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ON ATOMIC DISREGISTRY, MISFIT ENERGY, AND PEIERLS STRESS OF A CRYSTALLINE DISLOCATION

Abstract

Analytical determination of the Peierls stress required to move an edge dislocation in a crystalline lattice is studied from the combined atomistic and continuum elasticity points of view. Particular attention is given to the sinusoidal relationship between the shear stress and atomic disregistry across the glide plane, and the relationship between the dislocation width and the atomic interplanar separation across the glide plane. The analysis is based on the assumption that the dislocation core radius periodically varies during the glide of the dislocation between its consecutive equilibrium configurations. The resulting material parameters appearing in the expression for the lattice friction stress are related to those of a semi-discrete Peierls–Nabarro model and the corresponding calculation of the misfit energy based on either single or double-counting scheme.

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O RASPODJELI ATOMA, MISFIT ENERGIJI I PAIRLESOVOM NAPONU KRISTALNE DISLOKACIJE

I z v o d

U radu je data analiza Pairlesovog napona za pokretanje dislokacije u kristalnoj rešetki na bazi kombinovanog pristupa na nivou atoma i na nivou elastičnih deformacija kontinuuma. Posebna pažnja je posvećena sinusoidnoj relaciji izmedju smičućeg napona i atomskog misfita preko ravni klizanja, kao i relaciji izmedju širine jezgra dislokacije i medjuatomskog rastojanja u pravcu normale na ravan klizanja. Analiza je bazirana na pretpostavci da se radijus dislokacionog jezgra periodično mijenja tokom klizanja dislokacije izmedju njenih ravnotežnih položaja. Materijalni parametri u izvedenom izrazu za otpor klizanju su povezani sa odgovarajućim parametrima semi-diskretne Pairles–Nabaro analize i korespondentnog sračunavanja misfit energije koristeći dva različita pristupa.

1. INTRODUCTION

In the Peierls [1] model of a crystal dislocation the crystal is imagined to be divided along the glide plane into two elastic half-spaces. These are separated by the distance h, which is the normal distance between the atomic planes across the glide plane, and are subjected to surface displacements of the dislocation in an infinite elastic continuum. The resulting shear stresses on the faces $y = \pm h/2$ are balanced by the nonlinear atomic interactions across the glide plane. If the Frenkel sinusoidal force-displacement expression is adopted, the shear stress is

$$\tau_{xy}(x,0) = \frac{\mu b}{2\pi h} \, \sin \frac{2\pi \delta(x)}{b} \,, \qquad (1.1)$$

where $\delta(x)$ is the slip discontinuity across the glide plane. The associated atomic disregistry across the glide plane is $b/2 - \delta(x)$ (for $x > 0$; the negative sign precedes the expression for $x < 0$). The length of

the Burgers vector of the dislocation is b, and μ is the elastic shear modulus. The atomistic effects and the lattice discreteness are thus incorporated into the analysis approximately, by considering them to be confined within a thin layer consisting of two atomic planes around the glide plane $y = 0$. By equating (1.1) to the shear stress due to an appropriate continuous distribution of infinitesimal Volterra dislocations along the glide plane in an infinite elastic medium, it follows that

$$\delta(x) = \frac{b}{\pi} \tan^{-1} \frac{x}{\rho}, \quad \rho = \frac{h}{2(1 - \nu)}, \quad (1.2)$$

where ν is the Poisson ration, and $\rho = w/2$ is the half-width of the dislocation, which defines the region $(-\rho, \rho)$ where $\delta(x) < b/4$. This model of a crystal dislocation was used by Peierls [1] and Nabarro [2] to make the first estimates of the minimum external stress required to move a dislocation in a perfect crystalline lattice (without thermal agitation). This stress is called the Peierls–Nabarro stress or, in short, the Peierls stress (τ_{PS}). Its determination is of significance for the physical theories of plasticity and creep [3-5], dislocation-based plasticity theory [6-10], fracture mechanics [11,12], strain relaxation in thin films [13,14], etc. The Peierls–Nabarro expression for the critical stress required to move an edge dislocation is

$$\tau_{PS} = \frac{2\mu}{1 - \nu} \exp\left(-\frac{2\pi}{1 - \nu} \frac{h}{b}\right). \quad (1.3)$$

Due to the unrealistic sinusoidal interatomic force expression adopted in the model, and an over-simplified calculation of the atomic misfit energy in the glide plane, used to derive (1.3), the calculated values for τ_{PS} are an order of magnitude or more higher than those experimentally observed [15-17], or those calculated by the atomistic models [18-20]. Consequently, continuing attempts were made to improve the Peierls–Nabarro model and to better link the atomistic and continuum models of crystal dislocations and their properties. Ohsawa [21] introduced a dislocation into an array of nonlinear shear springs with different potentials, and calculated the critical stress as the applied stress beyond which no stable solution could be found. Bulatov and

Kaxiras [22] constructed a variational approach which incorporates the discrete nature of the lattice and which is particularly suitable for narrow core dislocations. Joós and Duesbery [23] derived simple closed form expressions for the misfit energy and lattice friction stress for both wide and narrow dislocations, which showed improved agreements with observations over the classical formulation. Miller *et al.* [24] devised a non-local version of the Peierls–Nabarro model in which the atomic level stresses in the slip plane depend in a non-local way on the slip degrees of freedom. Lu [25] analyzed single vs. double counting schemes (in which the misfit energies on either one or both sides of the glide plane are summed), as well as the effect of sampling scheme for different (facing or alternating) crystal lattices, in which the atoms above and below the glide plane face each other, or alternate across the glide plane. A two-dimensional extension of the Peierls–Nabarro dislocation model for straight dislocations of a mixed character was developed by Mryasov *et al.* [26] and Schoeck [27,28]. Joós and Zhou [29] presented a new analytical model for calculating the stress required to move a straight dislocation and a kink in the dislocation line. Other issues were also addressed in the literature recently, but their discussion is beyond the present scope of this paper. A recent review by Schoeck [30] can be consulted in this regard.

In this paper we analyze the determination of the Peierls stress studied from the combined atomistic and continuum elasticity points of view. A particular attention is given to the study of the sinusoidal relationship between the shear stress and atomic disregistry across the glide plane, and the relationship between the dislocation width or the dislocation core radius and the atomic plane separation across the glide plane. The analysis is based on the assumption that the dislocation core radius periodically varies during the glide of the dislocation between its consecutive equilibrium lattice positions. The resulting material parameters appearing in the expression for the lattice friction stress are related to those of a semi-discrete Peierls–Nabarro analysis and their calculation of the misfit energy based on a single or double-counting scheme. The comparison with some related work

and with experimental data for both wide and narrow dislocations is also given.

