Shape change and Peierls barrier of dislocation

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Shape change and Peierls barrier of dislocation are investigated theoretically in the framework of the improved Peierls-Nabarro model in which the lattice discreteness is considered fully. We found that the dislocation will become narrow as it moves from the energy valley to the barrier top. An expression for the Peierls barrier is proposed based on our calculations without the rigid translation assumption. The results enable us to relate the Peierls stress to the bulk properties of crystals directly and can be easily used in the evaluation of material plasticity. © *2015 AIP Publishing LLC*.
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I. INTRODUCTION

Dislocation is a kind of structural defect in crystals. The plasticity of crystals is dominated by the mobility of dislocation. In the continuum approximation of the crystals, there exists the continuous translation symmetry. As a result, dislocations in the continuum can move freely in an invariant shape. In the real crystal, a dislocation will change its shape when it moves because the continuous translation symmetry is broken into discrete translation symmetry. Furthermore, a dislocation cannot move through crystal unless the applied stress exceeds a critical value that is referred to as Peierls stress.[1] Theoretically, the structure and the mobility of dislocations are usually studied by the famous Peierls-Nabarro model (P-N), which was proposed by Peierls and later elucidated by Nabarro.[1–4] The P-N model is characterized by a nonlinear integro-differential equation (Peierls equation) used to determine the structure of a dislocation and a rigid dislocation assumption used to obtain the energy fluctuation. Because the Peierls equation is invariant under continuous translation transformation, the dislocation shape does not change as it moves. Under the rigid dislocation assumption, the discrete structure of a dislocation is proposed to be such that its continuous envelope is always identical with the solution of the Peierls equation. Although the shape is never changed in the P-N model, the energy changes periodically as a function of the dislocation position because the dislocation actually lives in a periodic world due to the periodic structure of a crystal. As a topological excitation, it is reasonable to expect that the shape change should be small because the major feature of a dislocation shape is preserved by its topology. However, while the P-N model can be well applied to the wide dislocation, it becomes increasingly inaccurate for narrow dislocations of which the shape change is not negligible and the Peierls stress is modified remarkably.[5]

Shape change caused by discreteness is a fundamental issue in physics. It is interesting to know how a dislocation changes its shape when it moves, and how the Peierls barrier is modified when the shape change is taken into account, and what the condition is under which the shape is nearly invariant? The issue has attracted a lot of attention, and considerable effort has been exerted to make progress.[5–10] However, due to complexity of the discrete system, the issues are still not been explored systematically in a fundamental way. And the major effects of discreteness on the shape change still need to be clarified. In this paper, a fully discrete equation is proposed on the general basis of the lattice dynamics, and an approximated method is developed to obtain discrete solutions. By using the free energy of dislocation given in the theory, shape change and the Peierls barrier of dislocation are studied in a reliable way. The results provide new insights into what is happening during the dislocation motion.

II. THE CHARACTERISTIC SCALES

The characteristic scale of a crystal is the lattice constant. It is assumed that the lattice constant $a \to 0$ in the continuum theory of solids. In fact, this assumption should be understood as that $\zeta/a \gg 1$, where ζ is the length scale involved in problems. A solid can be approximated as continuum provided that the length scale ζ is much larger than the lattice constant a. It is significant to clarify the length scale of dislocations.

In the classical P-N theory of dislocations, the fundamental equation is the famous Peierls equation[1]

$$-\frac{\mu}{2\pi(1-\nu)}\int_{-\infty}^{+\infty}\frac{dx'}{x'-x}\left(\frac{du}{dx}\right)\Big|_{x=x'}=\frac{\mu b}{2\pi d}\sin\left(\frac{2\pi u}{b}\right), \quad (1)$$

where u is the mismatch field, μ is the shear modulus, ν is the Poisson ratio, b is the Burger's vector, and d is the space between the glide planes. The Peierls equation has an exact solution[1]

$$u(x)=\frac{b}{\pi}\arctan(q), \quad q=k_p x, \quad k_p=\frac{2(1-\nu)}{d}. \quad (2)$$

