_0 + \gamma_1 + \gamma_2 = 0, \tag{9}$$

$$\gamma_0 - \gamma_1 + \gamma_2 = \gamma_I. \tag{10}$$

Generally, the actual displacement for γ_{us} is deviated from the geometrically symmetric displacement point $u = b/2$ due to the skewed properties of generalized stacking fault energy curve ($\gamma_I \neq 0$). However, the deviation is small for Ag due to the large γ_{us}/γ_I [15]. Here, the deviation is neglected and we have

$$\gamma_0 - \gamma_2 = \gamma_{us}. \tag{11}$$

Combining Eqs. (9)-(11), the coefficients of generalized stacking fault energy curve can be obtained and the GSF energy curve can be written as

$$\gamma(u) = \frac{\gamma_I}{2}(1 - \cos(\pi u/b)) - \frac{(\gamma_I - 2\gamma_{us})}{4}(1 - \cos(2\pi u/b)). \tag{12}$$

The expression (12) is only related to the unstable stacking fault energy γ_{us} and the intrinsic stacking fault energy γ_I. While the displacement $u = b$, the stacking fault energy is not equals to zero, but $\gamma(b) = \gamma_I$. Thus, the above expression is termed as skewed sinusoidal force law. For fcc Ag with lattice parameters a_0=0.409 nm, the shear modulus and Poisson's ratio are $\mu = 3.38 \times 10^{10}$ GPa and $\nu = 0.354$, respectively. The intrinsic stacking fault energy and the unstable stacking fault energy along <112> direction in {111} slip plane are 0.021 Jm^{-2} and 0.219 Jm^{-2}.

According to the definition of the restoring force, one obtains

$$f(u) = -\frac{\pi \gamma_I}{2b}\sin(\pi u/b) + \frac{\pi(\gamma_I - 2\gamma_{us})}{2b}\sin(2\pi u/b). \tag{13}$$

It is transparent that the skewed sinusoidal force law reduces to the sinusoidal force law while $\gamma_I = 0$. In Fig.1, the skewed sinusoidal shape force law is pictured. The unstable
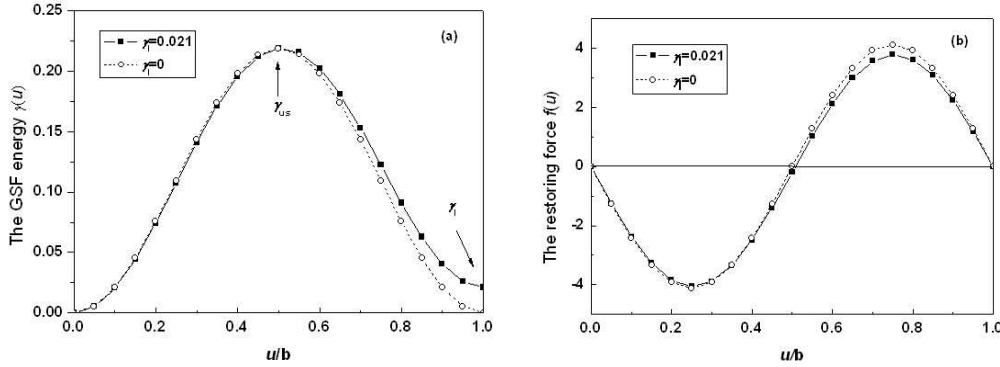
Figure 1: Skewed sinusoidal force law related to intrinsic stacking fault energy γ_I and the unstable stacking fault energy γ_{us}, (a)generalized stacking fault energy (in Jm^{-2}), (b) the restoring force law (in GPa).

stacking fault energy is nearly the same ($0.219 \, Jm^{-2}$) for the intrinsic stacking fault energy $\gamma_I = 0$ and $\gamma_I = 0.021 \, Jm^{-2}$ (as show in Fig. 1a). The difference of two restoring force is delimitated while $u > b/2$, see Fig. 1b.