2. PEIERLS DISLOCATION MODEL

An edge dislocation of idealized Volterra type can be introduced in an infinite elastic medium by making a cut along the y-axis and by horizontally displacing the two cut surfaces, relative to each other, by the constant amount b. The Airy stress function for this plane strain self-equilibrated state of stress is

$$\Phi^{\mathrm{V}} = -\frac{\mu b}{4\pi(1-\nu)}\, y\, \ln(x^2 + y^2)\,, \tag{2.4}$$

where the superscript $^{\mathrm{V}}$ stands for the Volterra type dislocation. The corresponding in-plane stress components are deduced from

$$\sigma_{xx}^{\mathrm{V}} = \frac{\partial^2 \Phi^{\mathrm{V}}}{\partial y^2}\,, \quad \sigma_{yy}^{\mathrm{V}} = \frac{\partial^2 \Phi^{\mathrm{V}}}{\partial x^2}\,, \quad \tau_{xy}^{\mathrm{V}} = -\frac{\partial^2 \Phi^{\mathrm{V}}}{\partial x \partial y}\,. \tag{2.5}$$

In particular, the shear stress is

$$\tau_{xy}^{\mathrm{V}}(x,y) = \frac{\mu b x}{2\pi(1-\nu)}\, \frac{x^2 - y^2}{(x^2 + y^2)^2}\,, \tag{2.6}$$

so that, along the x-axis,

$$\tau_{xy}^{\mathrm{V}}(x,0) = \frac{\mu}{2\pi(1-\nu)}\, \frac{b}{x}\,. \tag{2.7}$$

This becomes infinitely large as $x \to 0$, the order of singularity being $1/x$. The singularity is physically due to excessive shearing of the material produced at the center of dislocation $x = y = 0$ by the displacement discontinuity b. To eliminate this singularity, it was proposed in [31] that the displacement discontinuity b along the y-axis is achieved gradually – by a linear increase over the distance ρ, as sketched in Fig. 1a. (The consideration of a non-linear increase of the displacement discontinuity over the distance ρ may also be of interest, particularly in simulating a non-sinusoidal force-displacement
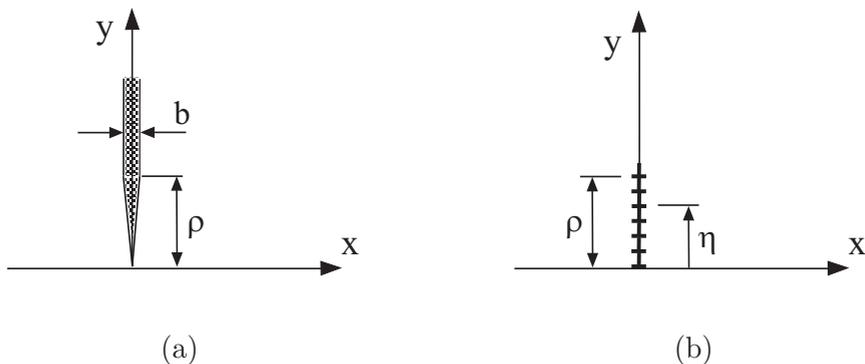
Figure 1: (a) A disclinated dislocation produced by a gradual displacement discontinuity from 0 to b along the distance ρ. (b) A continuous distribution of infinitesimal dislocations simulating a disclinated dislocation from part (a).

relation along the glide plane, inherent to semi-discrete treatments of the problem). The physical interpretation of ρ will be given in the sequel, although it is anticipated from the outset that ρ is related to the extent of the dislocation core – severely deformed region around the center of the dislocation. The linear increase of the displacement discontinuity along the distance ρ can be viewed as a part of the disclination (wedge dislocation), so that the complete displacement discontinuity along the y-axis can be figuratively referred to as being associated with a disclinated dislocation. More precisely, in the context of the general dislocation theory, a variable displacement discontinuity in Fig. 1a represents a Somagliana type dislocation. In any case, this type of dislocation can be modeled by a continuous distribution of infinitesimal dislocations of constant density $1/\rho$ and, thus, the specific Burgers vector b/ρ. This is sketched in Fig. 1b. By superposition of the stress fields of infinitesimal dislocations, the total shear stress along the x-axis is

$$\tau_{xy}(x,0) = \frac{\mu b}{2\pi(1-\nu)} \frac{x}{x^2 + \rho^2} \,, \tag{2.8}$$

which is plotted for several values of ρ in Fig. 3. If $x \gg \rho$, then

$\tau_{xy}(x,0) \to \tau_{xy}^{\mathrm{V}}(x,0)$. The shear stress is maximum at $x = \pm\rho$, with the magnitude

$$\tau_{xy}^{\mathrm{max}} = \frac{\mu}{4\pi(1-\nu)} \frac{b}{\rho} \,. \tag{2.9}$$

This maximum stress is only half the shear stress of the Volterra dislocation at $x = \rho$, *i.e.*,

$$\tau_{xy}^{\mathrm{max}} = \frac{1}{2} \tau_{xy}^{\mathrm{V}}(\rho,0) \,. \tag{2.10}$$

For example, if $\rho = 2b$ and $\nu = 1/3$, $\tau_{xy}^{\mathrm{max}} = 0.06\,\mu$. If $\rho = h/2(1-\nu)$,
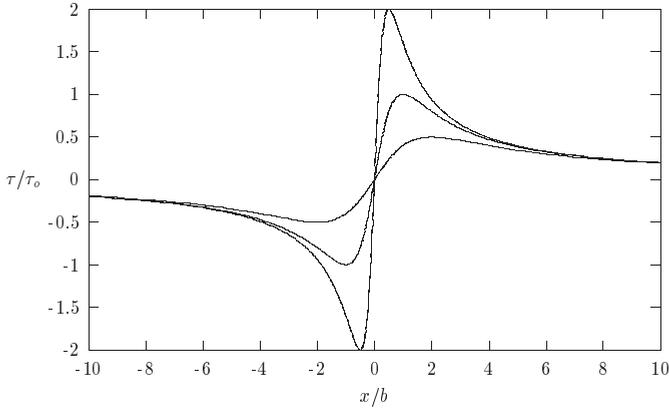

Figure 2: The normalized shear stress along the x-axis according to Eq. (2.8). The normalization factor is $\tau_o = \mu/4\pi(1-\nu)$. The curves correspond to $\rho = b/2, b$ and $2b$. The maximum stress in each case occurs at $x = \pm\rho$ and is equal to $\tau_{xy}^{\mathrm{max}} = \tau_o b/\rho$.

where h is the atomic interplanar separation across the slip plane (introduced in the Peierls semi-discrete analysis of the crystal dislocation), then $\tau_{xy}^{\mathrm{max}} = \mu b/2\pi h$, the theoretical shear strength of the crystal.

The shear stress (2.8), depicted in Fig. 2, has no singularity at the center of the dislocation core and has the physically anticipated behaviour away from the center, reproducing there the Volterra dislocation. This shear stress can thus be reasonably adopted as the shear

stress of the crystal dislocation, produced by a gradual slip disconti-
nuity along the slip plane $y = 0$. It is precisely the shear stress of the
Peierls dislocation model, provided that ρ is interpreted as one half
the width of the Peierls dislocation, $\rho = w/2$, $w = h/(1-\nu)$, where h
is the atomic interplanar distance across the glide plane [32,33].

