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RESEARCH ARTICLE

On approaches to modelling lattice dislocations

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By proposing a sinusoidal relationship between slip discontinuity and the associated mismatch force, Peierls and Nabarro famously developed a dislocation model that eliminates the stress singularity from the Volterra dislocation model. Recently, Lubarda and Markenscoff (*Appl. Phys. Lett.* 89:151923, 2006) developed a model in which the Burgers vector of the dislocation is applied over some finite distance, ρ, described as the 'core radius'. They found that the shear stress on the glide-plane predicted in the Lubarda-Markenscoff model is identical to that predicted by the Peierls-Nabarro model. In this paper, we investigate generalisations of both the Lubarda-Markenscoff and Peierls-Nabarro models, demonstrating that different distributions of infinitesimal dislocations in a generalised Lubarda-Markenscoff model can be associated with different expressions for the misalignment force in a generalised Peierls-Nabarro model. Our results indicate that the generalised Lubarda-Markenscoff framework is a versatile and useful method for modelling the core of a dislocation that neatly complements the well established Peierls-Nabarro framework.

Keywords: dislocation theory; dislocations; lattice defects; dislocation core radius; Peierls-Nabarro model

1. Introduction

In the 1940s, Peierls [11] and Nabarro [10] proposed a model of edge dislocations in cubic lattices that incorporates the effects of lattice discreteness within a narrow region around the glide plane. The Peierls-Nabarro model depends on a balance between the elastic forces in each half-crystal and a misalignment force that depends on the slip discontinuity across the glide plane. By analogy with the Frenkel model of crystal shear strength, Peierls and Nabarro modelled the relationship between slip discontinuity and misalignment force using a sinusoidal function [5]. However, there is no essential reason why the relationship between force and slip discontinuity should be sinusoidal rather than some other periodic function. The main advantage of using the sinusoidal function is that it enables analytic results to be obtained, and the Peierls-Nabarro model continues to be of interest as a bridge between continuum models and fully atomistic models [6].

Unlike the Peierls-Nabarro model, the Lubarda-Markenscoff model does not explicitly consider the relationship between slip discontinuity and misalignment force. Instead, a Lubarda-Markenscoff edge dislocation is modelled as a uniform distribution of infinitesimal Volterra dislocations along a short line segment orthogonal to the glide plane. The length of this line segment is associated with the size of the dislocation core, and it is assumed to vary with the position and environment of

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the dislocation [8, 9]. This spreading of incompatibility along a line is reminiscent of Eshelby's representation of a Volterra edge dislocation as a dipole of wedge dislocations [3], and the Lubarda-Markenscoff is effectively an extension of this model to the case where there is a finite distance between the two wedge dislocations.

The Lubarda-Markenscoff model is also motivated by experimental observations of dislocation core structure and by results from atomistic simulations. For example, Bassani *et al.* [2] used atomistic simulations to investigate the core of a $1/2\langle 111\rangle$ screw dislocation in a bcc lattice. They found that the dislocation core is smeared along the $\{110\}$ planes that intersect the screw dislocation, and that the extent of smearing depends on the applied stress. Moreover, they concluded that this smearing affects the dislocation mobility, leading to deviations from Schmid's law [2, 4]. This means that the changing size and shape of the dislocation core has a practical significance for dislocation motion and the Peierls stress, which Lubarda and Markenscoff [8, 9] derive as a configurational force in their model.

Interestingly, the stresses and displacements on the glide plane obtained in the Lubarda-Markenscoff model are identical to those observed in the Peierls-Nabarro model. However, just as Peierls and Nabarro considered only a sinusoidal misalignment force, Lubarda and Markenscoff considered only the case where the density of infinitesimal dislocations is uniform throughout the dislocation core. In this paper, we investigate the effect of using a general distribution of dislocations in the Lubarda-Markenscoff model, and we compare this with the effect of using a general periodic misalignment force in the Peierls-Nabarro model.

2. A generalised Lubarda-Markenscoff dislocation

Consider an isotropic material containing an infinite, straight dislocation running along the z-axis with a Burgers vector of $\hat{b}\,\boldsymbol{i}$. In the Lubarda-Markenscoff model [8], the x-y shear stress on the $y = 0$ plane due to this dislocation is given by

$$\tau_{xy}(x,\,0) = \frac{\mu}{2\,\pi\,(1-\nu)} \int_0^{\rho} \frac{\hat{b}}{\rho}\, \frac{x^3 - \eta^2\, x}{(x^2+\eta^2)^2}\, d\eta,$$

where μ is the shear modulus, ν is Poisson's ratio and ρ is the core width parameter.