This solution is uniquely characterized by a length scale

$$\zeta_p=\frac{1}{k_p}=\frac{d}{2(1-\nu)},$$

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and the related distribution is the Lorentz type

$$\rho(x) = \frac{du}{dx} = \frac{b}{\pi}\frac{k_p}{1+q^2} = \frac{b}{\pi}\frac{\zeta_p}{\zeta_p^2 + x^2}. \tag{3}$$

The length scale ζ_p is referred to as the width of the dislocation. It is proportional to the space with a factor slightly small than one, $\zeta_p \sim d$. For the SC lattice, the glide set is consisted of the {100} planes that has the maximum space, $d = a$, the dislocation width is $\zeta_p = 3a/4$, for $\nu = 1/3$. For the FCC lattice, the {111} planes are glide planes with the space $d = a/\sqrt{3}$, the dislocation width $\zeta_p = \sqrt{3}a/4$ for $\nu = 1/3$. For the glide dislocation in the diamond structure, $d = \sqrt{3}a/12$ and $\zeta_p = \sqrt{3}a/16$, for $\nu = 1/3$. The dislocations predicted by the classical Peierls equation are very narrow, in particular, for those in the covalent materials.

The classical Peierls equation is improved by using the generalized stacking-fault energy (γ-surface) and by taking the lattice discreteness correction into account. The improved equation is[11,12]

$$-\frac{\beta}{2}\frac{d^2u}{dx^2} - \frac{K}{2\pi}\int_{-\infty}^{+\infty}\frac{dx'}{x'-x}\frac{du}{dx'} = f, \tag{4}$$

where β is a constant describing the discreteness correction, K is the energy factor, $K = \frac{\mu}{1-\nu}$ for the edge dislocation, $K = \mu$ for the screw dislocation, f is the force on a unit area and given by gradient of γ-surface

$$f = -\frac{d\gamma}{du}, \quad \gamma = \frac{\mu b^2}{2\pi^2 d}\cos^2\frac{\pi u}{b}\left(1 + \Delta\cos^2\frac{\pi u}{b}\right), \tag{5}$$

Δ is a dimensionless parameter introduced to have a correct unstable stacking-fault energy.[13–16] The related variational functional is

$$F = \frac{\beta}{4}\int_{-\infty}^{+\infty}\rho^2(x)dx - \frac{K}{4\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\rho(x)\rho(x')\ln\frac{|x-x'|}{b}dxdx' + \int_{-\infty}^{+\infty}\gamma(u)dx. \tag{6}$$

The improved Peierls equation is a nonlinear integro-differential equation that can be hardly solved exactly. However, it is observed that the dislocation solution can be formally expressed as[17]

$$u = \frac{b}{\pi}\left[\arctan q + q\left(c_1 y + c_2 y^2 + \cdots\right)\right], \tag{7}$$

with

$$q = kx, \quad y = \frac{1}{1+q^2},$$

where k and $c_1, c_2, \ldots$ are constants need to be determined. It is not difficult to confirm this assertion. Substituting the formal solution equation (7) into Eq. (4), the left-hand side can be written as a polynomial of y with q as its pre-factor, and meanwhile, similar result can be obtained for the right-hand side when it is expanded as a power series of y. One can always make the left-hand side equals to the right-hand side by suitably selecting the constants k and $c_1, c_2, \ldots$.

From Eq. (7), it is easy to show that the distribution can be expressed in a series of y

$$\rho(x) = \alpha_1 y + \alpha_2 y^2 + \cdots, \tag{8}$$

where the coefficients $\alpha_1, \alpha_2, \ldots$ are the functions of the constants k and c_i. The formal solution equation (7) or Eq. (8) is a kind of series and can be truncated rationally to obtain the approximated solutions.[17,18] In the region far from the dislocation core $|x| \to \pm\infty$, the effects of the details of a dislocation structure should be negligible. Furthermore, the results obtained in the continuum elastic theory should be valid far from the dislocation core. This implies that the asymptotic behavior of the dislocation solution should be identical with that given in the classical Peierls equation

$$\rho(x) \to \frac{kb}{\pi}\frac{1-c_1}{1+q^2} \to \frac{b}{\pi}\frac{1-c_1}{kx^2}, \quad \text{as } x \to \infty. \tag{9}$$