Since the normal stresses at $y = 0$ and $y = \rho$ for the dislocation
model of Fig. 1 are divergent, we adopt from that problem only
the shear stress distribution along the x-axis, and (in the spirit of
a semi-inverse method) search for the corresponding (Taylor-type)
dislocation having the slip discontinuity along the x-axis. Following
Eshelby's [34] method, we therefore seek the continuous distribution
of infinitesimal dislocations of the specific Burgers vector $\beta(x)$ along
the x-axis which reproduces the shear stress (2.8). This gives

$$\beta(x) = \frac{b}{\pi} \frac{\rho}{x^2 + \rho^2} \,, \tag{2.11}$$

satisfying the normalization condition

$$\int_{-\infty}^{\infty} \beta(x) \, \mathrm{d}x = b \,. \tag{2.12}$$

The corresponding slip discontinuity along the x-axis, which is defined
as $\delta(x) = u(x,0^-) - u(x,0^+)$, where $u = u(x,y)$ is the horizontal
component of the displacement field, is obtained from

$$\delta(x) = \int_0^x \beta(\xi) \, \mathrm{d}\xi = \frac{b}{\pi} \tan^{-1} \frac{x}{\rho} \,. \tag{2.13}$$

Note that $\delta(\rho) = b/4$, while for the corresponding Volterra dislocation
$\delta^{\mathrm{V}}(\rho) = b/2$. The width of the crystal dislocation is, therefore, for-
mally defined as the distance $w = 2\rho$ over which the displacement dis-
continuity across the slip plane is less than $b/4$ (Fig. 3) (and thus the
atomic disregistry, defined in the Peierls model as $\phi(x) = b/2 - \delta(x)$,
is greater than $b/4$). Note also that in the presented derivation the
radius ρ (referred to in the sequel as the core radius) is a free (material
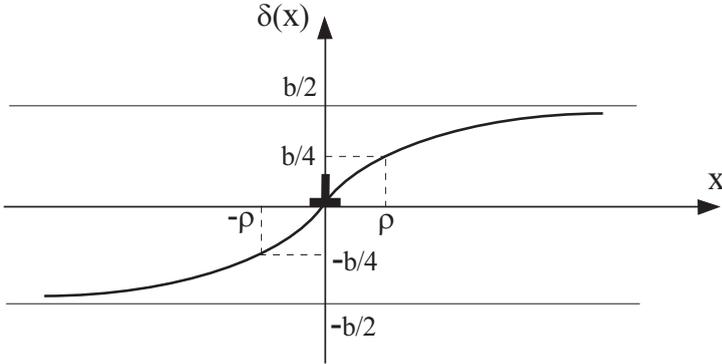dependent) parameter that can be specified by the actual dislocation

Figure 3: The slip discontinuity across the glide plane. The width of the dislocation is defined as the region $|x| \leq \rho$ within which the slip discontinuity is less than $b/4$.

spreading in the material, rather than being constrained by the relationship $2\rho = h/(1-\nu)$, as in the classical formulation of the Peierls dislocation model. [†]

The Airy stress function for the crystal dislocation is obtained by integrating the Airy stress function due to infinitesimal dislocations along the x-axis. Thus, by using Eq. (2.4), we write

$$\Phi = -\int_{-\infty}^{\infty} \frac{\mu\beta(\xi)\mathrm{d}\xi}{4\pi(1-\nu)}\, y\, \ln[(x-\xi)^2 + y^2]\,, \qquad (2.14)$$

which gives

$$\Phi = -\frac{\mu b}{4\pi(1-\nu)}\, y\, \ln\left[x^2 + (y \pm \rho)^2\right]. \qquad (2.15)$$

[†]If the gradient of the vertical displacement component, $\partial v/\partial x$, is included in the Peierls model [32], then $4\rho = (3-2\nu)h/(1-\nu)$, which predicts $(1.5-\nu)$ times larger core radius than in the case when $\partial v/\partial x$ is neglected. Both are, however, usually underestimates of the dislocation spreading in the crystal, although the dislocation width is indeed expected to be greater for crystals and slip systems characterized by larger values of h and ν. More realistic, non-sinusoidal, interatomic force expressions give rise to higher estimates of ρ.

The corresponding in-plane stress components are

$$\sigma_{xx} = -\frac{\mu b}{2\pi(1-\nu)}\left\{\frac{y \pm 2\rho}{x^2 + (y \pm \rho)^2} + \frac{2x^2 y}{[x^2 + (y \pm \rho)^2]^2}\right\}, \quad (2.16)$$

$$\sigma_{yy} = -\frac{\mu b}{2\pi(1-\nu)}\left\{\frac{y}{x^2 + (y \pm \rho)^2} - \frac{2x^2 y}{[x^2 + (y \pm \rho)^2]^2}\right\}, \quad (2.17)$$

$$\tau_{xy} = \frac{\mu b}{2\pi(1-\nu)}\left\{\frac{x}{x^2 + (y \pm \rho)^2} - \frac{2xy(y \pm \rho)}{[x^2 + (y \pm \rho)^2]^2}\right\}. \quad (2.18)$$

The upper placed sign corresponds to $y > 0$, and the lower placed sign to $y < 0$. Upon calculating the corresponding strains and integration, the displacement components are found to be[‡]

$$u = \frac{b}{2\pi}\left(\tan^{-1}\frac{y \pm \rho}{x} \mp \frac{\pi}{2}\frac{|x|}{x}\right) + \frac{b}{4\pi(1-\nu)}\frac{xy}{x^2 + (y \pm \rho)^2}, \quad (2.19)$$

$$v = -\frac{b(1-2\nu)}{8\pi(1-\nu)}\ln\frac{x^2 + (y \pm \rho)^2}{b^2} + \frac{b}{4\pi(1-\nu)}\frac{y(y \pm \rho)}{x^2 + (y \pm \rho)^2}. \quad (2.20)$$

In particular,

$$u(x,0^-) = -u(x,0^+) = \frac{b}{2\pi}\left(\frac{\pi}{2} - \tan^{-1}\frac{\rho}{x}\right) = \frac{b}{2\pi}\tan^{-1}\frac{x}{\rho}, \quad (2.21)$$

and

$$\delta(x) = u(x,0^-) - u(x,0^+) = \frac{b}{\pi}\tan^{-1}\frac{x}{\rho}. \quad (2.22)$$

3. SINUSOIDAL FORCE VS. DISREGISTRY RELATIONSHIP

In view of the trigonometric identity

$$\sin\frac{2\pi\delta(x)}{b} = \sin\left(2\tan^{-1}\frac{x}{\rho}\right) \equiv \frac{2\rho x}{\rho^2 + x^2}, \quad (3.23)$$

we conclude, by comparing (2.8) and (3.23), that $\tau(x,0)$ and $\delta(x)$ are related by

$$\tau_{xy}(x,0) = \frac{\mu}{4\pi(1-\nu)}\frac{b}{\rho}\sin\frac{2\pi\delta(x)}{b}. \quad (3.24)$$

[‡]In the Peierls–Nabarro model y is measured from the surface of each half-space, a distance $h/2$ from the glide plane in the middle of the thin atomic layer between the two half-spaces.

Therefore, we deduce rather than assume the sinusoidal relationship between the shear stress and the slip discontinuity along the glide plane. Furthermore, if $\rho = 0$ in the above expression, then $\delta(x) = (b/2)|x|/x$ (Volterra dislocation). The parameter h does not appear explicitly in our continuum analysis, except that in a crystal dislocation ρ is reasonably expected to depend on the glide system and therefore on the glide plane spacing h.

