Variable core model and the Peierls stress for the mixed (screw-edge) dislocation

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A variable core model of a moving crystal dislocation is proposed and used to derive an expression for the Peierls stress. The dislocation width varies periodically as a dislocation moves through the lattice, which leads to an expression for the Peierls stress in terms of the difference of the total energies in the crystal corresponding to stable and unstable equilibrium configurations of the dislocation, rather than the difference in the misfit energies alone. Results for both edge and mixed dislocations are given and proposed to be used in conjunction with *ab initio* calculations. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2361277]

In the Peierls model of a crystal dislocation, the atomistic effects and the lattice discreteness are incorporated into the analysis approximately by considering them to be confined within a layer consisting of two atomic planes around the glide plane. This model of a crystal dislocation was used by Peierls[1] and Nabarro[2] to make the estimates of the minimum external stress required to move a dislocation in a perfect lattice, which is called the Peierls stress (τ_{PS}). Its determination is of significant interest for the physical theories of plasticity and creep, fracture mechanics, strain relaxation in thin films, etc.[3–5] However, the calculated values for τ_{PS} are an order of magnitude or higher than those experimentally observed or those calculated by atomistic models,[6–9] and continuing attempts were made to improve the Peierls-Nabarro model.[10–14]

In the present letter we derive an expression for the Peierls stress without using the concept of misfit energy. The Peierls stress is found to be $\tau_b^{\mathrm{PS}}=\pi(E_*-E_o)/ab$, where E_*-E_o is the difference between the energies of a whole stressed crystal when a dislocation is in its unstable and stable equilibrium positions, a is the interatomic distance in the glide plane normal to the dislocation line, and b is the magnitude of the Burgers vector.

An edge dislocation of a Volterra type has a singularity of order $1/x$. To eliminate this singularity, a linear increase of the Burgers vector over the distance ρ is assumed, where ρ is related to the extent of the dislocation core—severely deformed region around the center of the dislocation. (Lothe[15] used a linearly spread-out dislocation core for a screw dislocation to eliminate the divergence in the core energy, while the stresses remained singular at the core boundary. In this letter we use the wedge dislocation along the vertical axis, but only to produce a nonsingular shear stress distribution along the glide plane of an edge dislocation. This is then used in conjunction with a semi-inverse method to derive the corresponding displacement discontinuity along the glide plane.) This can be modeled by a continuous distribution of infinitesimal dislocations of specific Burgers vector b/ρ. The corresponding shear stress along the x axis is

$$\tau_{xy}(x,0)=\frac{\mu b}{2\pi(1-\nu)}\frac{x}{\rho}\int_0^{\rho}\frac{x^2-\eta^2}{(x^2+\eta^2)^2}d\eta$$

$$=\frac{\mu b}{2\pi(1-\nu)}\frac{x}{x^2+\rho^2}, \tag{1}$$

which has no singularity at $x=0$ and which coincides with the Volterra dislocation for $x\gg\rho$. If $\rho=h/2(1-\nu)$, where h is the atomic interplanar separation across the glide plane, as in the Peierls semidiscrete model, then $\tau_{xy}^{\max}=\mu b/2\pi h$, the theoretical shear strength of the crystal. Alternatively, if γ_{us} is Rice's[16] unstable stacking energy, then $\tau_{xy}^{\max}=\pi\gamma_{\mathrm{us}}/b$, where $\gamma_{\mathrm{us}}=\mu b^2/2\pi^2 h$ for the Frenkel sinusoidal function.

Assuming that the shear stress distribution is given by Eq. (1), we seek the continuous distribution of infinitesimal dislocations of the specific Burgers vector $\beta(x)$ along the glide plane $y=0$, so that

$$\tau_{xy}(x,0)=\frac{\mu}{2\pi(1-\nu)}\mathrm{p.v.}\int_{-\infty}^{\infty}\frac{\beta(\xi)}{x-\xi}d\xi, \tag{2}$$

where p.v. denotes the Cauchy principal value. The solution of the above Cauchy singular integral equation is

$$\beta(x)=\frac{b}{\pi}\frac{\rho}{x^2+\rho^2}, \tag{3}$$

with the corresponding slip discontinuity

$$\delta(x)=\int_0^x\beta(\xi)d\xi=\frac{b}{\pi}\tan^{-1}\frac{x}{\rho}. \tag{4}$$

As in the Peierls model, from Eq. (4) it follows that the width of the dislocation $w=2\rho$ defines the region over which the displacement discontinuity is less than $b/4$.