Comparing with Eq. (3) in the limit $x \to \infty$, one obtains an important relation for constants k and c

$$k = k_p(1-c_1), \quad k_p = \frac{2\mu}{Kd}. \tag{10}$$

This relation is irrelevant to the specific form of the dislocation structure. Far from the dislocation core, the asymptotic behavior of dislocation is uniquely controlled by k_p, dislocation features are independent of constants $c_1, c_2, \ldots$. It is rational to interpret the constant c_i as the structure constants and to interpret the scale factor in the expression

$$\zeta = \frac{1}{k} = \frac{\zeta_p}{1-c_1},$$

as the characteristic length scale of a dislocation. Generally, the characteristic scale of the dislocation predicted from the improved equation is quite different from that given in the classical Peierls equation. For the $\langle 100\rangle\{010\}$ edge dislocation in BCC Fe, the structure constant is about $c_1 \sim 0.77$, and the characteristic length, $\zeta \sim 4\zeta_p \approx a$, is about four times of that given in the classical P-N theory.[12] For the glide dislocation (p-h pair) in graphene, $c_1 \sim 0.37$ and $\zeta \approx 0.31a$,[19] and for the glide partial dislocation in silicon, $c_1 \sim 0.6$ and $\zeta \approx 0.24a$.[20] Although the characteristic length ζ of dislocations is increased considerably comparing with that given in the classical P-N theory, it is still much smaller than the lattice constant a especially for the covalent materials. It is necessary to develop a fully discrete theory to investigate the dislocation properties.

III. FULLY DISCRETE EQUATION OF A STRAIGHT DISLOCATION

Within the harmonic approximation of the interaction among the atoms in a solid, the discrete equation of a straight dislocation can be generally written as[11,21]

$$\sum_{l'=-\infty}^{\infty}\Omega(l-l')u(l') = f(l), \tag{11}$$

where integers l and l' are used to label the atoms on the mismatched lattice plane, $u(l)$ is the mismatch field defined as the relative displacement, and $\Omega(l)$ is the discrete kernel. In physics, the kernel $\Omega(l)$ represents the force field produced by a unit mismatch $u(0)=1$ at the origin $l'=0$.

While the dislocation equation (11) can be formally obtained from the lattice dynamics, the key problem is how to clearly specify the discrete kernel Ω in a model-independent way, with which the Peierls equation can be recovered in the continuous limit. In fact, the discrete kernel Ω can be properly dealt within the wave-vector space (k-space)

$$\Omega(l)=\frac{\lambda}{2\pi}\int_{-\frac{\pi}{\lambda}}^{\frac{\pi}{\lambda}}\tilde{\Omega}(k)e^{ilk\lambda}dk,$$

where λ is the period in the direction perpendicular to dislocation line. It is crucial to observe that $\tilde{\Omega}(k)$ consists of the regular part $\tilde{\Omega}_r(k)$ and the singular part $\tilde{\Omega}_s(k)$[11,21,22]

$$\tilde{\Omega}(k)=\tilde{\Omega}_s(k)+\tilde{\Omega}_r(k). \tag{12}$$

The regular part represents the interaction between the atoms on a mismatched plane and can be expanded into the Fourier series

$$\tilde{\Omega}_r(k)=\omega_0^r+\omega_1^r\cos(k\lambda)+\cdots.$$

The singular part results from the interaction with the atoms in the interior and should be expanded into the following Fourier series:

$$\tilde{\Omega}_s(k)=\tilde{\Omega}_s(-k)=\omega_0^s\sin\left(\frac{1}{2}k\lambda\right)+\omega_1^s\sin\left(\frac{3}{2}k\lambda\right)+\cdots,\ k\geq 0. \tag{13}$$