In P-N model, the method of residua in the complex plane introduced by Lejček is used to construct the planar dissociated dislocation core for arbitrary form of the GSF energy [23] . However, the Eq. (5) with a second order derivation term can no longer be considered as an example of a Hilbert transformation. Hereafter, the variational method is used to deal with the nonlinear integro-differential dislocation equation. It can be easily verified that the variational functional of the dislocation equation takes the following form [24]

$$J = \frac{\beta_b}{4} \int_{-\infty}^{+\infty} \left(\frac{du}{dx}\right)^2 dx - \frac{K_b}{4\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{du}{dx} \left(\frac{du}{dx}\right)\bigg|_{x=x'} \ln\left|\frac{x-x'}{b}\right| dxdx' + \int_{-\infty}^{+\infty} \gamma(u)dx. \quad (14)$$

The trial solution of the variational problem can take the following form

$$u(x) = \frac{b}{\pi} \left(\arctan p + \frac{cp}{1+p^2}\right) + \frac{b}{2}, \quad (15)$$

where $p = \kappa x$. Eq. (15) must assure the correct asymptotic behavior far from the core region as obtained in the continuum elastic theory. Consequently, we have

$$\kappa = \kappa_0 (1-c), \quad (16)$$

with

$$\kappa_0 = \frac{2}{d} \left(\frac{\sin^2 \varphi}{1-\nu} + \cos^2 \varphi\right)^{-1}. \quad (17)$$

The trial solution is appropriate for describing edge, mixed and screw dislocations with different dislocation angle.

By substituting the trial solution Eq. (15) into the variational functional Eq. (14), the results of the first two terms can be easily obtained by contour integration

$$J_1 = \frac{\beta_b \kappa b^2}{4\pi} \left(1 + c + \frac{c^2}{2} \right), \tag{18}$$

$$J_2 = \frac{K_b b^2}{2\pi} \left[\ln \left(\frac{\kappa b}{2} \right) + c + \frac{c^2}{4} \right]. \tag{19}$$

In order to obtain the third term, the parametric derivation method is employed [25], and we have

$$J_3 = \alpha \left\{ e^{\frac{\partial}{\partial \alpha}} \int_{-\infty}^{+\infty} f(\theta_0) d\widetilde{p} - \int_{-\infty}^{+\infty} \left[\left(\frac{R}{2} - \frac{R^2}{3} + \frac{1}{6} \frac{\partial R}{\partial \alpha} \right) \frac{\partial f(\theta_0)}{\partial \alpha} + \frac{R}{2} \frac{\partial^2 f(\theta_0)}{\partial \alpha^2} \right] d\widetilde{p} \right\}, \tag{20}$$

where

$$f(\theta_0) = \frac{\gamma_I}{2} (1 - \sin\theta_0) - \left(\frac{\gamma_I - 2\gamma_{us}}{2} \right) \cos^2 \theta_0, \tag{21}$$

$$R = \frac{\partial^2 \theta_0}{\partial \alpha^2} \left(\frac{\partial \theta_0}{\partial \alpha} \right)^{-1}, \tag{22}$$

with $\theta_0 = \arctan \alpha \widetilde{p}$ and $\alpha = 1/c$. After calculation and arrangement, we have

$$J_3 = -\frac{\pi}{\kappa} \left(\frac{\gamma_I - 2\gamma_{us}}{2} \right) \left(1 - c + \frac{c^2}{4} + \frac{c^3}{12} \right). \tag{23}$$

The term J defined in (4) is now given by $J_1 + J_2 + J_3$. The geometric variational parameters can be determined by the following algebra equations

