Edge dislocation core structures in FCC metals determined from \textit{ab initio} calculations combined with the improved Peierls–Nabarro equation

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Abstract

We have employed the improved Peierls–Nabarro (P–N) equation to study the properties of \(1/2\langle110\rangle\) edge dislocation in the \{111\} plane in face-centered cubic (FCC) metals Al, Cu, Ir, Pd and Pt. The generalized-stacking-fault energy surface entering the equation is calculated by using first-principles density functional theory (DFT). The accuracy of the method has been tested by calculating the values for various stacking fault energies that favorably compare with previous theoretical and experimental results. The core structures, including the core widths of the edge and screw components, and dissociation behavior have been investigated. The dissociated distance between two partials for Al in our calculation agrees well with the values obtained from numerical simulation with DFT and molecular dynamics simulation, as well as experiment. Our calculations show that it is preferred to create partial dislocations in Cu, and easily observed full dislocations in Al, Ir, Pd and especially Pt.

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1. Introduction

It is widely accepted that dislocations have a direct influence on the deformation mechanism of materials [1], and there has been a great deal of interest in describing accurately the dislocation core structure on an atomic scale because of its important role in many phenomena of crystal plasticity [2, 3]. In FCC metals, dislocations can reduce the elastic energy by dissociating into Shockley partial dislocations connected by a stacking fault (SF) [1]. But as the core regions of two partials overlap, whether the partials can be observed is not only governed by stacking-fault energy (SFE) but also generally by atomic interactions. Dislocations in Al have been a focus of research over the last 20 years [4–13]. An accurate prediction of the atomic-scale core geometries for dislocations in Al is needed for informing higher-length scale models of plasticity in Al alloys, as well as other FCC metals [4]. In addition, it is well known that the nature of slip cannot be described in terms of the absolute value of SFE and a correct interpretation requires the generalized SFE (GSFE) curve, involving both intrinsic (stable) SFE (ISFE) and unstable SFE (USFE) [14].

There are usually two types of theoretical approaches employed to study the core properties of dislocations. The first method is based on direct atomistic simulations or first-principles calculations, and the second method is based on the framework Peierls–Nabarro (P–N) model. Empirical interatomic potentials involve the fitting of parameters to a predetermined database and hence may not be reliable in describing the core properties. On the other hand, first-principles calculations, although considerably more accurate, are computationally expensive for studies of dislocation properties. The P–N model, in which the discreteness of the crystal is neglected, is essentially a continuum treatment, but the dislocation core, the region of inelastic displacement, is given an approximate atomistic description. In addition, the partials in FCC metals are mixed dislocations with both edge and screw components [4].
Schoeck [8, 15] and Mryasov et al [16] adopted the generalized two-dimensional (2D) P–N model for the consideration of the two-component displacement field of dissociated dislocation, but the discreteness of the crystals was neglected. Recently, the 2D improved P–N dislocation equation has taken into account the discreteness of crystals based on the lattice dynamics, and the symmetry principle has been obtained [17, 18]. Both for the P–N model and the improved P–N equation [18], the forces in the dislocation core, where the atomic-scale discreteness really counts, are currently approximated with the GSFE surface ($\gamma$-surface) [3, 13, 19, 20]. The GSFE surface is the interplanar potential energy, which can currently be calculated accurately from \textit{ab initio} calculations, for sliding one half of a crystal over the other half.

In this paper, we perform first-principles calculations on the GSFE surfaces ($\gamma$-surface) for the FCC metals Cu, Al, Ir, Pd and Pt. The $\gamma$-surfaces are applied in the improved P–N equation to the edge dislocations. The accuracy of the method has been tested by calculating the values for various SFEs which compare favorably with previous theoretical and experimental results. Dislocation structures are calculated, including the core widths and dissociated distance between two partials.

This paper is organized as follows. In section 2, we carry out the first-principles calculation of the GSFE surface on the (111) plane in the FCC metals Cu, Al, Ir, Pd and Pt. In section 3, the core structure of dissociated dislocation is obtained from the improved P–N equation with the variational method, and dislocation properties are also discussed.

