# The Peierls Stress of Dislocations: An Analytic Formula

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A simple and rigorous analytic formula is derived for the Peierls stress of a dislocation within the Peierls-Nabarro model. This is both a generalization and a correction of the previously known formula valid only for wide dislocations. Our formula is shown to have quantitative predictive capabilities, and to permit estimation of the Peierls stress directly from the generalized stacking fault energy surface, for both narrow and wide dislocations. [S0031-9007(96)02187-4]

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Modern technological pressure for improved electronic and high-temperature materials has led to rapid expansion of research into the properties of synthetic structures, such as layered semiconductors, intermetallic compounds, and the transition metal silicides. While these materials promise great potential for engineering and economic benefits, they share common problems of mechanical instability and/or room temperature brittleness, drawbacks which severely limit their utility and impose substantial cost handicaps. The understanding and elimination of these undesirable physical characteristics, all rooted in the nucleation and transport of dislocations, are of prime importance.

These strategic materials, with strongly directional, hybridized *s-p* or *s-d* bonding, and often complex structures, are not readily amenable to the atomistic methods which have been so successful in evaluating dislocation properties in metals [1]. As a consequence, there has been a resurgence of interest in the simple and tractable Peierls-Nabarro (PN) model of dislocation structure and mobility. The purpose of this Letter is to introduce new methods within the aperiodic PN framework which permit easy estimation of the key dislocation characteristics of nucleation and mobility, directly from quantities accessible through standard quantum mechanical computations for periodic systems.

In the classical PN formalism [2–4], the dislocation misfit is assumed to be confined to a single plane, the glide plane, separating two semi-infinite linear elastic continua. Between these half-spaces is placed a dislocation, conveniently represented as a continuous distribution of infinitesimal dislocations [5] with density $\rho(x)$, where $x$ is a coordinate lying in the glide plane and normal to the dislocation line. A discrete lattice of arbitrary structure, deformed by the dislocation displacement field, is superimposed on the elastic half-spaces. At a given point along the interface, the resultant displacement, due to all the infinitesimal dislocations, is then balanced against the lattice restoring stresses across the glide plane. In the original formulation of the model [2,3], and in some later works [6,7], the restoring stresses in each of the half-spaces are treated as independent functions of the lattice displacements. This leads to a predicted Peierls stress (PS) $\sigma_p$, the minimum stress required to move a dislocation one lattice site, which is several orders of magnitude smaller than those either observed or calculated by atomistic methods [8]. The well known formula, on which these estimates are based, is

$$\sigma_p = A \exp\left(-\frac{\alpha\zeta}{b}\right). \tag{1}$$

In the original PN model [2,3] $\alpha = 4\pi$, and, for an edge dislocation, $A = 2\mu/(1-\nu)$. $\zeta$ is the dislocation half-width, $\mu$ the shear modulus, and $\nu$ the Poisson ratio.

Later developments recognized that a physically more realistic description of the restoring stresses is in terms of the relative displacements between the two half-spaces [4,9,10]; this modification, as will be shown, brings the predicted Peierls stresses into fair agreement with experimental measurements and atomistic calculation. In particular, for an edge dislocation, $\alpha = 2\pi$ and $A = \mu/(1-\nu)$.

The above formula (1) is, however, approximate. It is valid only in the limit of wide dislocations, much wider than commonly observed, but is nevertheless applied indiscriminately. The denominator in the exponent should be $a'$, the lattice period normal to the dislocation line.

We show in this Letter that the PS, the crucial quantity characterizing the mobility of a dislocation, can be calculated rigorously and exactly within the PN model. Simple, closed form expressions are obtained for the misfit (or core) energy and the PS; these are shown to be in agreement with numerical calculations for both narrow and wide dislocations in model systems and Si. The PN model has previously not been thought to be applicable to narrow dislocations.

*Peierls-Nabarro model.*—In a Cartesian set of coordinates $xyz$, we choose the $y$ axis as perpendicular to the $x0z$ glide plane. For the purposes of this Letter we assume the core to be confined within this plane. The