The series of $\tilde{\Omega}$ converges rapidly when it is expanded in this way.[22] In the leading term approximation

$$\tilde{\Omega}_r(k)=\omega_0^r(1-\cos k\lambda),\quad \tilde{\Omega}_s(k)=\tilde{\Omega}_s(-k)$$
$$=\omega_0^s\sin\left(\frac{1}{2}k\lambda\right),$$

where $\omega_0^r+\omega_1^r=0$ has been used,[11] the dislocation equation (11) becomes

$$-\frac{1}{2}\omega_0^r\left[\rho(l)-\rho(l-1)\right]-\frac{\omega_0^s}{2\pi}\sum_{l'=-\infty}^{\infty}\frac{\rho(l')}{l'-l+\frac{1}{2}}=f(l), \tag{14}$$

where $\rho(l)=u(l+1)-u(l)$ is the dislocation density. This equation is a fully discrete dislocation equation. It is obtained in a model-independent way. In the continuous approximation, the discrete equation (14) becomes an integro-differential equation

$$-\frac{1}{2}\omega_0^r\lambda^2\frac{d^2u(x)}{dx^2}-\frac{\omega_0^s\lambda}{2\pi}\int_{-\infty}^{+\infty}\frac{dx'}{x'-x}\frac{du}{dx}\bigg|_{x=x'}=f(x), \tag{15}$$

where $x=l\lambda$ is the coordinates. Comparing with the dislocation equation given previously,[11,12] we have

$$\omega_0^s=\frac{K}{\lambda},\quad \omega_0^s=\frac{\beta}{\lambda^2}, \tag{16}$$

where K is the energy factor of a straight dislocation and β is the effective force constant between the neighbor atoms.

It is straightforward to show that the energy functional of the dislocation equation (14) is

$$F=\frac{\beta}{4\lambda^2}\sum_{l=-\infty}^{\infty}\rho(l)^2$$
$$-\frac{K}{4\pi\lambda}\sum_{l=-\infty}^{\infty}\sum_{l'=-\infty}^{\infty}\rho(l)\rho(l')\psi^{(0)}\left(|l-l'|+\frac{1}{2}\right)$$
$$+\sum_{l=-\infty}^{\infty}\gamma(u), \tag{17}$$

where $\psi^{(0)}(z)$ is the Polygamma function

$$\psi^{(0)}(z)=\frac{1}{\Gamma(z)}\frac{d\Gamma(z)}{dz}.$$

It is interesting to see that the interaction potential between two dislocations is given by the Polygamma function $\psi^{(0)}(|l|+\frac{1}{2})$ in the lattice theory. The interaction potential $\psi^{(0)}(l+\frac{1}{2})$ is coincided with $\ln(l)$ appeared in continuum theory for $l\gg 1$.

IV. SHAPE CHANGE AND PEIERLS BARRIER OF DISLOCATION

The fully discrete equation of dislocation can be hardly solved exactly. The Ritz variational method is an efficient way to find the solution. The key point of the Ritz variational method is finding a good trial solution with correct asymptotic-behavior. Instead of the mismatch field, we first focus on the density distribution. If the density $\rho(l)$ is given, the field $u(l)$ can be obtained

$$u(l)=\sum_{-\infty}^{l-1}\rho(l')+u(-\infty).$$

For the Lorentz distribution around point t characterized by the width ζ

$$Y=\frac{1}{\bar{\zeta}^2+(l-t)^2},\quad \bar{\zeta}=\frac{\zeta}{\lambda},$$

we have

$$u_0(l)=\sum_{-\infty}^{l-1}Y(l')$$
$$=\frac{i}{2\bar{\zeta}}\left[\psi^{(0)}(-l+t-i\bar{\zeta}+1)-\psi^{(0)}(-l+t+i\bar{\zeta}+1)\right]$$

and normalization constant of the distribution

$$Q_0(l)=\sum_{-\infty}^{+\infty}Y(l')=\frac{\pi}{\bar{\zeta}}\times\Gamma_0,\quad \Gamma_0=\frac{\sinh(2\pi\bar{\zeta})}{\cosh(2\pi\bar{\zeta})-\cos(2\pi t)}.$$

The term $\pi/\bar{\zeta}$ is the normalization constant of the Lorentz distribution in the continuum approximation, and the term Γ_0 is the correction from lattice discreteness. For the wide distribution $\zeta \gg \lambda$, the correction term $\Gamma_0 \sim 1$. If the width $\zeta < \lambda/2$, the correction is not negligible, and it is also dependent on position coordinates t of the distribution.