2. First-principles calculations of the GSFE surface

2.1. Computational methodology

In the present study, total-energy calculations based on density functional theory (DFT) embodied in the Vienna \textit{ab initio} simulation package (VASP) [21–23] are employed. The Perdew–Burke–Ernzerhof (PBE) [24, 25] exchange-correlation functional for generalized gradient approximation (GGA) is used. A plane-wave basis set is employed within the framework of the projector augmented wave (PAW) method [26, 27]. On the basis of our tests, we chose the plane-wave energy cutoff of 500 eV for all the calculated metals. An initial calculation is performed to determine the optimum lattice constants as well as the elastic constants. For the first-Brillouin-zone integrals, reciprocal space is represented by the Monkhorst–Pack special $k$-point scheme [28] with $15 \times 15 \times 15$ grid meshes for these initial calculations, while the GSFE calculations employ $21 \times 21 \times 3$ grid meshes for our calculated FCC metals Cu, Al, Ir, Pd and Pt. The equilibrium theoretical lattice structures are determined by minimizing the Hellmann–Feynman force on the atoms and the stress on the unit cell. The convergence of energy and force is set to $1.0 \times 10^{-6}$ eV and $1.0 \times 10^{-4}$ eV Å$^{-1}$, respectively. In Table 1, we give all the equilibrium lattice constants and elastic moduli for all the studied FCC metals in our calculation, and it is shown that the results agree well with the experimental values [29, 30].

2.2. The GSFE surfaces

In the present study, we calculate the GSFE surfaces in the close-packed (111) surface that is the trigonal lattice, since the slip between the close-packed surfaces is most easy for FCC metals. Ideal FCC structures have the configuration $\cdots ABCABC\cdots$ stacking sequence of the atomic planes. To simulate the block shearing process, we use a slab consisting of 12 atomic layers in the (111) direction. Between periodically repeated slabs the vacuum space of 15 Å normal to the (111) plane is chosen to avoid interactions between two slabs. The SFEs for the slab consisting of 12 and 14 atomic layers are reasonably close. In addition, we find that the fluctuations of the calculated results for a vacuum gap of 15 and 18 Å are less than 1.0%. So, adequate convergence with respect to the supercell size consisting of a 12 atomic-layers-thick slab and a vacuum gap of 15 Å is indicated. The slab calculation is appropriate since the fault interactions are short ranged [13]. In comparison with a six-atomic-layers-thick slab calculation of intrinsic SF (ISF) performed by Hartford et al [13], our 12-atomic-layers-thick slab calculation is more accurate, but with great computational consumption.

The SFEs are determined as the difference of total energies for the two sides of the slab, in which there are six atomic layers below and above, designed to simulate faults with vectors $\mathbf{u} = 0$ and $\mathbf{u} \neq 0$. The SF vector $\mathbf{u}$, which is a 2D vector ($u_x, u_y$), is the displacement of the upper half-crystal relative to the one below. The ISF configuration corresponds to a slip of $\frac{\mathbf{a}}{\sqrt{6}}$ in the (112) direction, resulting in the SF vector $\mathbf{u} = \frac{\mathbf{a}}{\sqrt{6}} (\sqrt{3}, \frac{1}{2})$ (where $a$ is the lattice constant). The USFE $\gamma_{\text{USFE}}$ corresponds to the lowest-energy barrier that needs to be crossed for the slip from the ideal configuration to the ISF configuration in the (112) direction. In order to obtain the correct SFEs, structural optimizations must be considered in this study. The relaxations perpendicular to the (111) plane are carried out by a combined optimization of supercell volume and atomic coordinates in shifted configuration.

### Table 1. The calculated equilibrium lattice parameters $a$ (Å) and elastic constants (GPa), in comparison with the experimental and previously calculated results.

| Material | $a$ | $c_{11}$ | $c_{12}$ | $c_{44}$ | $\mu$ | $\nu$ |
|----------|-----|---------|---------|---------|-------|-------|
| Al       | 4.05, 4.05$^a$ | 112.3, 114.3$^b$ | 60.7, 61.3$^b$ | 30.2, 31.6$^b$ | 25.8, 26.3$^b$ | 0.350, 0.349$^b$ |
| Cu       | 3.64, 3.62$^a$ | 175.3, 176.2$^b$ | 124.4, 124.9$^b$ | 80.9, 81.8$^b$ | 25.5, 25.7$^b$ | 0.415, 0.415$^b$ |
| Ir       | 3.88, 3.84$^a$ | 579.6, 582.3$^b$ | 240.8, 241.3$^b$ | 261.2, 262.0$^b$ | 167.9, 170.5$^b$ | 0.294, 0.293$^b$ |
| Pd       | 3.96, 3.90$^a$ | 232.1, 234.1$^b$ | 175.2, 176.1$^b$ | 70.5, 71.2$^b$ | 28.5, 29.0$^b$ | 0.430, 0.420$^b$ |
| Pt       | 3.99, 3.92$^a$ | 356.8, 358.0$^b$ | 252.2, 253.6$^b$ | 76.3, 77.4$^b$ | 52.3, 52.2$^b$ | 0.414, 0.415$^b$ |