An alternative derivation of the shear stress expressions (2.8) and (3.24), entirely within the continuum elasticity framework, is as follows. We start with the assumption that the shear stress in the glide plane is a sinusoidal function of the slip discontinuity along the glide plane, *i.e.*,

$$\tau_{x,y}(x,0) = A\mu\frac{b}{\rho}\,\sin\frac{2\pi\delta(x)}{b}\,. \qquad (3.25)$$

If the slip discontinuity would be $(b/2)|x|/x$, this would reduce to the Volterra dislocation ($\rho = 0$). Thus, we introduce the core radius ρ in the denominator of the term b/ρ in front of the sinusoidal function, so that $\tau_{xy}(x,0) \sim 0/0$ for the Volterra dislocation. The shear modulus μ and the Burgers vector b appear in front of the sinusoidal function by the dimensional analysis. To determine the parameter A, we impose the condition

$$\tau_{xy}^{\max}(x,0) = \tau_{xy}(\rho,0)\,. \qquad (3.26)$$

This can be viewed as the condition that specifies the core radius, within the framework based on the shear stress expression (3.25). Geometrically, the assumption (3.26) implies, from (3.25), that $\delta(\rho) = b/4$. To employ this condition, we apply the method of distributed infinitesimal Volterra dislocations along the slip plane, and write

$$\frac{\mu}{2\pi(1-\nu)}\int_{-\infty}^{\infty}\frac{d\delta(\xi)/d\xi}{x-\xi}\,d\xi = A\mu\frac{b}{\rho}\,\sin\frac{2\pi\delta(x)}{b}\,. \qquad (3.27)$$

The solution of this integro-differential equation, for any non-zero A, is

$$\delta(x) = \frac{b}{\pi}\,\tan^{-1}\left[\frac{1}{4\pi A(1-\nu)}\frac{x}{\rho}\right]\,. \qquad (3.28)$$

To determine A, we now impose the condition

$$\delta(\rho) = \frac{b}{4} \quad \Rightarrow \quad A = \frac{1}{4\pi(1-\nu)} \, . \qquad (3.29)$$

The relationship between the shear stress and the slip displacement along the glide plane (3.24) is obtained when (3.29) is substituted into (3.25). The expression (2.8) follows from (3.25) and (3.28).

Introducing the disregistry immediately across the glide plane as $\phi_o(x) = b/2 - \delta(x)$, and observing that $\phi_o \to 0$ as $x \to \infty$, (3.24) simplifies at large x to

$$\tau_{xy}(x,0) = \frac{\mu}{2(1-\nu)} \frac{\phi_o}{\rho}, \quad x \gg \rho. \qquad (3.30)$$

4. ATOMIC DISREGISTRY ACROSS THE GLIDE PLANE

The horizontal displacements immediately above and below the glide plane are opposite and equal to

$$u(x,0^-) = -u(x,0^+) = \frac{b}{2\pi}\left(\frac{\pi}{2} - \tan^{-1}\frac{\rho}{x}\right) = \frac{b}{2\pi}\tan^{-1}\frac{x}{\rho}, \quad (4.31)$$

so that

$$\delta(x) = u(x,0^-) - u(x,0^+) = \frac{b}{\pi}\tan^{-1}\frac{x}{\rho}. \qquad (4.32)$$

At large x we have

$$\tan^{-1}\frac{x}{\rho} = \frac{\pi}{2} - \frac{\rho}{x} + \frac{1}{3}\left(\frac{\rho}{x}\right)^3 - \cdots, \qquad (4.33)$$

and (4.32) reduces to

$$\delta(x) \approx \frac{b}{2} - \frac{b\rho}{\pi}\frac{1}{x}, \quad x \gg \rho. \qquad (4.34)$$

The disregistry between geometric points immediately above and below the glide plane $y = 0$ will be denoted by $\phi_o(x)$, Fig. 4. This is defined by

$$\phi_o(x) = \frac{b}{2} - \delta(x) = \frac{b}{\pi}\tan^{-1}\frac{\rho}{x}. \qquad (4.35)$$
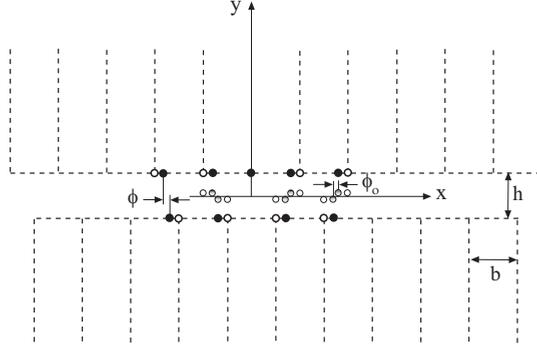
Figure 4: The atomic disregistry $\phi(x)$ between the atoms on the planes $y = \pm h/2$. The disregistry between geometric points immediately above and below the glide plane $y = 0$ is $\phi_o(x)$. Initially, the horizontal distance between the corresponding pairs of atoms, or geometric points, is $b/2$. If the slip discontinuity across the slip plane is $\delta(x)$, then $\phi_o(x) = b/2 - \delta(x)$.

Since

$$\tan^{-1} \frac{\rho}{x} = \frac{\rho}{x} - \frac{1}{3}\left(\frac{\rho}{x}\right)^3 + \frac{1}{5}\left(\frac{\rho}{x}\right)^5 - \cdots, \tag{4.36}$$

from (4.35) we obtain

$$\phi_o(x) \approx \frac{b\rho}{\pi}\frac{1}{x}, \quad x \gg \rho, \tag{4.37}$$

which can also be recognized directly from (4.34).

Suppose that we have discretized the whole continuum by identifying the atomic planes, two of which that are closest to the glide plane $y = 0$ being depicted in Fig. 5. The white circles indicate the initial positions of the atoms, and the black circles their positions after the creation of the dislocation. The normal distance between the atomic planes is h. The initial atomic disregistry across the glide plane, $b/2$, is reduced by the creation of the dislocation to

$$\phi(x) = \frac{b}{2} - \left[u\left(x, -\frac{h}{2}\right) - u\left(x + \frac{b}{2}, \frac{h}{2}\right)\right]. \tag{4.38}$$
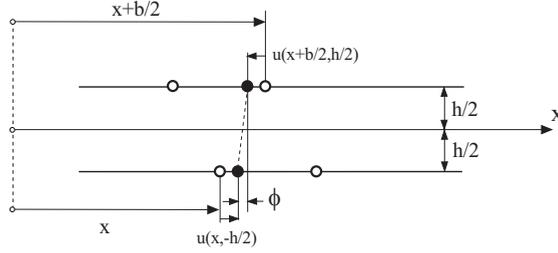
Figure 5: The atomic disregistry $\phi(x)$ between the atoms on the planes $y = \pm h/2$. The white circles indicate the initial positions of atoms, and the black circles the positions of displaced atoms, after the creation of the dislocation.