Based on the knowledge learned from the continuous approximation, we assume that the distribution ρ of a dislocation can be expressed as a polynomial of Y

$$\rho(l) = \alpha_1 Y + \alpha_2 Y^2 + \cdots.$$

Keeping the terms up to the second order, the normalized density distribution can be written as

$$\rho(l) = \frac{\hat{D}Y}{Q}, \quad Q = \hat{D}Q_0, \tag{18}$$

where parametric derivative

$$\hat{D} = (1-c)\bar{\zeta}^2 - c\bar{\zeta}^3 \frac{\partial}{\partial \bar{\zeta}}$$

is introduced for convenience. This density is similar to that generally used in the continuous approximation. The parameter ζ is the characteristic width of dislocation. The parameter c is the structure constant of the dislocation. The parameter t is the coordinate of dislocation. The mismatch field of the distribution is

$$u(l) = \frac{\hat{D}u_0}{Q}.$$

Substituting $u(l)$ and $\rho(l)$ into Eq. (14) and letting the left-hand sides equals to the right-hand sides to the order $1/l$, we obtain a relation between the structure constant c and the characteristic width $\bar{\zeta}$

$$c = \frac{2\bar{\zeta}\phi + i\left(-\pi\cot\left[\pi\left(t-i\bar{\zeta}\right)\right] + \pi\cot\left[\pi\left(t+i\bar{\zeta}\right)\right]\right)}{\bar{\zeta}\left(2\phi + \pi^2\csc\left[\pi\left(t-i\bar{\zeta}\right)\right]^2 + \pi^2\csc\left[\pi\left(t+i\bar{\zeta}\right)\right]^2\right)}, \tag{19}$$

where ϕ is a constant related to the second derivative of the γ-surface at the equilibrium position

$$\phi = \frac{2\pi\lambda}{K}\frac{df}{du}\bigg|_{eq} = -\frac{2\pi\lambda}{K}\frac{d^2\gamma}{du^2}\bigg|_{eq}.$$

The approximated solution of the discrete equation of dislocation can be obtained by finding the minimum of the energy F as a function of the characteristic width ζ

$$F(\zeta) = \frac{\beta}{4\lambda^2}s(0) + \sum_{l=-N}^{l=N}\left[-\frac{K}{4\pi\lambda}s(l)\psi^{(0)}\left(|l|+\frac{1}{2}\right) + \gamma(u)\right], \quad N \to \infty,$$
$$s(l) = \sum_{l'=-\infty}^{\infty}\rho(l')\rho(l'-l), \tag{20}$$

where the summation in the expression of $s(l)$ can be obtained exactly, but its analytic expression is very long and omitted here. In the following, the period $\lambda = b$ is assumed, the stress is measured by the shear modulus, $\mu = 1$, the length is measured by the Burgers vector, $b = 1$.

For the quasi-static process where the dislocation moves slowly, the dislocation shape changes periodically. In the leading term approximation, the characteristic width ζ and the structure constant c can be expressed as

$$\zeta(t) = \frac{1}{2}(\zeta_B + \zeta_O) + \frac{1}{2}(\zeta_B - \zeta_O)\cos 2\pi t,$$
$$c(t) = \frac{1}{2}(c_B + c_O) + \frac{1}{2}(c_B - c_O)\cos 2\pi t. \tag{21}$$

The constants ζ_B (c_B) and ζ_O (c_O) are, respectively, the characteristic widths (structure constants) of the dislocation at the energy valley and the barrier top. The dislocation localized at the energy valley is a stable equilibrium. The dislocation localized at the barrier top is an unstable equilibrium. The stable dislocation will be referred to as B-type dislocation and the unstable dislocation will be referred to as O-type dislocation. The Peierls barrier E_p is the energy difference between the O-type and B-type dislocations.