We may generalise this model by introducing a non-constant Burgers vector distribution, $b(\eta)$, so that the x-y shear stress at $y = 0$ is given by

$$\tau_{xy}(x,\,0) = \frac{\mu}{2\,\pi\,(1-\nu)} \int_0^{\rho} b(\eta)\, \frac{x^3 - \eta^2\, x}{(x^2+\eta^2)^2}\, d\eta, \quad x \neq 0. \tag{1}$$

In order to ensure that the total Burgers vector of the dislocation is still $\hat{b}$, we impose the condition

$$\int_0^{\rho} b(\eta)\, d\eta = \hat{b}. \tag{2}$$

Additionally, we assume that $b(\eta)$ is nonnegative and nonsingular throughout $x \in [0,\,\rho]$, and that b is continuous in the neighbourhood of $\eta = 0$.

As described in the Appendix, we can use asymptotic techniques to obtain series

expansions for $\tau_{xy}(x,\,0)$ in the case where $|x| \gg \rho$. This yields

$$\tau_{xy}(x,\,0) \sim \frac{\mu}{2\,\pi\,(1-\nu)}\,\frac{\hat{b}}{x}.$$

Hence, the stress due to a generalised Lubarda-Markenscoff dislocation becomes identical to the stress due to a Volterra dislocation as $x \to \infty$. Similarly, asymptotic analysis of the case where $|x| \ll \rho$ reveals that $\tau_{xy} \to 0$ as $x \to 0$ as long as $b(\eta)$ is bounded as $\eta \to 0$. This shows that that the generalised Lubarda-Markenscoff dislocation avoids the stress singularity that is characteristic of the Volterra dislocation.

The slip discontinuity associated with a generalised Lubarda-Markenscoff dislocation can be obtained by reversing the original Peierls-Nabarro argument. We recall from [8] that the elastic shear stress on the glide plane and the slip discontinuity, $\delta(x)$, are related by

$$\tau_{xy}(x,\,0) = \frac{\mu}{2\,\pi\,(1-\nu)}\int_{-\infty}^{\infty} \frac{1}{x-x'}\,\frac{d\delta}{dx'}\,dx'. \tag{3}$$

Inverting the Hilbert transform then yields

$$\delta(x) = \frac{1}{\pi}\int_0^{\rho} b(\eta)\left(\tan^{-1}\frac{x}{\eta} - \frac{x\,\eta}{\eta^2+x^2}\right)\,d\eta, \quad x \neq 0. \tag{4}$$

Since the integrands in (1) and (4) are both odd functions of x, it follows that $\tau_{xy}(x,\,0)$ and $\delta(x)$ are also odd functions. As detailed in the Appendix, asymptotic techniques reveal that $\delta \to \pm\frac{\hat{b}}{2}$ as $x \to \pm\infty$, and it can also be shown that $\delta(x)$ is continuous at $x = 0$ with $\delta(0) = 0$. All of these observations are consistent with our physical expectation that the slip discontinuity will vary continuously and symmetrically from $-\frac{\hat{b}}{2}$ to $\frac{\hat{b}}{2}$.

Also, we note that

$$\frac{d\delta}{dx} = \frac{1}{\pi}\int_0^{\rho} b(\eta)\,\frac{2\,\eta\,x^2}{(\eta^2+x^2)^2}\,d\eta, \quad x \neq 0. \tag{5}$$

Since $b(\eta)$ is nonnegative and has a positive integral, it follows that $\delta'(x) > 0$ for all $x \neq 0$. The asymptotic analysis given in the appendix indicates that $\delta'(0) = \frac{1}{\pi}\,b(0)$, and we can therefore conclude that $\delta(x)$ is a monotone increasing function.

Hence, $\delta(x)$ has a unique inverse, $\tilde{x}(\delta)$, that maps $(-\frac{\hat{b}}{2},\,\frac{\hat{b}}{2})$ to the entire real line. We can use this to construct a further function, $\tilde{\tau}(\delta)$, that gives the shear stress associated with any particular slip discontinuity. As relating the stress to the slip discontinuity is fundamental to the Peierls-Nabarro approach, this suggests a method by which the two approaches might be related.

We also note that, for any given $b(\eta)$, there is only a single function $\tau_{xy}(x,\,0)$ that satisfies (1) and a single function $\delta(x)$ that satisfies (4). Thus, there is a unique $\tilde{\tau}(\delta)$ associated with each $b(\eta)$. As we discuss in Section 4, however, it is not clear that the converse is true.