In view of the trigonometric identity

$$\sin\frac{2\pi\delta(x)}{b}=\sin\left(2\tan^{-1}\frac{x}{\rho}\right)\equiv\frac{2\rho x}{\rho^2+x^2}, \tag{5}$$

we conclude, by comparing Eqs. (1) and (5), that $\tau(x,0)$ and $\delta(x)$ are related by

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$$\tau_{xy}(x,0)=\frac{\mu}{4\pi(1-\nu)}\frac{b}{\rho}\sin\frac{2\pi\delta(x)}{b}. \tag{6}$$

Thus, unlike the Peierls-Nabarro model, we deduce from the analysis rather than assume the sinusoidal relationship between the shear stress and the slip discontinuity along the slip plane. The core radius ρ enters Eq. (6) rather than the atomic interplanar distance h, although ρ is expected to depend on the glide system and therefore on the glide plane spacing h. Since we are not separating in our analysis the two elastic half spaces by the distance h, we do not have a strain measure ϕ/h in the thin layer around the glide plane. Therefore, we do not require that $\tau=\mu\phi/h$ at large x (as in the Peierls-Nabarro model), and our core radius is not necessarily related to h by $\rho=h/2(1-\nu)$.

The work of the stress $\tau_{xy}(x,0)$ on the slip discontinuity $\delta(x)$ from the cutoff distance $-R$ to R, is

$$W=\frac{1}{2}\int_{-R}^{R}\tau_{xy}(x,0)\delta(x)dx, \tag{7}$$

which is

$$W=\frac{\mu b^2}{4\pi^2(1-\nu)}\left[\ln\left(1+\frac{R^2}{\rho^2}\right)\tan^{-1}\left(\frac{R}{\rho}\right)-\int_0^{R/\rho}\frac{\ln(1+z^2)}{1+z^2}dz\right]. \tag{8}$$

In the limit $R\gg\rho$, we obtain

$$W=\frac{\mu b^2}{4\pi(1-\nu)}\ln\frac{R}{2\rho}. \tag{9}$$

Far from the center of the dislocation, the stresses and displacements are essentially those of the Volterra dislocation, so that the work of the corresponding traction over the circle of radius R is $\mu b^2/8\pi(1-\nu)$. The total strain energy within a large radius R around the dislocation is then

$$E=\frac{\mu b^2}{4\pi(1-\nu)}\ln\frac{e^{1/2}R}{2\rho}. \tag{10}$$

Under a sufficiently large externally applied remote shear stress τ, the dislocation glides along its glide plane between consecutive positions of stable and unstable equilibrium. We propose as an approximation a simple periodic variation of the core radius ρ with glide distance Δ,

$$\rho(\Delta)=\frac{1}{2}(\rho_o+\rho_*)+\frac{1}{2}(\rho_o-\rho_*)\cos\frac{2\pi\Delta}{b}. \tag{11}$$

The core radius at the stable configuration $\Delta=0$ is ρ_o and at the unstable $\Delta=b/2$ is ρ_*.

The potential energy of a dislocated crystal, apart from an independent potential energy due to uniform elastic shear strain $\gamma=\tau/\mu$, is

$$\Pi(\Delta)=E(\Delta)-\int_0^{\Delta}b\tau(\Delta)d\Delta. \tag{12}$$

The second term on the right-hand side is the load potential, calculated as for the Volterra dislocation, since the fields far away from the core of the dislocation are the same. During the quasistatic displacement of the dislocation, we have $d\Pi/d\Delta=0$ and $b\tau(\Delta)=dE/d\Delta$. Thus, considering Eq. (11),

$$\tau(\Delta)=\frac{1}{b}\frac{dE}{d\rho}\frac{d\rho}{d\Delta}=\frac{\mu}{4(1-\nu)}\frac{\rho_o-\rho_*}{\rho}\sin\frac{2\pi\Delta}{b}. \tag{13}$$