In order to reveal the features of phenomenon, the lattice version of the classical Peierls equation ($\beta = 0$ and $\Delta = 0$) is investigated first. The characteristic widths of dislocation have been evaluated for the different space that affects the dislocation structure. It is found that the structure constant is zero, $c = 0$, provided that the space is not too small. As shown in Fig. 1, for the small space $d < b$, the characteristic widths of the O-type and B-type dislocation are apparently different. The characteristic widths of the B-type dislocation with the minimum energy are always larger than that of O-type dislocation. The result indicates that the dislocation becomes narrow when moving from the energy valley to the barrier top. The characteristic width approaches to that given by the continuous approximation $\zeta = d/2(1-\nu)$ for the large space $d > b$. The converging as the characteristic width increases implies that the wide dislocation nearly does not change its shape when moving slowly. In Fig. 2, the density distributions are plotted for $d = 0.6b$ and $d = b$. For $d = b$, the

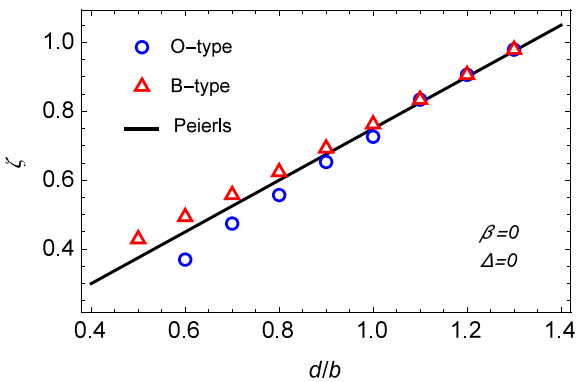

FIG. 1. The characteristic width ζ varies as a function of the space d for $\lambda = b$. The solid line is given by the continuous approximation obtained as an exact solution of the classical Peierls equation. The characteristic width of the B-type dislocation is wider than that of the O-type dislocation. Because the dislocation changes from the B-type to the O-type as it moves from energy valley to the barrier top, the dislocation in the ground state has a maximum width.

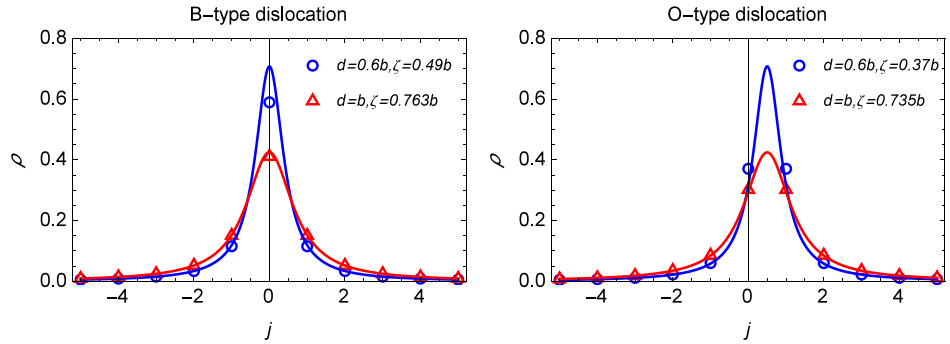

FIG. 2. The density distributions of dislocations for $\beta=0$ and $\Delta=0$. The lines are given by the Peierls solutions, the solid circles are evaluated from variational method presented in the text. The green lines (circles) are obtained for $d=0.6b$ and $\zeta_p=0.45b$, and the red lines (circles) are obtained for $d=b$ and $\zeta_p=0.75b$. For the wide dislocation $\zeta_p=0.75b$, the discrete distribution coincides with that from the Peierls solution. For the narrow dislocation $\zeta_p=0.45b$, there is discrepancy in particular, for the B-type dislocation.