Upon using (2.19), this is

$$\phi(x) = \frac{b}{2\pi}\left(\tan^{-1}\frac{\rho + h/2}{x} + \tan^{-1}\frac{\rho + h/2}{x + b/2}\right)$$

$$+ \frac{bh}{8\pi(1-\nu)}\left[\frac{x}{x^2 + (\rho + h/2)^2} + \frac{x + b/2}{(x + b/2)^2 + (\rho + h/2)^2}\right].$$

For large x, the so-defined disregistry becomes

$$\phi(x) = \phi_o(x) + \frac{3 - 2\nu}{4\pi(1-\nu)}\frac{bh}{x}, \quad x \gg \rho. \tag{4.39}$$

Geometrically, the difference between the disregistries $\phi(x)$ and $\phi_o(x)$ is sketched in Fig. 5. The second term on the right-hand side of (4.39) can be interpreted as the atomic disregistry between the atoms imagined on the planes $y = \pm h/2$, according to the Volterra dislocation model, *i.e.*,

$$\phi^{\mathrm{V}}(x) = \frac{b}{2} - \left[u^{\mathrm{V}}\left(x, -\frac{h}{2}\right) - u^{\mathrm{V}}\left(x + \frac{b}{2}, \frac{h}{2}\right)\right] = \frac{3 - 2\nu}{4\pi(1-\nu)}\frac{bh}{x}, \quad x \gg \rho.$$

An additional interpretation of (4.39) can be given in terms of the displacement gradient $\partial u/\partial y$. Since

$$\left(\frac{\partial u}{\partial y}\right)_{y=0} = \frac{3 - 2\nu}{4\pi(1-\nu)}\frac{bx}{x^2 + \rho^2}, \quad \left(\frac{\partial v}{\partial x}\right)_{y=0} = -\frac{1 - 2\nu}{4\pi(1-\nu)}\frac{bx}{x^2 + \rho^2},$$

we have

$$\left(\frac{\partial u}{\partial y}\right)_{y=0} = \frac{3-2\nu}{4\pi(1-\nu)}\frac{b}{x}, \quad \left(\frac{\partial v}{\partial x}\right)_{y=0} = -\frac{1-2\nu}{4\pi(1-\nu)}\frac{b}{x}, \quad x \gg \rho.$$

Thus, (4.39) can be recast as

$$\phi(x) = \phi_o(x) + h\left(\frac{\partial u}{\partial y}\right)_{y=0}, \quad x \gg \rho. \tag{4.40}$$

5. SHEAR STRESS VS. ATOMIC DISREGISTRY

For the sake of comparison with the original Peierls–Nabarro dislocation model, it is of interest to relate the shear stress $\tau_{xy}(x,0)$ to the atomic disregistry $\phi(x)$. A simple relationship is obtained for large $x \gg \rho$. By substituting

$$\phi_o(x) = \frac{b}{2} - \delta(x) \tag{5.41}$$

into (3.24), we obtain

$$\tau_{xy}(x,0) = \frac{\mu}{4\pi(1-\nu)}\frac{b}{\rho}\sin\frac{2\pi\phi_o}{b} \approx \frac{\mu}{4\pi(1-\nu)}\frac{b}{\rho}\frac{2\pi\phi_o(x)}{b}, \quad x \gg \rho.$$

After incorporating (4.39), this becomes

$$\tau_{xy}(x,0) = \frac{\mu}{2(1-\nu)}\left[\frac{\phi(x)}{\rho} - \frac{3-2\nu}{4\pi(1-\nu)}\frac{bh}{\rho x}\right], \quad x \gg \rho. \tag{5.42}$$

But, at large $x \gg \rho$ the dislocation has the features of the Volterra dislocation, so that

$$\tau_{xy}(x,0) = \frac{\mu}{2\pi(1-\nu)}\frac{b}{x} \quad \Rightarrow \quad \frac{1}{2\pi(1-\nu)}\frac{b}{x} = \frac{\tau_{xy}(x,0)}{\mu}, \quad x \gg \rho.$$

When this is substituted into (5.42), there follows

$$\frac{\phi(x)}{h} = \left[\frac{3-2\nu}{2} + 2(1-\nu)\frac{\rho}{h}\right]\frac{\tau_{xy}(x,0)}{\mu}, \quad x \gg \rho. \tag{5.43}$$

This is a desired relationship between $\tau_{xy}(x,0)$ and $\phi(x)$.

We can also establish the relationship between $\tau_{xy}(x,0)$ and $\phi_o(x)$ at large x. This follows by combining (4.39) and (5.42), with the end result

$$\tau_{xy}(x,0) = \mu \left[2(1-\nu)\frac{\rho}{h} \right] \frac{\phi_o(x)}{h}, \quad x \gg \rho. \tag{5.44}$$

In the Peierls–Nabarro model the two elastic half-spaces are separated by h, and one can require that $\tau_{xy}(x,0) = \mu\phi_o(x)/h$ at large x (ignoring the strain contribution from $\partial v/\partial x$). The dislocation core radius is then, from (5.44), necessarily equal to $\rho = h/2(1-\nu)$. 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_o/h in a thin layer around the glide plane, and therefore our core radius is not necessarily related to h by $\rho = h/2(1-\nu)$.

An improved estimate of the core radius in the Peierls–Nabarro model can be obtained as follows. If we assume that the elastic half-spaces are separated by h, and that

$$\left(\frac{\partial u}{\partial y} \right)_{y=0} = \frac{\phi_o(x)}{h} = \frac{b\rho}{\pi h}\frac{1}{x}, \quad x \gg \rho. \tag{5.45}$$

On the other hand, from (2.19),

$$\left(\frac{\partial u}{\partial y} \right)_{y=0} = \frac{b(3-2\nu)}{4\pi(1-\nu)}\frac{1}{x}, \quad x \gg \rho. \tag{5.46}$$

The comparison of (5.45) and (5.46) establishes the expression for the core radius

$$\rho = \frac{3-2\nu}{4(1-\nu)}\, h. \tag{5.47}$$

6. PEIERLS STRESS

The elastic strain energy in an infinite medium within a large radius R around the Peierls dislocation is

$$E = \frac{\mu b^2}{4\pi(1-\nu)} \ln \frac{e^{1/2}R}{2\rho}. \tag{6.48}$$

If a remote shear stress τ is applied, the dislocation will tend to glide along its slip plane against the lattice friction stress due to interatomic

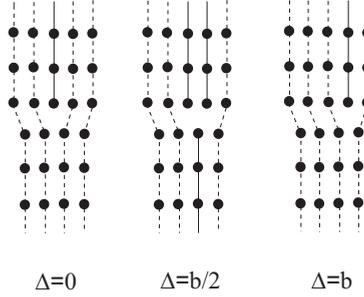$\Delta=0 \qquad \Delta=b/2 \qquad \Delta=b$

Figure 6: The glide of an edge dislocation within the distance $0 \leq \Delta \leq b$, indicating the change in atomic rearrangement around the center of the dislocation. Three consecutive equilibrium configurations are shown.

forces around the glide plane (Fig. 6). In [31] the assumption was introduced that the radius of the dislocation core changes with the glide distance Δ according to

$$\rho(\Delta) = \frac{1}{2}(\rho_o + \rho_*) + \frac{1}{2}(\rho_o - \rho_*)\cos\frac{2\pi\Delta}{b}\,, \qquad (6.49)$$

which is sketched in Fig. 7. This is motivated by the fact that the atomic disregistry across the glide plane near the center of the dislocation changes as the dislocation glides between its two consecutive equilibrium configurations (Fig. 8). The corresponding potential energy is

$$\Pi(\Delta) = E(\Delta) - \int_0^\Delta b\tau(\Delta)\,\mathrm{d}\Delta\,. \qquad (6.50)$$

