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Configurational force on a lattice dislocation and the Peierls stress

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Abstract The solution for a crystalline edge dislocation is presented within a framework of continuum linear elasticity, and is compared with the Peierls–Nabarro solution based on a semi-discrete method. The atomic disregistry and the shear stress across the glide plane are discussed. The Peach–Koehler configurational force is introduced as the gradient of the strain energy with respect to the dislocation position between its two consecutive equilibrium positions. The core radius is assumed to vary periodically between equilibrium positions of the dislocation. The critical force is expressed in terms of the core radii or the energies of the stable and unstable equilibrium configurations. This is used to estimate the Peierls stress for both wide and narrow dislocations.

Keywords Configurational force · Core radius · Disclination · Dislocation · Lattice friction · Peach–Koehler force · Peierls stress

1 Introduction

A semi-discrete model of a lattice dislocation by Peierls [1] and Nabarro [2] was introduced to estimate the minimum external stress required to surpass the lattice friction and drive a dislocation in a perfect crystal lattice. Due to various simplifications introduced in the original model, the calculated values of the Peierls stress were an order of magnitude or more higher than those experimentally observed or those calculated by atomistic models. Further refinements and improvements of the model were subsequently suggested by many researchers [3–12]. In the present paper, we derive a solution for the lattice dislocation in the framework of a linear elasticity by superposing the solutions of two disclinations in an infinite medium. The atomic disregistry and the shear stress across the glide plane are analyzed, with particular attention given to the relationship between the dislocation core radius and the interplanar atomic spacing. The Peach–Koehler configurational force is introduced as the gradient of the total strain energy with respect to dislocation position between two consecutive equilibrium configurations. The core radius is assumed to vary periodically between equilibrium positions of the dislocation. The critical configurational force is expressed in terms of the core radii or the energies of the stable and unstable equilibrium configurations. This yields the Peierls stress required to surpass the lattice friction due to atomic interactions. The results are applied to dislocations in metallic and covalently bonded crystals, characterized by wide and narrow dislocation cores.

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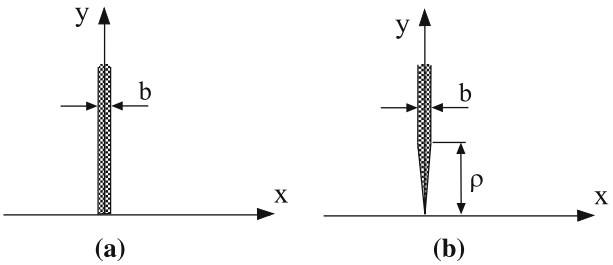

Fig. 1 **a** An edge dislocation produced by a horizontal displacement discontinuity of constant amount b along the positive y-axis. **b** A disclinated dislocation produced by a gradual displacement discontinuity from 0 to b along the height ρ

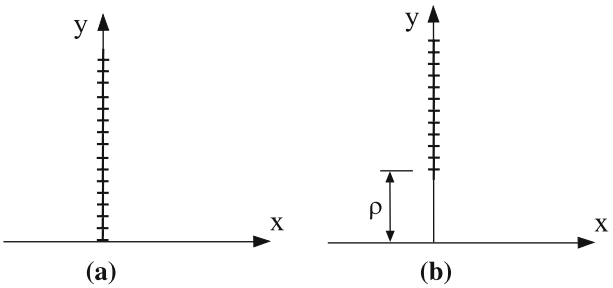

Fig. 2 **a** A semi-infinite dislocation wall with a continuous distribution of positive dislocations of density $1/\rho$ along the y-axis from $y = 0$ to ∞. **b** A semi-infinite dislocation wall with a continuous distribution of negative dislocations of density $1/\rho$ along the y-axis from $y = \rho$ to ∞

2 Lattice dislocation in the framework of linear elasticity

The stress field of the Volterra edge dislocation (Fig. 1a) is singular due to excessive straining produced by the constant displacement discontinuity b applied at the center of the dislocation. The shear stress along the x-axis has a characteristic $1/x$-type singularity as $x \to 0$. To eliminate this singularity, the simplest remedy is to assume that the displacement discontinuity b along the y-axis is achieved gradually – by a linear increase over some distance ρ, as sketched in Fig. 1b. [1] This type of wedge dislocation can be modeled by the superposition of two semi-infinite dislocation walls [14, 15]. These can also be viewed as two disclinations [16, 17], which consist of infinitesimal dislocations of density $1/\rho$ (Fig. 2). The corresponding shear stress is