The maximum value of this shear stress, with respect to Δ, is the shear stress required to move the dislocation in a perfect crystalline lattice by amount b and is referred to as the Peierls stress. Thus, $d\tau/d\Delta=0$ implies that

$$\tau_{\mathrm{PS}}=\frac{\mu}{4(1-\nu)}\frac{\rho_o-\rho_*}{\sqrt{\rho_o\rho_*}}. \tag{14}$$

In view of Eq. (10), we have

$$\frac{\rho_o}{\rho_*}=\exp\frac{E_*-E_o}{D},\quad D=\frac{\mu b^2}{4\pi(1-\nu)}, \tag{15}$$

where E_*-E_o is the energy difference between the unstable and stable equilibrium positions of the dislocation, which is the key quantity in the subsequent analysis. With a nondimensional parameter $\Gamma=(E_*-E_o)/2D$, the Peierls stress (14) is written as

$$\tau_{\mathrm{PS}}=\frac{\mu}{4(1-\nu)}\left(\sqrt{\frac{\rho_o}{\rho_*}}-\sqrt{\frac{\rho_*}{\rho_o}}\right)=\frac{\mu}{2(1-\nu)}\sinh(\Gamma). \tag{16}$$

For small values of Γ,

$$\tau_{\mathrm{PS}}=\pi\frac{E_*-E_o}{b^2}\left(1+\frac{\Gamma^2}{6}+\cdots\right)=\pi\frac{E_*-E_o}{b^2}+\text{higher order terms}. \tag{17}$$

An analogous expression exists in the classical Peierls-Nabarro formulation, but in terms of the Peierls energy $W_P=4D\exp(-2n\pi\rho/b)$, which is the difference between the misfit energies of the two neighboring equilibrium configurations and which has created the single versus double-counting controversy. Since the atomic distribution and the stress and strain fields away from the dislocation core are essentially equal for both stable and unstable equilibrium configurations of the dislocation, the energy difference E_*-E_o is due to the difference in the corresponding core energies, which can be determined by quantum mechanics calculations based on electron density functional theory, or, on a less fundamental level, by empirical atomic models based on either atomic pair potentials or embedded atom methods. Only relatively small number of atoms in the neighborhood of the center of the dislocation need to be considered since the far dislocation field is Volterra. The sensitive core radius does not appear in the final expression for the Peierls stress and was only used as an intermediate quantity.

If the dislocation is in a purely screw orientation, the slip discontinuity and the corresponding shear stress, in analogy with Eqs. (4) and (6), are

$$\delta_s(x)=\frac{b_s}{\pi}\tan^{-1}\frac{x}{\rho_s},\qquad \tau_s(x)=\frac{\mu}{4\pi}\frac{b_s}{\rho_s}\sin\frac{2\pi\delta_s(x)}{b_s}=\frac{\mu b_s}{2\pi}\frac{x}{\rho_s^2+x^2}, \tag{18}$$

where the index s designates the screw character. The strain energy within a large radius R around the dislocation center is $E=(\mu b_s^2/4\pi)\ln(R/2\rho_s)$. The analysis previously presented for dislocations of a pure edge type can be extended to dis-

locations of a mixed (screw-edge) type as follows. Since there is no coupling of the energy due to edge and screw components (b_e and b_s) in an isotropic crystal (the in-plane shear stresses from an edge component do no work on the out-of-plane displacements due to screw component), the total strain energy is

$$E=\frac{\mu b_e^2}{4\pi(1-\nu)}\ln\frac{e^{1/2}R}{2\rho_e}+\frac{\mu b_s^2}{4\pi}\ln\frac{R}{2\rho_s}. \tag{19}$$

Writing $\rho_s=c\rho_e$, where c is assumed to be a constant during the motion of the dislocation, Eq. (19) becomes

$$E=\frac{\mu\bar{b}^2}{4\pi(1-\nu)}\ln\frac{R}{2\rho_e}+\frac{\mu b_e^2}{8\pi(1-\nu)}-\frac{\mu b_s^2}{4\pi}\ln c,$$
$$\bar{b}^2=b_e^2+(1-\nu)b_s^2. \tag{20}$$

The value of the constant c does not appear in the final expression for the Peierls stress derived below, which involves only the difference between the relevant energy levels.