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Burgers vector, perpendicular to the $y$ axis, makes an angle $\theta$ with the dislocation line chosen as the $z$ axis direction. In the absence of anharmonic effects, the direction of displacement of the atoms around the dislocation line is along the Burgers vector. Within the glide plane, at each point a distance $x'$ from the dislocation line, the displacement $\vec{f}$ of the upper half of the crystal ($y > 0$) with respect to the lower half ($y < 0$) results from the continuous distribution of infinitesimal dislocations with Burgers vector density $\vec{\rho}(x')\,dx' = [d\vec{f}(x')/dx']\,dx'$. The component along $\vec{b}$ of the total resultant stress at a point $x$, $\sigma_{by}(x)$, is the sum of the contributions from all these infinitesimal dislocations. $\sigma_{by}(x)$ is balanced by the corresponding component of the periodic restoring force stress $\vec{F}_b(\vec{f}(x))$ acting between atoms on either side of the interface. Using the result of continuum theory, that a dislocation at $x'$ generates a stress field proportional to $1/(x - x')$ at other points $x$ along the interface [4], we obtain the integro-differential equation known as the PN equation,

$$\frac{K}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{x - x'}\frac{df(x')}{dx'}\,dx' = F_b(f(x)), \qquad (2)$$

with the normalization conditions $f(-\infty) = 0$, and $f(\infty) = b$. The elastic constant $K$ depends on the type of dislocation and the crystalline direction of the Burgers vector [for a pure edge, $\theta = 90°$, in an isotropic crystal $K = \mu/(1 - \nu)$] [10]. The restoring stress $\vec{F}(\vec{f})$ is given by the gradient of the so-called generalized stacking fault energy (gsf or $\gamma$) surface [11]. The gsf surface is obtained by cutting the crystal along the glide plane, displacing one half with respect to the other by a vector $\vec{f}$ and then rejoining them. As $\vec{f}$ sweeps out a repeat area on the glide plane, the energy of the displaced crystal generates the gsf surface $\gamma(\vec{f})$ (energy per unit area). The restoring stress is then simply, $\vec{F}(\vec{f}) = -\partial\gamma/\partial\vec{f}$. $\vec{F}(\vec{f})$ in general will have a complex functional form. In order to obtain a simple analytical solution, the original PN model assumes a sinusoidal restoring force,

$$F_b(f(x)) = \tau_{\max}\sin\frac{2\pi f(x)}{b}, \qquad (3)$$

and $\tau_{\max}$ is chosen so that, for small displacements, the elastic limit is recovered.

This latter approximation may, however, be very crude, since dislocation cores depend more on the value of the restoring stress at large displacements than in the limit of small displacement. A more physical interpretation of $\tau_{\max}$ is to take it as the maximum slope of the gsf surface, in the appropriate direction for the dislocation under study. This $\tau_{\max}$ can be identified as the theoretical shear strength of the lattice along that direction, and is a convenient parameter for the characterization of the interface restoring forces.

With the approximation in Eq. (3), the PN equation (2) has the solitonlike solution,

$$f(x) = \frac{b}{\pi}\tan^{-1}\frac{x}{\zeta} + \frac{b}{2}, \qquad (4)$$

where $\zeta = Kb/4\pi\tau_{\max}$ is the half-width of the dislocation.

*Misfit energy and the Peierls stress.*—Although a periodic restoring force has been incorporated into the PN model, it still considers the crystal above and below the glide plane as an elastic medium. Mass is homogeneously distributed at the interface. If $f(x)$ is a solution to the displacement field, so is $f(x - u)$ where $u$ is any constant [$f(x - u)$ corresponds to a dislocation translated by $u$]. This "continuum-mass" dislocation has no PS. However, a stress can be defined by restoring discreteness to the mass distribution. This is done by noting that the displacement function $f(x - u)$ corresponds to a real displacement only where an atomic plane is present. In the absence of a dislocation the spacing of atomic planes in the direction $x$ is defined as $a'$. When the dislocation is introduced at the position $u$, the planes, in the upper half of the crystal at a position $ma'$ in a direction perpendicular to the dislocation line, will be displaced with respect to the lower half by $f(ma' - u)$ along $\vec{b}$. The misfit energy can be considered as the sum of misfit energies between pairs of atomic planes [4,9,10] and can be written as

$$W(u) = \sum_{m=-\infty}^{+\infty}\gamma(f(ma' - u))a'. \qquad (5)$$

This formula focuses on the variation of the disregistry as one moves across the dislocation core along the interface in a direction perpendicular to the dislocation line. It has the correct period $a'$, and the right limit for very narrow dislocations, for which the amplitude of variation of $W(u)$ should be the same as that of $\gamma(u)a'$, i.e., $\gamma_{\max}a'$.