$^a$[29].

$^b$[30].
The projection of the GSFE surface in the (111) plane for FCC metals. The experimental and other calculated results are also listed. All values are in units of mJ m$^{-2}$.

|            | Cu  | Al  | Ir  | Pd  | Pt  |
|------------|-----|-----|-----|-----|-----|
| $\gamma_1$ | 160 | 158 | 615 | 167 | 171 |
| $\gamma_2$ | 260 | 213 | 928 | 243 | 188 |
| $\gamma_{ISF}$ | 43  | 158 | 359 | 122 | 262 |
| $\gamma_{SF}^d$ | 75  | 146 | 41  | 244 | 356 |
| $\gamma_{SF}^b$ | 43  | 150 |     | 101 | 111 |
| $\gamma_{SF}^c$ | 51  | 153 |     | 186 |     |
| $\gamma_{SF}^{d}$ | 40  | 45  | 169 | 300 | 322 |
| $\gamma_{USF}$ along (112) | 175 | 225 | 753 | 215 | 311 |
| $\gamma_{USF}$ along (110) | 638 | 633 | 2462| 668 | 685 |

Figure 3. Disregistry profile $u(x)$ (a) and dislocation density (b) for the edge dislocation in Al are obtained from our first-principles calculations combined with the improved P–N equation. The solid and dashed lines represent the edge and screw components of displacement, respectively. The black dot marks the displacement of the screw component of the crystallographic Shockley partial dislocation, which is about 0.29b. Here the maximum value of relative displacements of screw components of the partial dislocation is 0.13b.

The GSFE surface $\gamma(u)$ satisfies the translational symmetry $\gamma(R+u) = \gamma(u)$, (1) where $R$ is the lattice vector. The GSFE surface can be represented with the aid of the reciprocal lattice by a 2D
Fourier series that reflects the full symmetry of the (111) plane,

\[ \gamma'(u) = \sum_n \gamma_n e^{iG \cdot u}, \]  

where \( G \) is the reciprocal lattice vector. The nearest-neighbor approximation in reciprocal lattice space is taken into account,

\[ \gamma'(u', u'') = \gamma_0 + \gamma_1 \left\{ \cos \left( \frac{4\pi u'}{\sqrt{3}a} \right) + \cos \left( \frac{2\pi u^x}{a} + \frac{2\pi u^y}{\sqrt{3}a} \right) \right\} + \gamma_2 \left\{ \sin \left( \frac{4\pi u'}{\sqrt{3}a} \right) - \sin \left( \frac{2\pi u^x}{a} + \frac{2\pi u^y}{\sqrt{3}a} \right) \right\}. \]  

The coefficients \( \gamma_0, \gamma_1 \) and \( \gamma_2 \) can be determined by fitting to the GSFE surface that can be obtained by our first-principles calculations. \( \gamma_0 \) represents the ground state energy, which does not influence the shape of the GSFE surface and can be chosen to the zero, so only \( \gamma_1 \) and \( \gamma_2 \) need to be fixed. We list the fitted parameters \( \gamma_1 \) and \( \gamma_2 \) of equation (3) for all calculated FCC metals in table 2. Equation (3) is accurate for describing the translational and reflection symmetry of the GSFE surface on the (111) plane in FCC metals, and facilitates the computation of dislocation properties.