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

so that, along the x-axis,

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

The elastic shear modulus is μ, and the Poisson ration ν. This is clearly finite everywhere, being equal to zero at the origin, and diminishing again to zero as $x \to \pm\infty$, in the manner of the Volterra dislocation. We can then reasonably adopt (2) as the shear-stress distribution along the slip plane of a Taylor-type lattice dislocation, produced by a gradual slip discontinuity along the x-axis. Denoting by $\beta(x)$ the specific Burgers vector of a continuous distribution of infinitesimal Volterra dislocations along the x-axis, we require

$$\text{p.v.} \int_{-\infty}^{\infty} \frac{\beta(\xi)}{x - \xi} \, \mathrm{d}\xi = \frac{bx}{x^2 + \rho^2} \,, \quad \int_{-\infty}^{\infty} \beta(x) \mathrm{d}x = b \,, \tag{3}$$

[1] Lothe [13] 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 paper we use the wedge dislocation along the vertical axis, but only to produce a non-singular shear-stress distribution along the glide plane of an edge dislocation. This is then used in conjunction with a semi-inverse method to derive (through an integral equation approach) the corresponding displacement discontinuity along the glide plane.

which has the solution (derived in the Appendix)

$$\beta(x) = \frac{b}{\pi}\,\frac{\rho}{x^2+\rho^2}\,. \tag{4}$$

The corresponding slip discontinuity along the x-axis is

$$\delta(x) = \int_0^x \beta(\xi)\,\mathrm{d}\xi = \frac{b}{\pi}\,\tan^{-1}\frac{x}{\rho}\,. \tag{5}$$

The length ρ can now be interpreted as the distance from the center of the dislocation at which the slip discontinuity is $\delta(\rho) = b/4$, which is half of the maximum slip $\delta_{\max} = b/2$, infinitely far from the center of the dislocation.

The corresponding Airy stress function is

$$\Phi = -\frac{\mu b}{4\pi(1-\nu)}\,y\,\ln\left[x^2+\left(y+\frac{|y|}{y}\,\rho\right)^2\right], \tag{6}$$

with the in-plane stresses [18]

$$\sigma_{xx}(x,y) = -\frac{\mu b}{2\pi(1-\nu)}\left\{\frac{y\pm 2\rho}{x^2+(y\pm\rho)^2}+\frac{2x^2 y}{[x^2+(y\pm\rho)^2]^2}\right\}, \tag{7}$$

$$\sigma_{yy}(x,y) = -\frac{\mu b}{2\pi(1-\nu)}\left\{\frac{y}{x^2+(y\pm\rho)^2}-\frac{2x^2 y}{[x^2+(y\pm\rho)^2]^2}\right\}, \tag{8}$$

$$\tau_{xy}(x,y) = \frac{\mu b}{2\pi(1-\nu)}\left\{\frac{x}{x^2+(y\pm\rho)^2}-\frac{2xy(y\pm\rho)}{[x^2+(y\pm\rho)^2]^2}\right\}, \tag{9}$$

and the displacements [19, 20]

$$u(x,y) = \frac{b}{2\pi}\left(\tan^{-1}\frac{y\pm\rho}{x}\mp\frac{\pi}{2}\,\frac{|x|}{x}\right)+\frac{b}{4\pi(1-\nu)}\,\frac{xy}{x^2+(y\pm\rho)^2}\,, \tag{10}$$

$$v(x,y) = -\frac{b(1-2\nu)}{8\pi(1-\nu)}\,\ln\frac{x^2+(y\pm\rho)^2}{b^2}+\frac{b}{4\pi(1-\nu)}\,\frac{y(y\pm\rho)}{x^2+(y\pm\rho)^2}\,. \tag{11}$$

The upper sign corresponds to $y > 0$, and the lower sign to $y < 0$.[2]

By comparing (2) and (5) we establish the sinusoidal relationship between the shear stress and the slip displacement,

$$\tau_{xy}(x,0) = \frac{\mu}{4\pi(1-\nu)}\,\frac{b}{\rho}\,\sin\frac{2\pi\delta(x)}{b}\,. \tag{12}$$

This reveals that $\delta(x) = (b/2)|x|/x$ implies $\rho = 0$, which is the case of the Volterra dislocation.

[2] 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.