The Peach-Koehler formula [see Eq. (3.90) in Ref. [4]] relates the applied stress field $\vec{\sigma}$ to the force per unit length $\vec{F}$ generated on the dislocation

$$\vec{F} = (\vec{b}\cdot\vec{\sigma})\times\hat{z}. \qquad (6)$$

From this follows the Peierls stress $\sigma_p$, the maximum stress required to overcome the periodic barrier in $W(u)$,

$$\sigma_p = \max\{\sigma\} = \max\left\{\frac{1}{b}\frac{dW}{du}\right\}. \qquad (7)$$

When the restoring force is sinusoidal, an exact solution is possible. Integrating the restoring force in Eq. (3) to get an energy, and using Eq. (4), we have

$$W(u) = \sum_{m=-\infty}^{+\infty}\frac{\tau_{\max}a'b}{2\pi}\left\{\cos\left[2\tan^{-1}\left(\frac{ma' - u}{\zeta}\right)\right] + 1\right\}. \qquad (8)$$

Using the identities,

$$1 + \cos\left[2\tan^{-1}\frac{x}{\zeta}\right] = \frac{2\zeta^2}{x^2 + \zeta^2}, \qquad (9)$$

and $\zeta\tau_{\max} = Kb/4\pi$, and introducing the dimensionless quantities $\Gamma = \zeta/a'$ and $y = u/a'$, we have

$$W(y) = \sum_{m=-\infty}^{+\infty} \frac{Kb^2}{4\pi^2} \frac{\Gamma}{\Gamma^2 + (m - y)^2}. \quad (10)$$

$W(y)$ is an even periodic function of period 1, and its Fourier series has the form

$$W(y) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos 2\pi n y, \quad (11)$$

where

$$a_n = 2\int_0^1 \sum_{m=-\infty}^{+\infty} \frac{Kb^2}{4\pi^2} \frac{\Gamma}{\Gamma^2 + (m - y)^2} \cos(2\pi n y)\, dy. \quad (12)$$

With the change of variable $t = y - m$, this becomes a well known integral over $(-\infty, +\infty)$, such that the Fourier series has the form,

$$W(y) = \frac{Kb^2}{4\pi} + \sum_{n=1}^{\infty} \frac{Kb^2}{2\pi} e^{-2\pi n\Gamma} \cos 2\pi n y. \quad (13)$$

Using the fact that the cosine is a sum of exponentials, this series can be summed easily to yield

$$W(y) = \frac{Kb^2}{4\pi} \frac{\sinh 2\pi\Gamma}{\cosh 2\pi\Gamma - \cos 2\pi y}. \quad (14)$$

The maximum of this function is at $y = 0$ where $W(0) = Kb^2/4\pi^2\Gamma$ showing the expected divergence of $W$ as the dislocation gets narrower. To get the PS we first have to compute the stress associated with the misfit energy variation.

$$\sigma(y) = \frac{1}{b}\frac{dW}{du} = -\frac{Kb}{2a'} \frac{\sinh 2\pi\Gamma \sin 2\pi y}{(\cosh 2\pi\Gamma - \cos 2\pi y)^2}. \quad (15)$$

Maximizing this quantity yields the PS

$$\sigma_p = \sigma(y_m), \qquad \text{where}$$
$$2\cos 2\pi y_m = -\cosh 2\pi\Gamma + \sqrt{9 + \sinh^2 2\pi\Gamma}. \quad (16)$$

This is a relatively easy formula to use. Simpler formulas can be deduced in two limits, (i) narrow dislocations ($\Gamma \ll 1$), and (ii) wide dislocations ($\Gamma \gg 1$).

(i) *The limit for narrow dislocations* is achieved when the dislocation core is narrower than one lattice site. Returning to Eq. (5), we note that, in that limit, only one term in the sum contributes, and

$$W(u) = \gamma(f(-u))a' = \frac{Kb^2a'}{4\pi^2} \frac{\zeta}{\zeta^2 + u^2}; \quad (17)$$

and hence,

$$\sigma(u) = \frac{1}{b}\frac{dW}{du} = -\frac{Kba'}{2\pi^2} \frac{\zeta u}{(\zeta^2 + u^2)^2}, \quad (18)$$

leading to the maximum value

$$\sigma_p = \frac{3\sqrt{3}}{8}\tau_{\max}\frac{a'}{\pi\zeta}. \quad (19)$$

A more general form can be obtained in this limit, which is applicable to nonsinusoidal restoring forces. One starts again with the observation that, for narrow dislocations, only one atomic plane will be significantly displaced as the dislocation is moved, or the first part of Eq. (17), which when differentiated gives

$$\sigma(u) = \frac{1}{b}\frac{dW}{du} = \frac{a'}{b}\frac{d\gamma(f(-u))}{df}\frac{df}{du}. \quad (20)$$

Assuming a $\tan^{-1}$ profile for the dislocation, as in Eq. (4),

$$\sigma(u) = -\frac{a'}{\pi}\frac{d\gamma(f(-u))}{df}\frac{\zeta}{u^2 + \zeta^2}. \quad (21)$$

Inverting Eq. (4), Eq. (21) can be rewritten in terms of the displacement $f$ only, leading to

$$\sigma_p = \frac{a'}{\pi\zeta}\max\left\{\frac{d\gamma(f)}{df}\sin^2\frac{\pi f}{b}\right\}. \quad (22)$$

The quantity to be maximized is essentially proportional to $\tau_{\max}$. The appropriate coefficient in front will depend on the functional form of $d\gamma/df$. With a sinusoidal form, for instance, we recover Eq. (19).