A simple periodic variation of the core radius $\rho_e=\rho(\Delta)$ with the distance Δ in the glide plane and orthogonal to the dislocation line will be assumed, so that

$$\rho(\Delta)=\frac{1}{2}(\rho_o+\rho_*)+\frac{1}{2}(\rho_o-\rho_*)\cos\frac{2\pi\Delta}{a}, \tag{21}$$

where a is the interatomic distance in the glide plane in the direction of the dislocation motion.

The potential energy of a dislocated crystal under the remote shear stress τ parallel to the dislocation glide plane is

$$\Pi(\Delta)=E(\Delta)-\int_0^\Delta b\tau_b(\Delta)d\Delta,$$
$$b=(b_e^2+b_s^2)^{1/2}, \tag{22}$$

where τ_b is the resolved shear stress within the glide plane in the direction of the Burgers vector and b is the magnitude of the Burgers vector. For example, if φ is the angle that τ makes with the positive direction of the dislocation line and ψ is the angle between the Burgers vector and the dislocation line, then $\tau_b=\tau\cos(\varphi-\psi)$. From the equilibrium condition $d\Pi/d\Delta=0$, it follows that $b\tau_b(\Delta)=dE/d\Delta$, which yields

$$\tau_b(\Delta)=\frac{\mu}{4(1-\nu)}\frac{\bar{b}^2}{ab}\frac{\rho_o-\rho_*}{\rho(\Delta)}\sin\frac{2\pi\Delta}{a}. \tag{23}$$

The maximum value of this shear stress,

$$\tau_b^{\mathrm{PS}}=\frac{\mu}{4(1-\nu)}\frac{\bar{b}^2}{ab}\frac{\rho_o-\rho_*}{\sqrt{\rho_o\rho_*}}, \tag{24}$$

defines the shear stress required to move the dislocation in its glide plane by an interatomic distance a, normal to the dislocation line (again referred to as the Peierls stress). Since, from Eq. (19),

$$E_*-E_o=\bar{D}\ln\frac{\rho_o}{\rho_*},\quad \bar{D}=\frac{\mu\bar{b}^2}{4\pi(1-\nu)}, \tag{25}$$

Eq. (24) can be recast in the form

$$\tau_b^{\mathrm{PS}}=\frac{\mu}{2(1-\nu)}\frac{\bar{b}^2}{ab}\sinh(\bar{\Gamma}),$$
$$\bar{\Gamma}=\frac{E_*-E_o}{2\bar{D}}. \tag{26}$$

To the leading order term, therefore,

$$\tau_b^{\mathrm{PS}}=\pi\frac{E_*-E_o}{ab}+\text{higher order terms}, \tag{27}$$

where E_*-E_o is the energy difference between unstable and stable configurations of the dislocation, a is the interatomic distance in the glide plane normal to the dislocation line, and b is the magnitude of the Burgers vector. This generalizes the result (17) for an edge dislocation to a mixed one of arbitrary screw-edge type. If $b_s=0$ and $a=b_e$, Eq. (27) reduces to Eq. (17).

The considerations in this letter are restricted to a single straight dislocation in a perfect crystal. The curvature of the dislocation line, kinking of the dislocation, dissociation of the dislocation into partial dislocations, the stacking fault energy, and the nonplanar dislocation configurations also have obvious effects on the dislocation core structure and the resulting Peierls stress.[17] Such analysis is of interest for the study of nanocrystalline materials, in which some crystals are so small that dislocations in them may not be fully formed and where the dislocation core interactions, among themselves and with the nearby grain boundaries, represent an essential aspect of the deformation process.[18,19]

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