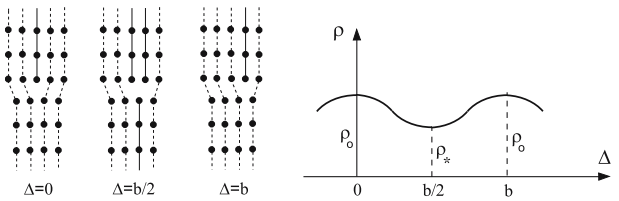

Fig. 3 **a** A glide of an edge dislocation within the distance $0 \le \Delta \le b$. Three consecutive equilibrium configurations are shown. **b** A periodic variation of the core radius ρ with the dislocation glide distance Δ, according to Eq. (15), in the case $k = 2$

3 Configurational force on a lattice dislocation

The total strain energy in an infinite medium within a large radius R around the center of the dislocation is [18, 21]

$$E = \frac{1}{2}\int_{-R}^{R} \tau_{xy}(x,0)\delta(x)\,\mathrm{d}x + E_R\,, \quad E_R = \frac{\mu b^2}{8\pi(1-\nu)}\,, \tag{13}$$

which is

$$E = \frac{\mu b^2}{4\pi(1-\nu)}\,\ln\frac{e^{1/2}R}{2\rho}\,. \tag{14}$$

If the uniform remote shear stress τ is applied, the dislocation will tend to glide along its glide plane, its consecutive equilibrium configurations being schematically shown in Fig. 3a. The lattice friction stress due to lattice periodicity and interatomic forces around the dislocation opposes this motion. Assuming that the radius of the dislocation core changes with the glide distance Δ, we consider a periodic variation

$$\rho(\Delta) = \frac{1}{2}(\rho_o + \rho_*) + \frac{1}{2}(\rho_o - \rho_*)\cos\frac{k\pi\Delta}{b}\,, \quad k = 2, 4, \tag{15}$$

with a period $2b/k$ (i.e., b or $b/2$). The core radius at $\Delta = 0$ is ρ_o and at $\Delta = b/k$ is ρ_*. In Fig. 3b it is assumed that $\rho_* < \rho_o$, so that $\Delta = 0$ is a stable and $\Delta = b/2$ an unstable equilibrium configuration of the dislocation [since then, from Eq. (14), $E_* > E_o$].

Assuming that the strain energy outside the large radius R remains unaltered by a small displacement Δ of the center of the dislocation, the configurational force[3] on the dislocation, according to the Eshelby concept of this force [24, 25], can be defined as the energy gradient with respect to the glide distance, i.e.,

$$F(\Delta) = \frac{\mathrm{d}E}{\mathrm{d}\Delta}\,. \tag{16}$$

Thus,

$$F(\Delta) = \frac{\mathrm{d}E}{\mathrm{d}\rho}\,\frac{\mathrm{d}\rho}{\mathrm{d}\Delta} = -\frac{\mu b^2}{4\pi(1-\nu)}\,\frac{1}{\rho}\,\frac{\mathrm{d}\rho}{\mathrm{d}\Delta}\,. \tag{17}$$

Since, from Eq. (15),

$$\frac{\mathrm{d}\rho}{\mathrm{d}\Delta} = -\frac{k\pi}{2b}\,(\rho_o - \rho_*)\sin\frac{k\pi\Delta}{b}\,, \tag{18}$$

the configurational force is

$$F(\Delta) = \frac{k\mu b}{8\pi(1-\nu)}\,\frac{\rho_o - \rho_*}{\rho}\,\sin\frac{k\pi\Delta}{b}\,. \tag{19}$$

[3] A comprehensive treatment of the configurational (material) forces can be found in [22, 23].

The maximum value of this force is obtained from

$$\frac{\mathrm{d}F}{\mathrm{d}\Delta} = 0 \quad \Rightarrow \quad \cos\frac{k\pi\Delta}{b} = -\frac{\rho_o - \rho_*}{\rho_o + \rho_*}\,, \quad \sin\frac{k\pi\Delta}{b} = 2\,\frac{\sqrt{\rho_o\rho_*}}{\rho_o + \rho_*}\,. \tag{20}$$

The corresponding radius, from (15), is given by $\rho = 2\rho_o\rho_*/(\rho_o + \rho_*)$, and substitution into (19) yields

$$F_{\max} = \frac{k\mu b}{8(1-\nu)}\,\frac{\rho_o - \rho_*}{\sqrt{\rho_o\rho_*}} = \frac{k\mu b}{8(1-\nu)}\,\frac{\rho_o - \rho_*}{\rho_o}\,\sqrt{\frac{\rho_o}{\rho_*}}\,. \tag{21}$$

This is the critical Peach–Koehler force required to drive a dislocation within its glide plane in a perfect crystal. In terms of the energy barrier between the stable and unstable equilibrium configurations, the Peach–Koehler force can be expressed as

$$F_{\max} = \frac{k\mu b}{4(1-\nu)}\,\sinh\frac{E_* - E_o}{2D}\,, \quad D = \frac{\mu b^2}{4\pi(1-\nu)}\,, \tag{22}$$

i.e.,

$$F_{\max} = \frac{k\pi}{2}\,\frac{E_* - E_o}{b} + \text{higher order terms}\,. \tag{23}$$

Peach–Koehler forces on dislocations within the theory of couple stress and nonlocal elasticity have been studied recently [26, 27].