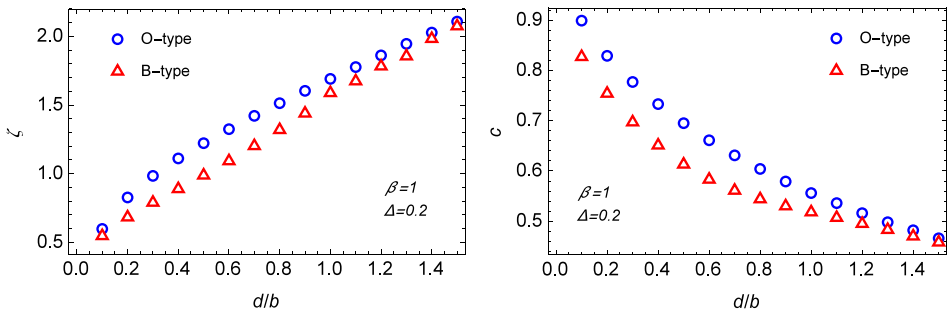

FIG. 3. The characteristic width ζ and structure constant c vs the space d. Similar to that shown in Fig. 1, the dislocation solution in the continuous approximation splits into the O-type and B-type solutions due to discreteness. The maximum difference in characteristic length ζ and the structure constant c occurs at $d\sim0.5$ for the two types of dislocation.

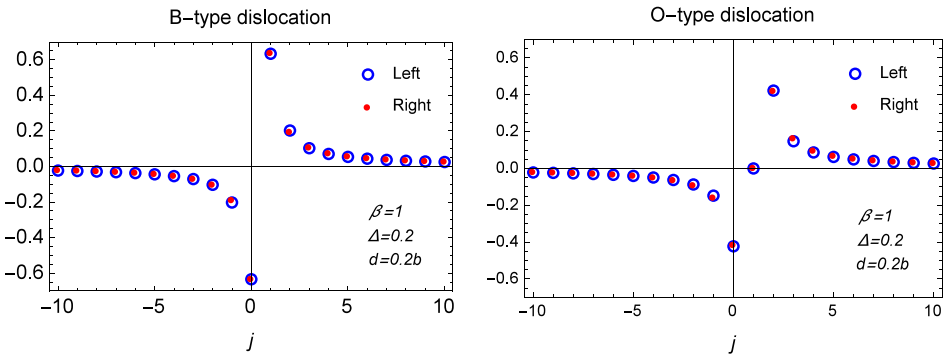

FIG. 4. In order to verify the accuracy of the solutions, the left-hand side and the right-hand side of the discrete equation are compared when the variational solutions are substituted into the dislocation equation (14). The agreement between them is satisfactory.

characteristic widths are, respectively, $\zeta=0.763b$ for the B-type and $\zeta=0.735b$ for the O-type, which are very close to $\zeta=0.75b$ given in the continuous approximation. For $d=0.6b$, the difference in core structure emerges clearly comparing with that given in the continuous approximation. The assumption of rigid dislocation cannot be used for the narrow dislocation.

The characteristic width ζ and structure constant c have been evaluated for $\beta=\mu b$ and $\Delta=0.2$. In this case, the lattice effects emerge even for wide dislocations. As shown in Fig. 3, the structures of B-type and O-type dislocations are different until $\zeta\sim2b$. In order to verify the accuracy of our calculation, the solutions have been substituted into Eq. (14) to see if the left-hand sides equals to the right-hand sides. As shown in Fig. 4, the solutions are quite good and the results are reliable. In the practical calculation, the summation range in Eq. (20) is chosen to be $N=200$. As shown in Table I, the results keep invariant except the energy F decreasing slightly as N increases from $N=200$ to $N=400$.

The Peierls barrier is the energy difference between the O-type and B-type dislocations. The Peierls barrier obtained in this way includes the contribution from the strain energy and the misfit energy. In Fig. 5, the Peierls barrier has been plotted as a function of the space d for some typical cases. The relation between the logarithm of Peierls barrier and the space is linear one.

The first two terms in the free energy Eq. (17) are the deformation energy caused by the dislocation. The last term in the free energy Eq. (17) is the mismatch energy between two sides of the cut-plane. For a dislocation, if the deformation energy is large, the dislocation width will be wide. In contrast, if the mismatch energy is large, the dislocation width will be narrow. The dislocation width actually results from the competition between the deformation energy and

TABLE I. The convergence test for selecting adequate summation range N in the calculation, with $\beta = 0.2$ and $\Delta = 0.2$.