3. The dissociation of dislocation and the governing equation

3.1. The improved P–N dislocation equation

In the (111) plane of FCC metals, the primary slip system is \( \langle 112 \rangle \langle 111 \rangle \), so dislocations with the Burgers’ vector \( \frac{1}{2}[110] \) will energetically favor dissociating into two Shockley partials connected by an SF ribbon according to Frank’s rule [1]. The dissociation process is described by the following reaction:

\[ \frac{1}{2}[110] \rightarrow \frac{1}{2}[\bar{1}2] + SF + \frac{1}{2}[\bar{1}1]. \]

The dissociation can be understood from the GSFE surfaces for the slip plane (111). Figure 2 shows that the lowest-energy path happens to be along the \( \langle 112 \rangle \) direction, and perfect dislocations (Burgers’ vector \( b_1 = \frac{1}{2}[\bar{1}2] \)) are likely to dissociate into partial dislocations (Burgers’ vectors are \( b_1 = \frac{1}{2}[\bar{1}2] \) and \( b_2 = \frac{1}{2}[\bar{1}1] \)) due to the lower-energy barrier. The two partial dislocations are 60° fractional dislocations, namely the included angle between the dislocation line and the Burgers’ vector is 60°. The magnitude of the total Burgers vector is \( b = \sqrt{a/2} \) and \( a \) is the lattice constant for FCC metal. The Burgers’ vectors of the two partial dislocations have magnitudes \( b_1 = b_2 = \sqrt{3b}/3 \). Hereafter, let the dislocation lines be parallel to the \( y \)-axis (\( \langle 112 \rangle \) direction) and perpendicular to the total Burgers’ vector of edge dislocation (\( \langle 110 \rangle \) direction). The x- and y-components, respectively, represent the edge and screw components of partial dislocations for dissociation from edge dislocation.

The 2D dislocation equation for straight dislocations that describes the balance of atoms on the border based on the lattice dynamics and the symmetry principle takes the following form [18]:

\[ -\beta_e \frac{d^2 u^x}{dx^2} - K_e \int_{-\infty}^{+\infty} \frac{dx'}{x^2-x} \left( \frac{du^y}{dx} \right) \bigg|_{x=x'} = f^x(u^x, u^y), \]

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

where \( K_e \) and \( K_s \) are the energy factors of the edge and screw dislocations, and \( u^x \) and \( u^y \) are the edge and screw components of displacements, respectively. For the isotropic solid, \( K_e = \mu \sigma/(1-\nu) \) and \( K_s = \mu \sigma \), with \( \mu \) being the shear modulus and \( \nu \) Poisson’s ratio and \( \sigma \) is the area of the primitive cell of the misfit plane. The shear modulus and Poisson’s ratio can be expressed as the second-order elastic constants \( c_{ij} \), i.e. \( \mu = (c_{11} - c_{12})/2 \) and \( \nu = c_{12}/(c_{11} + c_{12}) \) (the values as shown in table 1). The coefficients of the second-order derivations \( \beta_e \) and \( \beta_s \) relate to the acoustic phonon velocity and the lattice geometry structure

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

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

where \( \theta \) and \( \phi \) are the orientation angles of the relative positions of a pair of neighbor atoms in the intrinsic frame with the axes given by the polarization directions, \( \theta = \pi/4 \) and \( \phi = \pi/6 \) for FCC crystals, and \( \Omega \) is the volume of the primitive cell. Compared with the generalized 2D P–N equation in the P–N model, there are two extra second-order derivations that represent the discreteness effect of crystals in the new equation. From exactly solvable models [17, 18], in which the discreteness of a lattice can be fully considered, one clearly sees the discreteness correction appearing in terms of the second-differential of the displacement. Physically, the integral term in equation (5) represents a long-range interaction that is inversely proportional to the distance, and the differential term describes short-range interaction that results from the interaction among the atoms on the surface plane. When \( \beta_e \) and \( \beta_s \) are taken to be zero, namely the discreteness effect is neglected, the generalized 2D P–N equation can be obtained [16].

3.2. The core properties of dissociated dislocation with the variational method

The dislocation solution of the 2D dislocation equation is unknown. In this paper, the variational method is applied to the 2D dislocation equation [17, 35]. It can be straightforwardly verified that the variational functional of the
2D dislocation equation takes the following form:

\[
J = -\frac{\beta_e}{4} \int_{-\infty}^{+\infty} \left( \frac{du^y}{dx} \right)^2 dx - \frac{K_e}{4\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{du^y}{dx} \frac{du^x}{dy} |_{x=y} dx dy
\]

\[
\times \ln \frac{x-x'}{d} dx dy - \frac{\beta_s}{4} \int_{-\infty}^{+\infty} \left( \frac{du^y}{dx} \right)^2 dx
\]

\[
\times \ln \frac{x-x'}{d} dx dy + \int_{-\infty}^{+\infty} \gamma(u^x, u^y) dx,
\]

where \(d\) is the distance of the nearest atoms in the misfit plane.