$$\frac{\partial J}{\partial c} = 0. \tag{24}$$

The dislocation core width ζ is defined as the atomic distance over which u changes from $b/2$ to $3b/4$ (definition I) [19]. The core width may also be defined as the position reaching half maximum of the dislocation density (definition II) [20]. It is valuable to note that definitions I and II equate to each other only within the original Peierls-Nabarro model with sinusoidal force law (arctan-type dislocation solution). The core width for seven partial dislocations evaluated from the above two definitions are shown in Fig. 2. The core width increases monotonically with dislocation angle for both definition I and definition II. The core width obtained from definition I is smaller than that obtained form definition II. Fig. 3 illustrates that the core width decreases with the increase of the unstable stacking fault energy γ_{us} and the intrinsic stacking fault energy γ_I. The conclusion that the core width decreases monotonically with the increase of γ_{us}/γ_I can also be made from Fig. 3. It is well known that the stacking fault energy can be altered by solid-solution alloying [26–28]. Thus, the core structure is controllable for different mechanical property purpose of materials.
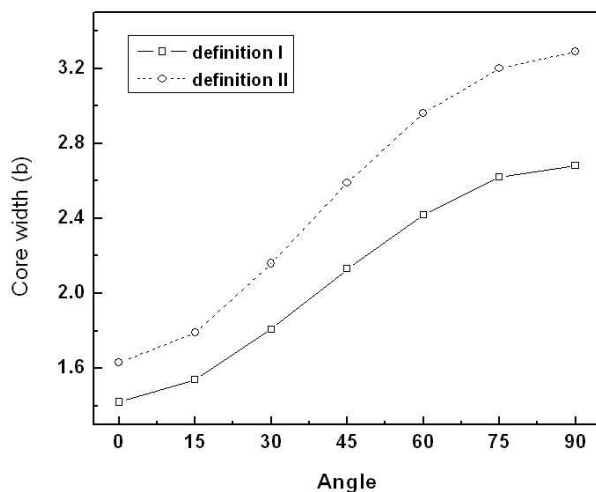
Figure 2: Half core width ς of $60°$ in Ag decreases with the increasing of the unstable stacking fault energy γ_{us}.
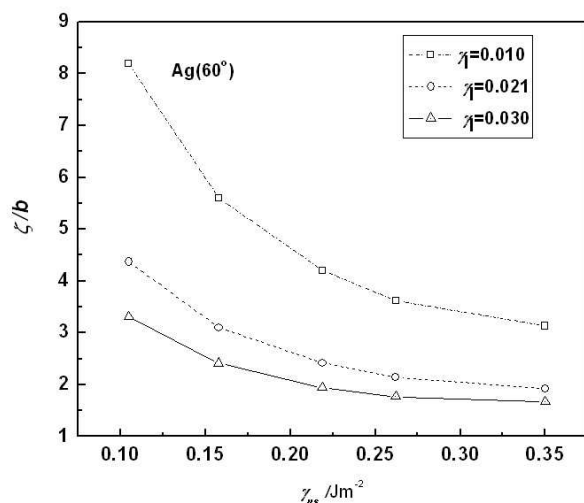

Figure 3: Half core width ς of dislocations increases with the increase of dislocation angle for definition I and II

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3   Peierls stress of $60°$ partial dislocations in Ag

It is well known that the core structure is difficult to be determined from experiments. Thus, it is useful to calculate the Peierls stress of partial dislocation to verify the above results. The Peierls stress is the crucial quantities characterizing the mobility of dislocations that controls the mechanical properties of materials. After the first estimation of the stress by Peierls and Nabarro, attempts to improve the prediction of the stress for-

mula have been made [29]. However, the elastic strain energy is neglected due to the continuous medium approximation in P-N model [30] . The contribution of the elastic strain energy are considered while calculating the Peierls stress in lattice theory and the dislocation energy associated with discreteness of lattice can be expressed as

$$E_d(l) = \sum_{m=-\infty}^{+\infty} \gamma[u(ma-l)] + \frac{1}{2}\sum_{m=-\infty}^{+\infty} f[u(ma-l)]u(ma-l), \tag{25}$$

where the first term and the second term are the misfit energy and the elastic strain energy, respectively, a is the interspacing in the direction of dislocation sliding and $a = b\sin\varphi$ in Ag, and l is the position of the dislocation. The assumption of Nabarro is reserved that the profile of dislocation core is independent of the position of the dislocation. Factor $\frac{1}{2}$ originates from that $u(x)$ is the relative displacement rather than the absolute displacement. By means of Poisson formula, the dislocation energy are