During the quasi-static displacement of the dislocation by an amount Δ, we have

$$\frac{\mathrm{d}\Pi}{\mathrm{d}\Delta} = 0 \quad \Rightarrow \quad \tau(\Delta) = \frac{1}{b}\frac{\mathrm{d}E}{\mathrm{d}\Delta}\,. \qquad (6.51)$$

Thus,

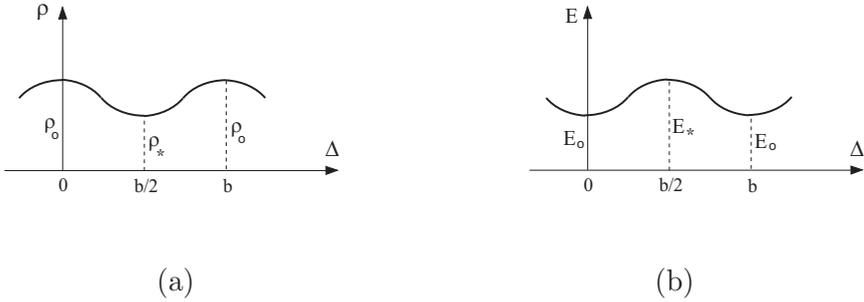$$\tau(\Delta) = \frac{\mu}{4\pi(1-\nu)}\frac{\rho_o - \rho_*}{\rho}\sin\frac{2\pi\Delta}{b}\,. \qquad (6.52)$$

(a)   (b)

Figure 7: (a) A periodic variation of the core radius ρ with the disloca-
tion glide distance Δ, according to Eq. (6.49). (b) The corresponding
periodic energy variation according to Eq. (6.48), with the minimum
$E_o = E(0)$ and maximum $E_* = E(b/2)$.

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. This is called the Peierls stress; the opposite
stress is the maximum lattice friction stress. Therefore,

$$\tau_{PS} = \frac{\mu}{4(1-\nu)} \frac{\rho_o - \rho_*}{\sqrt{\rho_o \rho_*}} = \frac{\mu}{4(1-\nu)} \left(\sqrt{\frac{\rho_o}{\rho_*}} - \sqrt{\frac{\rho_*}{\rho_o}} \right). \qquad (6.53)$$

The experimental evidence indicate that dislocations in softer met-
als are characterized by a wider dislocation core and a lower lattice
friction stress. An atomic disregistry across the slip plane for a wide
and a narrow dislocation is schematically shown in Fig. 9. We ex-
pect that the relative change of the dislocation width is far more
pronounced for a narrow than for a wide dislocation, because the
displacement of the center of the dislocation within the distance $b/2$
notably disturbs the narrow core, whose size is only about b. For
wide dislocations, the outermost atoms at the boundary of the core
are barely affected by the slight motion of the center of the dislocation,
and thus the width of the dislocation is almost unchanged in that case.
Furthermore, the uniform elastic shear strain due to external stress,
$\gamma = \tau/\mu$, increases the atomic disregistry across the glide plane by γh,
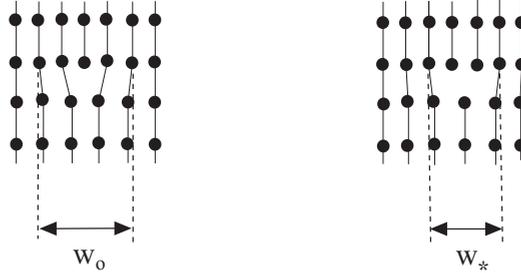
Figure 8: A schematic representation of atomic disregistry around the center of the dislocation in its two consecutive equilibrium configurations. Indicated is the change of the width of the dislocation (w_* vs. w_o).

which contributes to the decrease of the width $w = 2\rho$ within which the atomic disregistry is greater than $b/4$. For soft metals τ is small portion of μ and thus the contribution from γ to the change of the dislocation width is small, but for hard covalently bonded crystals τ can be much higher, which significantly affects the dislocation width. In view of this, an exponential function, which rapidly decreases with ρ_o, suggests itself to describe the relative change of the dislocation width,[§] and we propose that

$$\frac{\rho_*}{\rho_o} = 1 - c \exp\left(-k\pi\rho_o/b\right), \tag{6.54}$$

where c and k are the appropriate parameters, possibly dependent on Poisson's ratio and the temperature. Their values are constrained by the condition that the second term on the right-hand side of (6.54) is

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[§]An alternative, albeit less appealing, expression for the relative change of the dislocation width is in terms of an inverse power of the dislocation width, $m(b/w_o)^n$, where m and n are appropriate parameters. It can be shown that for wide dislocations this assumption leads to $\tau_{PS} \sim \mu(b/w_o)^n$, which is an expression of the type suggested in [35] on the basis of one-dimensional Frenkel–Kantorova dislocation model; see also [36,37].

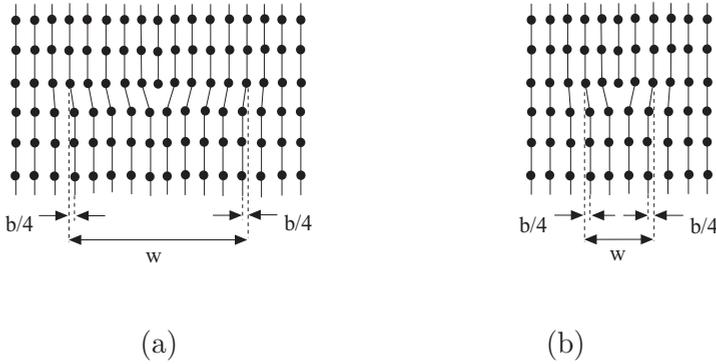(a)   (b)

Figure 9: A schematic representation of atomic disregistry for a wide
(a) and narrow (b) dislocation. The width is formally defined as the
distance over which the atomic disregistry across the slip plane is
greater than $b/4$.

small comparing to one, for both wide and narrow dislocations. The
factor of π is included in the argument of the exponential function for
convenience; alternatively it could be absorbed in the parameter k.
Thus, with a good approximation, we can write

$$\sqrt{\frac{\rho_*}{\rho_o}} = 1 - \frac{c}{2}\exp\left(-k\pi\rho_o/b\right), \quad \sqrt{\frac{\rho_o}{\rho_*}} = 1 + \frac{c}{2}\exp\left(-k\pi\rho_o/b\right). \quad (6.55)$$

When this is substituted into Eq. (6.52), we obtain the following
expression for the Peierls stress

$$\tau_{\mathrm{PS}} = \frac{\mu}{4(1-\nu)}\, c\,\exp\left(-k\pi\rho_o/b\right). \quad (6.56)$$

Knowing that the Peierls–Nabarro formula ($k = 4$), based on a double-
counting scheme to calculate the misfit energy around the glide plane,
significantly underestimates the lattice friction stress for realistic val-
ues of the core radius, although it overestimates the lattice friction
stress if ρ is constrained to be $h/2(1-\nu)$, and knowing that a single-
counting scheme (described in the Appendix) decreases the parameter
k by a factor of 2, we adopt the value $k = 2$. This greatly increases

τ_{PS}. Theoretical elaborations in [38] also support this choice of k. Assuming that the narrowest dislocations have the core radius $\rho_0 \approx b/2$ (and thus the width $w \approx b$), and assuming that the upper bound for the lattice friction stress is of the order of $0.1\,\mu$, we specify $c = 4$.