To obtain the structure of the dissociated dislocation, we represent each of the two partials by two closely spaced Peierls dislocations (or arctan type) that can ensure the correct asymptotic behavior. Thus, the trial dislocation solution for dissociated dislocation can be written as

\[
u^x = \frac{b}{2\pi} \left\{ \arctan \left( \frac{x+d_{eq}/2}{\xi_e} \right) + \arctan \left( \frac{x-d_{eq}/2}{\xi_e} \right) \right\} + \frac{b}{2},
\]

\[
u^y = \frac{\sqrt{3}b}{6\pi} \left\{ \arctan \left( \frac{x+d_{eq}/2}{\xi_e} \right) - \arctan \left( \frac{x-d_{eq}/2}{\xi_e} \right) \right\}.
\]

where \(d_{eq}\) is the equilibrium separation of two partial dislocations and \(\pm d_{eq}/2\) are the positions of the two partials, and \(\xi_e\) and \(\xi_s\) represent the core widths of the edge and screw components, respectively. The relation between the edge and screw components of the relative displacement determines the dissociation path in the glide plane. Generally, the width of the edge component \(\xi_e\) is not equal to that of the screw component \(\xi_s\) and the dissociation path deviations from the crystallographic Burgers’ vector \(\mathbf{b}\). Thus, the dissociated dislocations cannot be dealt with by the 1D dislocation equation.

Substituting the trial solution into the variational functional equation (8), the total variational functional \(J\) is a function of \(d_{eq}\), \(\xi_e\) and \(\xi_s\). The separation and the width of the edge and screw components can be determined by solving the following equations:

\[
\frac{\partial J}{\partial d_{eq}} = 0,
\]

\[
\frac{\partial J}{\partial \xi_e} = 0.
\]
Table 4. The predicted core structures, including core widths of both the edge and screw components, and dissociated distance in the FCC metals Cu, Al, Ir, Pd and Pt are listed. For completeness, we also list the results obtained from the P–N model in which the second-derivative term is neglected. For discussion, we give the $\gamma_{\text{ISF}}/\gamma_{\text{PF}}$ ratios along the (112) direction. The $\gamma_{\text{ISF}}/\gamma_{\text{PF}}$ ratio is dimensionless, and $\xi_e$, $\xi_s$ and $d_{\text{ISF}}$ are in units of the length of the Burgers’ vector $b = \sqrt{2}/2a$.

|       | Cu  | Al  | Ir  | Pd  | Pt  |
|-------|-----|-----|-----|-----|-----|
| $\xi_e$ | 2.6$^a$, 2.1$^a$ | 2.5$^a$, 2.0$^a$ | 3.5$^a$, 3.1$^a$ | 3.1$^a$, 2.4$^a$ | 4.8$^a$, 4.0$^a$ |
| $\xi_s$ | 1.9$^b$, 1.5$^b$ | 2.1$^b$, 1.6$^b$ | 2.9$^b$, 2.5$^b$ | 2.4$^b$, 1.8$^b$ | 3.9$^b$, 3.0$^b$ |
| $d_{\text{ISF}}$ | 5.5$^a$, 3.7$^a$ | 3.6$^a$, 2.6$^a$ | 5.6$^b$, 4.6$^b$ | 5.4$^b$, 3.5$^b$ | 5.5$^a$, 4.0$^a$ |
| $\gamma_{\text{ISF}}/\gamma_{\text{PF}}$ | 4.07 | 1.42 | 2.10 | 1.76 | 1.10 |

$^a$ Obtained from the improved P–N equation (with second-derivative term).

$^b$ Obtained from the P–N equation (without second-derivative term).

Figure 4. The same as in figure 3, but for Cu. Here the maximum value of relative displacements of screw components of the partial dislocation is 0.20b.