$$E_d(l) = \sum_{s=-\infty}^{+\infty} \left[(\Lambda_m(s) + \Lambda_e(s)) \right] e^{-\frac{2\pi isl}{b\sin\varphi}}, \tag{26}$$

where $\Lambda_m(s)$ and $\Lambda_e(s)$ take the following form after arrangement

$$\Lambda_m(s) = -\frac{1}{\pi i s} \int_{-\infty}^{+\infty} f[u(x)]\rho(x) e^{\frac{2\pi isx}{b\sin\varphi}} dx, \tag{27}$$

$$\Lambda_e(s) = \frac{1}{2b\sin\varphi} \int_{-\infty}^{+\infty} f[u(x)]u(x) e^{\frac{2\pi isx}{b\sin\varphi}} dx. \tag{28}$$

While calculating dislocation energy, it is sufficient to consider the lowest harmonic contributions. Then, if the parity properties of $f[u(x)]$, $u(x)$ and $\rho(x)$ are taken into account, the dislocation energy can be written as

$$E_d(l) = E_d^0 + 2\Lambda_p(1)\cos\left(\frac{2\pi l}{b\sin\varphi}\right), \tag{29}$$

with $\Lambda_p(1) = \Lambda_m(1) + \Lambda_e(1)$. The Peierls energy is the energy variation while the dislocation slip along the Burgers vector and that can be obtained from Eq. (29) expediently, $E_p = 4\Lambda_p(1)$. The Peierls stress σ_p is given by the maximum slop of the Peierls energy according to the definition that the smallest external applied stress to move a dislocation

$$\sigma_P = \frac{\pi\xi(2\gamma_{us} - \gamma_I)}{b\sin\varphi} |A(\xi)| e^{-\xi}, \tag{30}$$

where

$$A_m(1) = \left(2 - \frac{5c^2}{8} + \frac{c^3}{72} + 2c\xi - \frac{5c^2\xi}{8} + \frac{c^3\xi}{72} + \frac{3c^2\xi^2}{8} - \frac{c^3\xi^2}{36} + \frac{5c^3\xi^3}{216}\right), \tag{31}$$

$$A_e(1) = (0.5772 + \ln 2\xi)\left(-1 + c - c\xi + \frac{3c^2\xi}{4} - \frac{c^3\xi}{6} - \frac{c^2\xi^2}{4} + \frac{c^3\xi^2}{6} - \frac{c^3\xi^3}{36}\right), \tag{32}$$

with

$$\xi = \frac{2\pi}{\kappa b \sin\varphi}.$$
(33)

While the contribution of elastic strain energy is not taken into account, Peierls stress $\sigma_P = 5.7 \times 10^{-6}\mu$ for $60°$ partial dislocation in Ag is smaller than the experimental measurements, $2.0 \times 10^{-5}\mu$ and $2.6 \times 10^{-5}\mu$ [31]. After considering the elastic strain energy, Peierls stress $\sigma_P = 1.0 \times 10^{-5}\mu$ is in accordance with the experimental results. The accordance show that both the core structure and Peierls stress obtained with the modified P-N dislocation equation are acceptable.

4   Conclusions

The 2D modified P-N dislocation equation is reduce to 1D dislocation equation based on the assumption $\frac{u^x}{u^y} = \tan\varphi$. The reduced dislocation is applied to determined the core structure and Peierls stress of the partial dislocation in Ag. The generalized stacking fault energy curve along the Burgers vector of the partial dislocation is a skewed sinusoidal force law that is related to the intrinsic stacking fault energy γ_I and the unstable stacking fault energy γ_{us}. After sloving the dislocation with the variational method, the results show that the half core width of partial dislocations increases as the increasing of dislocation angle. A increase in the ratio between unstable stacking fault energy and intrinsic stacking fault energy results in the narrowing of the half core width. Peierls stress calculated for partial dislocation is in agreement with the experimental result.

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