If $\nu = 1/3$ and $\rho_0 = 2b$, the Peierls stress is $\tau_{PS} = 5.25 \times 10^{-6}\,\mu$, while for a narrow dislocation with $\rho_o = b/2$ and $\nu = 1/5$, $\tau_{PS} = 5.4 \times 10^{-2}\,\mu$. The experimental values at low temperature for τ_{PS} in a closed-packed Cu is about $5 \times 10^{-6}\,\mu$, while in a covalent Si is about $0.1\,\mu$. The lower values of the parameter k increase the lattice friction stress. For example, if the value $k = 1.75$ is selected (which may be more suitable at a lower temperature), then $\tau_{PS} = 8 \times 10^{-2}\,\mu$ for $\rho_o = b/2$ and $\nu = 1/5$ (Si). The effects of temperature on the Peierls stress were discussed in [39,40]. The temperature driven vibrations of atoms lead to uncertainty in their positions, which affects the dislocation size and the core structure, and thus the lattice friction stress.

7. CONCLUSIONS

We have presented in this paper the solution for the crystalline dislocation without assuming in advance the sinusoidal relationship between the shear stress across the glide plane and the corresponding slip discontinuity. This was accomplished by using a semi-inverse method based on an auxiliary elasticity problem of a disclinated dislocation. In the presented analysis the core radius ρ is a free material dependent parameter, specified by the actual dislocation spreading in a crystalline lattice, rather than being constrained by the relationship $2\rho = h/(1 - \nu)$, as in the classical formulation of the Peierls dislocation model. Upon introducing the assumption that the core radius depends on the glide distance of the dislocation between its consecutive equilibrium configurations, we derived an expression for the Peierls stress. The elastic strain energy of the whole crystal was used, rather than the localized misfit energy across the glide plane, as in the Peierls–Nabarro model. An expression for the Peierls stress is constructed based on a proposed periodic variation of the dislocation width between its two equilibrium configurations. The material

parameters appearing in the expression for the lattice friction resistance are related to those of a semi-discrete Peierls–Nabarro analysis and the corresponding calculation of the misfit energy based on either single or double-counting scheme. An encouraging agreement with experimental data for both wide and narrow dislocations is obtained.

The considerations in this paper were restricted to a single edge dislocation in a perfect crystal. The extension of the analysis to a dislocation of mixed edge-screw character will be reported elsewhere [41]. The structure of the dislocation core and the width of the dislocation is affected by the interaction of the dislocation with other dislocations or crystalline defects, free surfaces, and grain boundaries. For example, it is well-known that dislocation core broadens as two opposite dislocations approach each other; an incipient dislocation ahead of the crack tip has a broader core than an isolated dislocation away from the crack tip; the curvature of the dislocation line, kinking of the dislocation, dissociation of the dislocation into partial dislocations, the stacking fault energy, and the non-planar dislocation configurations also have obvious effects on the dislocation core structure and the resulting Peierls stress. Atomistic simulations of some of these phenomena have already been performed and reported in the literature [42-44]. The extension of the analysis is also of interest for the study of nanocrystalline, grain boundary abundant materials [45], 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 overall deformation process.

Acknowledgments

REFERENCES

[1] Peierls, R. (1940), Proc. Phys. Soc. 52, 34.
[2] Nabarro, F.R.N. (1947), Proc. Phys. Soc. 59, 256.

[3] Cottrell, A.H. (1961), Dislocations and Plastic Flow in Crystals, Oxford University Press, London.

[4] Havner, K.S. (1992), Finite Plastic Deformation of Crystalline Solids, Cambridge University Press, Cambridge.

[5] Asaro, R.J. and Lubarda, V.A. (2006), Mechanics of Solids and Materials, Cambridge University Press, Cambridge.

[6] Lubarda, V.A., Blume, J.A., and Needleman, A. (1993), Acta Metall. Mater. 41, 625.

[7] Needleman, A. and Van der Giessen, E. (2001), Mater. Sci. Engng. A 309, 1.

[8] Zbib, H.M., de la Rubia, T.D., and Bulatov, V.V. (2002), J. Eng. Mater. Tech. 124, 78.

[9] Deshpande, V.S., Needleman, A., and Van der Giessen, E. (2003), J. Mech. Phys. Solids 51, 2057.

[10] Lubarda, V.A. (2006), Int. J. Solids Struct. 43, 3444.

[11] Rice, J.R. (1992), J. Mech. Phys. Solids 40, 239.

[12] Rice, J.R. and Beltz, G.E. (1994), J. Mech. Phys. Solids 42, 333.

[13] Beltz, G.E. and Freund, L.B. (1994), Phil. Mag. A 69, 183.

[14] Freund, L.B. and Suresh, S. (2003), Thin Film Materials: Stress, Defect Formation and Surface Evolution, Cambridge University Press, New York.

[15] Hirth, J.P. and Lothe, J. (1982), Theory of Dislocations (2nd ed.), John Wiley & Sons, New York.

[16] Wang, J.N. (1996), Mater. Sci. Engng. A 206, 259.

[17] Nabarro, F.R.N. (1997), Phil. Mag. A 75, 703.

[18] Zhou, S.J., Carlsson, A.E., and Thomson, R. (1994), Phys. Rev. B 49, 6451.

[19] Pasianot, R.C. and Moreno-Gobbi, A. (2004), Phys. Stat. Sol. B 241, 1261.

[20] Anglade, P.M., Jomard, G., Robert, G., and Zerah, G. (2005), J. Phys. Cond. Matter. 17, 2003.

[21] Ohsawa, K., Koizumi, H., Kirchner, O.K., and Suzuki, T. (1994), Phil. Mag. A 69, 171.

[22] Bulatov, V.V. and Kaxiras, E. (1997), Phys. Rev. Lett. 78, 4221.

[23] Joós, B. and Duesbery, M.S. (1997), Phil. Mag. A 81, 1329.

[24] Miller, R., Phillips, R., Beltz, G., and Ortiz, M. (1998), J. Mech. Phys. Solids 46, 1845.

[25] Lu, G., Kioussis, N., Bulatov, V.V., and Kaxiras, E. (2000), Phil. Mag. Lett. 80, 675.

[26] Mryasov, O.N., Gornostyrev, Y.N., and Freeman, A.J. (1998), Phys. Rev. B 58, 11927.

[27] Schoeck, G. (2001), Comp. Mater. Sci. 21, 124.

[28] Schoeck, G. (2001), Acta Mater. 49, 1179.

[29] Joós, B. and Zhou, J. (2001), Phys. Rev. Lett. 78, 266.

[30] Schoeck, G. (2005), Mater. Sci. Engng. A 400-401, 7.

[31] Lubarda, V.A. and Markenscoff, X. (2006), Arch. Appl. Mech., in press.