Burgers’ vector of the partial $\frac{1}{2}(112) = 0.29b$ (the black dot in figure 3(a)). This means that the area within two partials is not a pure SF ribbon, where the core regions of the two partials overlap and the displacement of the $\gamma$-components annihilate each other due to the opposite direction [8, 36]. The structure of dislocations in Al cannot be dealt with using the 1D model due to the strong overlap of two partials as illustrated in figure 3(b). The two partial dislocations cannot be identified due to the large overlap that is consistent with the experiment and the first-principles simulation [4].

In this work, the core structures of edge dislocation in other FCC metals Cu, Ir, Pd and Pt have also been calculated by using first-principles calculations GSFE surfaces based on the improved P–N equation. The core widths of both the edge and screw components and the dissociated distances are listed in table 4, and the registry and the dislocation density for Cu, Ir, Pd and Pt are shown in figures 4–7, respectively. We have listed in table 4 the results obtained from the P–N model in which the second-derivative term is neglected. One can see that the discrete effects always increase the widths of both the edge and screw components. Physically, the improved P–N equation, equation (5), is more functional to determine the structures of dislocation than the classical P–N equation [18], but for the calculated FCC metals we regret not being able to find any experimental data that would clearly demonstrate that the results with the second-derivative term are superior to those without the second-derivative term. We cannot be sure which model is a better one at the present level of knowledge. However, we believe that the new experimental results will clarify this question.

It is known that the deformation mechanism cannot be explained by the absolute value of ISFE $\gamma_{\text{ISF}}$ alone and the entire behavior has to be understood in terms of the ratio $\gamma_{\text{ISF}}/\gamma_{\text{PF}}$ along $(112)$ [14], so we also list the $\gamma_{\text{ISF}}/\gamma_{\text{PF}}$ ratios in table 4. When this ratio is low, the energy barrier that has to be overcome for creating a trailing partial is very low and therefore it will be possible to observe the full dislocation. Pt has the lowest $\gamma_{\text{ISF}}/\gamma_{\text{PF}}$ ratio 1.10 in our calculation, so the overlap of two partials is so strong that one cannot distinguish them although dissociation behavior exists. In figure 7, we can see that the maximum value of $u_x$ for Pt is 0.11b and the two-peak of the dislocation density for the edge component $\rho_x$ vanishes. But when this ratio is large, the energy increase...
necessary for nucleating the trailing partial is substantial, which is the case for Cu with the large $\gamma_{\text{USF}}/\gamma_{\text{ISF}}$ ratio 4.07. In figure 4, we can see that the overlap of two partials is weak in Cu. It has been verified in simulations [37] that extended partial dislocations in Cu have been observed as the predominant deformation mechanism at nanocrystalline grains. It is worth noting that although the dissociated distance of 5.5$b$ for Pt is larger than the 5.4$b$ for Pd, the core width of Pt is larger than that of Pd. This explains why figure 6 for Pd shows the two-peak of $\rho_x$, but figure 7 for Pt does not. Our detailed calculations demonstrate that whether full dislocations or Shockley partials can easily be observed, an FCC lattice must be understood in terms of the $\gamma_{\text{USF}}/\gamma_{\text{ISF}}$ ratio.

4. Conclusion

In conclusion, we have performed first-principles calculations to obtain the GSFE surface for the [111] glide plane in the FCC metals Cu, Al, Ir, Pd and Pt. The accuracy of the method has been tested by calculating the values for various SFEs, which favorably compare with previous theoretical and experimental results. From these calculations, we extract the core properties for the edge dislocation of dissociation into partials, using the improved P–N equation that includes the discreteness effect of crystals. The Ritz variational method is presented to solve the dislocation equation and the trial solution is constituted by two arctan-type functions, which represents the dislocation dissociating into two partials. The core structures, including the core widths of both the edge and screw components, and dissociation behavior for edge dislocations have been investigated. The dissociated distance between two partials for Al in our calculation agrees well with the values obtained from the numeric simulation with DFT and MD methods, as well as experiment. Our detailed calculations demonstrate that whether full dislocations or Shockley partials will easily be observed, an FCC lattice must be understood in terms of the $\gamma_{\text{USF}}/\gamma_{\text{ISF}}$ ratio, and show that it is preferred to create partial dislocation in Cu, and easily observed full dislocation in Al, Ir, Pd and especially Pt.

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Figure 7. The same as in figure 3, but for Pt. Here the maximum value of relative displacements of screw components of the partial dislocation is 0.11$b$. 

![Graph](image_url)