N	ζ_B	ζ_O	F_B	F_O	E_p
100	0.683	0.827	0.4882	0.3447	0.1435
200	0.683	0.827	0.4877	0.3440	0.1437
300	0.683	0.827	0.4875	0.3438	0.1437
400	0.683	0.827	0.4874	0.3437	0.1437

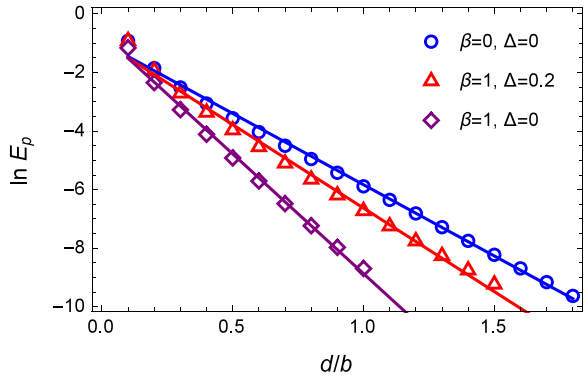

FIG. 5. The logarithm of Peierls barrier $\ln E_p$ vs the space d. The linear relation maintains for typical values of the β and Δ. There is a tendency that the straight lines converge together at small d.

the mismatch energy. A wide dislocation has a low Peierls barrier and a narrow dislocation has a high Peierls barrier. Therefore, the slope of the lines in Fig. 5 should proportional to $Kb + \beta$, which is the factor of the deformation energy, and inversely proportional to the unstable stacking fault energy γ_u, which measures the magnitude of the mismatch energy. The data obtained suggest the following expression:[3]

$$E_p = F_O - F_B = \frac{AKb^2}{4} e^{-\frac{Kb+\beta}{2\pi\gamma_{us}}} = \frac{AKb^2}{4} e^{-\frac{1+\frac{\beta}{Kb}}{1+\Delta}} e^{-\frac{\pi d}{(1-\nu)b}}, \quad (22)$$

where factor A is

$$A = 1 + \frac{1}{2\pi}\left(\frac{\beta}{Kb} - \Delta\right) \sim 1. \quad (23)$$

The Peierls stress is

$$\sigma_p = \frac{\pi E_p}{b^2} = \frac{\pi AK}{4} e^{-\frac{1+\frac{\beta}{Kb}}{1+\Delta}} e^{-\frac{\pi d}{(1-\nu)b}} = \frac{\pi AK}{4} e^{-\frac{1+\frac{\beta}{Kb}}{1+\Delta}} e^{-\frac{2\pi\zeta_p}{b}}, \quad (24)$$

where ζ_p is the Peierls width given in the classical Peierls equation. This expression enables us to directly relate the Peierls stress to the properties of bulk material and can be used easily in practice. For the $\frac{1}{2}\langle 111\rangle(110)$ screw dislocation in BCC Ta, $\zeta_p = d/2$, $\Delta \approx -0.33$, $\mu \approx 61$ GPa, $\beta \approx \mu b$, the Peierls stress from Eq. (24) is $\sigma_p = 226$ MPa. For the 90° partial dislocation in silicon, $\zeta_p = d/2(1-\nu)$, $d = b/2\sqrt{2}$, $\nu \approx 0.256$, $\Delta \approx 0.23$, $\mu \approx 69$GPa, $\beta \approx \mu b/2$, $\sigma_p = 5.4$GPa.[23,24] The results are close to the values given previously.[5,12,25,26]

V. SUMMARY AND DISCUSSION

A full discrete theory of dislocation is presented in a model-independent way and an efficient method of solving the dislocation equation is proposed. The theory can be generalized to include the higher order contribution in the Fourier series of Eq. (14) and in the polynomial of density, and the method can be applied to dislocations with complex structure like the dissociated dislocation. In the light of the variational evaluation, it is found that the dislocation in the ground state has its maximum width, and the dislocation will become narrow as it moves from the energy valley to the barrier top. Furthermore, based on our evaluation result, we propose a new expression for the Peierls barrier which directly relates to the physical constants of a material.

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