[32] Nabarro, F.R.N. (1967), Theory of Crystal Dislocations, Oxford University Press, Oxford.

[33] Christian, J.W. and Vitek, V. (1970), Rep. Prog. Phys. 33, 307.

[34] Eshelby, J.D. (1949), Phil. Mag. 40, 903.

[35] Indenbom, V.L. and Orlov, A.N. (1962), Usp. Fiz. Nauk 76, 557.

[36] Hobart, R. (1965), J. Appl. Phys. 36, 1944.

[37] Nabarro, F.R.N. (1989), Mater. Sci. Engng. A 113, 315.

[38] Huntington, H.B. (1955), Proc. Phys. Soc. Lond. B 68, 1043.

[39] Kuhlmann-Wisdorf, D. (1960), Phys. Rev. 120, 773.

[40] Seeger, A. (2002), Z. Metallkd. 93, 760.

[41] Lubarda, V.A. and Markenscoff, X. (2006), Appl. Phys. Lett., in press.

[42] Teodosiu, C. (1982), Elastic Models of Crystal Defects, Springer-Verlag, Berlin.

[43] Tadmor, E.B., Ortiz, M., and Phillips, R. (1996), Phil. Mag. A 73, 1529.

[44] Wang, G.F., Strachan, A., Cagin, T., and Goddard, W.A. (2004), Modelling Simul. Mater. Sci. Eng. 12, S371.

[45] Asaro, R.J. and Suresh, S. (2005), Acta Mater. 53, 3369.

APPENDIX: MISFIT ENERGY BASED ON A SINGLE-COUNTING SCHEME

In the Peierls–Nabarro analysis, ignoring the strain contribution from the gradient of the vertical component of the displacement, $\partial v/\partial x$, the shear strain in the thin layer between two adjacent atomic planes across the glide plane ($y = 0$, $x > 0$) is

$$\gamma(x,0) = \frac{b/2 - \delta(x)}{h}, \quad \mathrm{d}\gamma = -\frac{1}{h}\,\mathrm{d}\delta(x). \tag{A.1}$$

The misfit energy within the area $h\Delta x$ is

$$\frac{\Delta W}{h\Delta x} = \int_0^\gamma \tau(x,0)\,\mathrm{d}\gamma(x,0) = -\int_{b/2}^{\delta(x)} \tau(x,0)\,\frac{1}{h}\,\mathrm{d}\delta(x). \tag{A.2}$$

Upon multiplying by h, and by using the expression (3.24), we obtain

$$\frac{\Delta W}{\Delta x} = -\frac{\mu b}{4\pi(1-\nu)}\frac{1}{\rho}\int_{b/2}^{\delta(x)} \sin\frac{2\pi\delta(x)}{b}\,\mathrm{d}\delta(x). \tag{A.3}$$

The substitution of Eq. (2.13) for $\delta(x)$, and integration, gives

$$\frac{\Delta W}{\Delta x} = \frac{\mu b^2}{4\pi^2(1-\nu)}\frac{1}{\rho}\cos^2\left(\tan^{-1}\frac{x}{\rho}\right) \equiv \frac{\mu b^2}{4\pi^2(1-\nu)}\frac{\rho}{\rho^2 + x^2}. \tag{A.4}$$

The continuum approximation of the total misfit energy is

$$D = \frac{\mu b^2}{4\pi^2(1-\nu)}\int_{-\infty}^\infty \frac{\rho\,\mathrm{d}x}{\rho^2 + x^2} = \frac{\mu b^2}{4\pi(1-\nu)}. \tag{A.5}$$

In a semi-discrete method of Peierls and Nabarro, the misfit energy per length $\Delta x = b$, around the dislocation at $x = nb$ within the atomic plane just above the slip plane is, from (A.4),

$$\Delta W = \frac{\mu b^3}{4\pi^2(1-\nu)}\frac{\rho}{\rho^2 + n^2 b^2}. \tag{A.6}$$

If the dislocation center has moved by αb ($0 \le \alpha \le 1$), then according to the so-called single-counting scheme, in which all atoms above the slip plane moved by αb, the strain energy of the displaced configuration is

$$W(\alpha) = \frac{\mu b \rho}{4\pi^2(1-\nu)} \sum_{n=-\infty}^{\infty} \frac{1}{(\rho/b)^2 + (n+\alpha)^2} . \tag{A.7}$$

Upon the summation, this becomes

$$W(\alpha) = \frac{\mu b^2}{4\pi(1-\nu)} \frac{\sinh(2\pi\rho/b)}{\cosh(2\pi\rho/b) - \cos(2\pi\alpha)} . \tag{A.8}$$

It can be easily verified that for all ρ greater than about $b/2$, W is very nearly equal to

$$W(\alpha) = \frac{\mu b^2}{4\pi(1-\nu)} \left[1 + 2\exp(-2\pi\rho/b)\cos(2\pi\alpha)\right], \tag{A.9}$$

which is the Peierls–Nabarro expression corresponding to a single-counting scheme, with the periodicity of $W(\alpha)$ being equal to 1. The energy

$$W_{\mathrm{P}} = W(0) - W(1/2) = 4D\exp(-2\pi\rho/b) \tag{A.10}$$

is called the Peierls energy. In a double-counting scheme, the argument $-2\pi\rho/b$ is replaced by $-4\pi\rho/b$, and the periodicity of $W(\alpha)$ is equal to 1/2. The Peierls energy in this case is $W_{\mathrm{P}} = 4D\exp(-4\pi\rho/b)$.

Returning to the exact expression (A.8), the lattice friction stress is defined by

$$\tau_{\mathrm{LF}} = -\frac{1}{b^2} \frac{\partial W}{\partial \alpha} = \frac{\mu}{2(1-\nu)} \frac{\sinh(2\pi\rho/b)\sin(2\pi\alpha)}{\left[\cosh(2\pi\rho/b) - \cos(2\pi\alpha)\right]^2} . \tag{A.11}$$

Its maximum value is obtained from

$$\frac{\partial \tau_{\mathrm{LF}}}{\partial \alpha} = 0 \quad \Rightarrow \quad \cos(2\pi\alpha) \approx \frac{2}{\cosh(2\pi\rho/b)} . \tag{A.12}$$

Consequently, the Peierls stress, based on a single-counting scheme, is

$$\tau_{\mathrm{PS}} = \tau_{\mathrm{LF}}^{\mathrm{max}} = \frac{\mu}{2(1-\nu)} \frac{\sinh(2\pi\rho/b)}{\sinh^2(2\pi\rho/b) - 1} . \tag{A.13}$$

Two consecutive approximations of this are

$$\tau_{\mathrm{PS}} \approx \frac{\mu}{2(1-\nu)} \frac{1}{\sinh(2\pi\rho/b)} \approx \frac{\mu}{1-\nu} \exp(-2\pi\rho/b). \qquad (A.14)$$

The last expression is sufficiently accurate approximation of (A.13) for any $\rho > b/2$. Thus, the coefficient $k = 2$ in the exponential argument of Eq. (6.54) is supported by the Peierls–Nabarro model based on a single-counting scheme to calculate the misfit energy across the glide plane. By combining (A.10) and (A.14), we find that $\tau_{\mathrm{PS}} = \pi W_{\mathrm{P}}/b^2$.