4 A simple estimate of the Peierls stress

The Peierls stress, required to surpass the lattice friction stress and move a dislocation in a perfect crystal lattice, is $\tau_{\mathrm{PS}} = F_{\max}/b$. Before precise evaluations of the energy difference between stable and unstable equilibrium configurations are available, an estimate of the Peierls stress can be obtained from the expression (21) with $k = 2$ as follows. The experimental evidence indicates that dislocations in softer metals are characterized by a broader dislocation width ($w = 2\rho$) and a lower lattice friction stress. It can then be reasonably anticipated that the relative change of the dislocation width is much 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, which contributes to the decrease of the dislocation width. 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 [4]

$$\frac{\rho_*}{\rho_o} = 1 - k_1\,\exp\left(\frac{-k_2\pi\rho_o}{b}\right). \tag{24}$$

The parameters k_1 and k_2 in general depend on Poisson's ratio and the temperature. When (24) is substituted into (21), we obtain the Peierls stress as

$$\tau_{\mathrm{PS}} \approx \frac{\mu}{4(1-\nu)}\,k_1\,\exp\left(\frac{-k_2\pi\rho_o}{b}\right). \tag{25}$$

In Table 1 we list the specifications of k_1 and k_2 that reduce this expression to some of the well-known expressions for the Peierls stress reported in the literature. The specifications in the table correspond to $\rho_o = b/2(1-\nu)$ in Eq. (25). The parameter β in Foreman's et al. formula is defined by $\beta = 2\pi(\alpha - 1)/(1-\nu)$, where $\alpha > 1$ is a fitting parameter.

[4] 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 $\tau_{\mathrm{PS}} \sim \mu(b/w_o)^n$, which is an expression of the type suggested in [28, 29] on the basis of the one-dimensional Frenkel–Kantorova dislocation model.

Table 1 Peierls stress expressions

Parameters: $k_1,\ k_2$	Formula
$k_1 = 8,\ k_2 = 4$	Peierls–Nabarro [1,2]
$k_1 = 8[1 + \beta + \beta^2/6],\ k_2 = 4\alpha$	Foreman et al. [30]
$k_1 = [2.3 + 0.98(1 - \nu)]/4,\ k_2 = 2$	Huntington [31]
$k_1 = 8,\ k_2 = 2(3 - 2\nu)$	Lee and Dundurs [32]

Knowing that the Peierls–Nabarro formula ($k_2 = 4$), based on a double-counting scheme to calculate the misfit energy around the glide plane, significantly underestimates the lattice friction stress for realistic values 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 halves the parameter k_2, we adopt the value $k_2 = 2$. Theoretical elaborations in [4, 30] also support this choice of k_2. Assuming that the narrowest dislocations have width $2\rho \approx b$, and expecting that the upper bound for the lattice friction stress is of the order of $0.1\,\mu$, we specify $k_1 = 4$.

If $\nu = 1/3$ and $\rho_0 = 2b$, the Peierls stress is $\tau_{\rm PS} = 5.25 \times 10^{-6}\,\mu$, while for a narrow dislocation with $\rho_o = b/2$ and $\nu = 1/5$, $\tau_{\rm PS} = 5.4 \times 10^{-2}\,\mu$. The experimental values at low temperature for $\tau_{\rm PS}$ in closed-packed Cu is about $5 \times 10^{-6}\,\mu$, while in covalent Si it is about $0.1\,\mu$. If $\rho_o = 1.7b$ and $\nu = 1/3$, $\tau_{\rm PS} = 3.4 \times 10^{-5}\,\mu$, which is close to an experimentally observed value for hexagonal close-packed (HCP) Zn ($2 \times 10^{-5}\,\mu$ for the basal plane). If $\rho_o = b$ and $\nu = 0.3$, $\tau_{\rm PS} = 2.67 \times 10^{-3}\,\mu$, which is close to an experimentally observed value for a base-centered cubic (BCC) α-Fe ($5 \times 10^{-3}\,\mu$).