(ii) *The limit for wide dislocations* can be most easily derived from Eq. (13), where only the first exponential term in the series is kept [2–4,6], yielding a sinusoidal variation in the misfit energy

$$W(u) = \frac{Kb^2}{4\pi}\left(1 + 2e^{-2\pi\zeta/a'}\cos\frac{2\pi u}{a'}\right), \quad (23)$$

from which follows

$$\sigma_p = \frac{Kb}{a'}e^{-2\pi\zeta/a'}. \quad (24)$$

[This last term can be obtained directly from Eq. (16) by taking the limit $\Gamma \gg 1$.] The exponential factor is in agreement with the result found numerically for the Frenkel-Kontorowa model, the simplest model for dislocation motion [12], but differs, by a factor of 2, from what is given in the original derivations [2,3] and in some recent work [7]. In these papers, the displacements of the top and bottom of the crystal are added up as separate entities. This is fine for the calculation of the total stress, but it yields an unphysical result for the misfit energy, which does not combine linearly.

Verification of the model is possible in several ways. Atomistic calculations sometimes provide both PS and dislocation core width information. The latter can be used to predict the PS from Eqs. (19) or (24). Zhou, Carlsson, and Thomson [8] calculated the PS in a model close-packed hexagonal lattice (wide dislocations) using pair potentials and found $\sigma_p = 10^{-4}\mu$ for a dislocation width of $\zeta = 1.6b$. Using the same width, with $\nu = 1/4$ in Eq. (24), which is the appropriate formula to use in

systems with wide dislocations, yields a predicted $\sigma_p = 0.57 \times 10^{-4}\mu$, within a factor of 2 of the atomistic value. This agreement demonstrates that the dislocation width-PS relationship of Eq. (24) is consistent with atomistic theory. Use of the classical expression [2,3] in this case leads to an underestimate of the atomistic PS by a factor of $10^4$.

The typical experimental value for the PS in a close-packed metal (Cu) is about $5 \times 10^{-6}\mu$ [13]. Our PN model can be compared with this value by using the value of $\tau_{\max} = 0.04\mu$ calculated by Kelly [14] (comparable with the value of $0.031\mu$ measured in Ag whiskers by Brunner [15]). Inserting this value for $\tau_{\max}$, with $\nu = 0.324$ [4] and $b/a' = 2/3$ into Eq. (24) predicts $\sigma_p = 1.99 \times 10^{-6}\mu$, within a factor of 2.5 of the experimental measurement. The classical PN model gives a value of $\sigma_p \approx 10^{-11}\mu$.

The expression for narrow dislocations Eq. (22), or more simply Eq. (19), applicable to covalent materials, can be tested on Si, using a recent numerical solution of the PN model [10] based on realistic restoring forces obtained from a first principles calculation of the gsf surface [16]. The results of this work have been confirmed by simulations using an empirical potential [17], and by an effective-medium tight-binding calculation [18]. Comparing the values reported in Ref. [10] with predictions of Eq. (19) yields an agreement within less than a percent for the glide partials for which $\zeta/a' \approx 0.3$ [Ref. [10] gives $0.450\mu$ and $0.561\mu$ for the 90° and 30° glide partials, respectively, while Eq. (19) yields $0.446\mu$ and $0.561\mu$]. Even for the shuffle set where $\zeta/a'$ is close to 1 the agreement is within 10% [$\sigma_p = 0.076\mu$ and $0.103\mu$ for the 60° and screw dislocations from Ref. [10], and $0.072\mu$ and $0.090\mu$ from Eq. (19)]. Experimental information is also available for Si [19,20]. Extrapolation to 0 K gives a value of $\sigma_p$ between 0.1 to $0.5\mu$ [21,22], covering the range of values predicted by Eq. (19) for the relevant glide partials.

These verifications of our expressions for the PS demonstrate that they provide a rapid and inexpensive alternative to atomistic calculations. They restore credibility to the PN model as a simple model for dislocations with the capability of quantitative predictions. The only required inputs are the maximum of the restoring stress $\tau_{\max}$, for the glide plane under study, and the corresponding elastic constant $K$. $\tau_{\max}$ should become increasingly available as first principles calculations of materials properties become more routinely performed.

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