The radius ρ_o in the preceding analysis is a free parameter, to be specified for a given crystal and glide system from the observations of the extent of the dislocation core spreading. Alternatively, ρ_o may be related to an estimate of the maximum shear stress along the glide plane of the dislocation. Denoting this by $\tau_{\max}$, it follows that

$$\rho_o = \frac{\mu b}{4\pi(1 - \nu)\tau_{\max}}\,. \tag{26}$$

It is reasonable to assume that $\tau_{\max}$ is equal to the actual shear strength of the pure crystal under uniform straining, either experimentally determined or estimated from atomistic calculations, which is a fraction of the theoretical shear strength $\mu b/2\pi h$ of the pure crystal [33]. Guided by experimental data on the lattice friction stress, we take $\tau_{\max}$ to be one half of the theoretical shear strength, i.e., $\tau_{\max} = \mu b/4\pi h$. For a face-centered cubic (FCC) crystal ($\langle 211\rangle\,\{111\}$ partial, $h/b = \sqrt{2}$), we obtain $\tau_{\max} = 0.056\,\mu$. With $\nu = 1/3$, Eq. (26) gives $\rho_o = 2b$. For a BCC crystal ($\langle 111\rangle\,\{110\}$ glide system, $h/b = \sqrt{2/3}$), we obtain $\tau_{\max} = 0.1\,\mu$ and, with $\nu = 0.3$, Eq. (26) gives $\rho_o = 1.1b$. For an HCP crystal ($\langle 11\bar{2}0\rangle\,\{0001\}$ glide system, $h/b = 1.093$), we obtain $\tau_{\max} = 0.07\,\mu$. With $\nu = 1/3$, Eq. (26) gives $\rho_o = 1.7b$. Finally, for a diamond cubic crystal ($\langle 110\rangle\,\{111\}$ shuffle plane, $h/b = 0.4083$), we obtain $\tau_{\max} = 0.2\,\mu$ and, with $\nu = 1/5$, Eq. (26) gives $\rho_o = 0.5b$.

5 Conclusions

A solution for the lattice dislocation was derived in the framework of a continuum linear elasticity, and is compared with the Peierls–Nabarro solution based on a semi-discrete model. The atomic disregistry and the shear stress across the glide plane are discussed, with particular attention given to the relationship between the dislocation width and the atomic spacing across the glide plane. The Peach–Koehler configurational force on the lattice dislocation, defined as the gradient of the strain energy with respect to the dislocation position between consecutive equilibrium configurations, was used, in conjunction with the periodic variation of the core radius, to derive an expression for the critical configurational force and the Peierls stress required to overcome the lattice friction due to atomic interactions. The obtained results are applied to edge dislocations with both narrow and wide cores. The comparison with typical experimental data for metallic and covalently bonded crystals is given.

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Appendix: Solution of the singular integral equation

The singular Cauchy-type integral equation

$$\frac{1}{\pi}\,\text{p.v.}\int_{-\infty}^{\infty}\frac{f(\xi)\,\mathrm{d}\xi}{x-\xi}=g(x) \tag{27}$$

has the solution

$$f(x)=\frac{1}{\pi}\,\text{p.v.}\int_{-\infty}^{\infty}\frac{g(\xi)\,\mathrm{d}\xi}{\xi-x}\,. \tag{28}$$

The functions $f(x)$ and $g(x)$ are referred to as the Hilbert pair. Since

$$\int_{-\infty}^{\infty}\frac{g(x)\,\mathrm{d}\xi}{\xi-x}=g(x)\int_{-\infty}^{\infty}\frac{\mathrm{d}\xi}{\xi-x}=0\,, \tag{29}$$

the integral in (28) can be rewritten as

$$f(x)=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{g(\xi)-g(x)}{\xi-x}\,\mathrm{d}\xi\,, \tag{30}$$

which is an ordinary integral whenever g is Hölder continuous [34]. Thus, letting

$$\frac{1}{\pi}\,f(\xi)=\beta(\xi)\,,\quad g(x)=\frac{bx}{x^2+\rho^2}\,, \tag{31}$$

it follows that

$$\beta(x)=\frac{b}{\pi^2}\,\frac{1}{x^2+\rho^2}\int_{-\infty}^{\infty}\frac{\rho^2-\xi x}{\xi^2+\rho^2}\,\mathrm{d}\xi=\frac{b}{\pi}\,\frac{\rho}{x^2+\rho^2}\,. \tag{32}$$

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