3. A generalised Peierls-Nabarro dislocation

In the Peierls-Nabarro model, the slip discontinuity on the glide plane is obtained by balancing the force associated with macroscopic elastic effects with a force due to the misalignment between the planes of atoms on either side of the glide plane. Its pivot is its constitutive assumption about the function that relates the misalignment force to the disregistry (or, equivalently, to the slip discontinuity).

Based on the symmetry of the atomic lattice, Peierls and Nabarro argued that the misalignment force should be periodic in the slip discontinuity with a period of $\hat{b}$ and zeros at integer multiples of $\frac{\hat{b}}{2}$. In their original work, Peierls and Nabarro suggested a misalignment force of the form

$$\tilde{\tau}(\delta) = K \sin\left(\frac{2\,\pi\,\delta(x)}{\hat{b}}\right), \tag{6}$$

where K is a constant. In order to match with linear elasticity at small displacements, they determined that $K = \frac{\mu}{2\,\pi}$.

We now wish to extend this idea to a general periodic function, $\tilde{\tau}(\delta)$. We note from both Section 2 and the original Peierls-Nabarro model that the slip discontinuity actually only varies between $-\frac{\hat{b}}{2}$ and $\frac{\hat{b}}{2}$. This means that it is appropriate to define $\tilde{\tau}(\delta)$ only on the range $-\frac{\hat{b}}{2} < \delta < \frac{\hat{b}}{2}$, and impose the conditions

$$\tilde{\tau}\left(-\frac{\hat{b}}{2}\right) = \tilde{\tau}\left(\frac{\hat{b}}{2}\right) = 0, \tag{7a}$$

and

$$\left.\frac{d^n\tilde{\tau}}{d\delta^n}\right|_{\delta=-\frac{\hat{b}}{2}} = \left.\frac{d^n\tilde{\tau}}{d\delta^n}\right|_{\delta=\frac{\hat{b}}{2}}, \tag{7b}$$

for all positive integers n. Condition (7a) implies that the stress associated with a regular lattice is zero, while (7b) implies that $\tilde{\delta}(x)$ can be extended into a periodic function without introducing any discontinuities in derivatives.

In order to match with linear elasticity at small displacements, we also require that the derivative of stress with respect to slip discontinuity tend to $\frac{\mu}{\hat{b}}$ for a regular lattice. Hence,

$$\tilde{\tau}'\left(-\frac{\hat{b}}{2}\right) = \tilde{\tau}'\left(\frac{\hat{b}}{2}\right) = -\frac{\mu}{\hat{b}}. \tag{7c}$$

Following the Peierls-Nabarro approach with a general $\tilde{\tau}(\delta)$ leads to a nonlinear, hypersingular integral equation of the form

$$\frac{\mu}{2\,\pi\,(1-\nu)} \text{⨍}\!\!\!\!\!-_{-\infty}^{\infty} \frac{\delta(x')}{(x-x')^2}\,dx' = \tilde{\tau}(\delta). \tag{8}$$

Except for special cases, such as where $\tilde{\tau}(\delta)$ is a sinusoidal function, this equation cannot be solved analytically. Indeed, equations of this form are also difficult to solve numerically, although some effective methods have been developed for dealing with nonlinear equations of this type [7].

In order to be physically realistic, we expect $\delta \to \pm\infty$ as $x \to \pm\frac{\hat{b}}{2}$. However, it is not immediately clear whether this follows from the conditions in (7), or whether additional restrictions on $\tilde{\tau}$ are required. Moreover, it is not clear whether solutions to (8) will exist for any given choice of $\tilde{\tau}(\delta)$ that satisfies (7), and, if so, whether they will be unique. We leave these questions as open problems.

4. The relationship between the two dislocation models

Since Lubarda and Markenscoff [8] observed that their method of smearing the dislocation core led to identical expressions for slip discontinuity and stress as obtained from the Peierls-Nabarro model, we now investigate whether different choices of $b(\eta)$ in the generalised Lubarda-Markenscoff model can be associated with different choices of $\tilde{\tau}(\delta)$ in the generalised Peierls-Nabarro model. It was established in Section 2 that any $b(\eta)$ can be used to construct a function $\tilde{\tau}(\delta)$ that satisfies (8). In Section 3, however, we imposed the conditions in (7) on any proposed $\tilde{\tau}(\delta)$. What restrictions, if any, are implied for $b(\eta)$?

Firstly, we recall from Section 2 that $\delta(x) \to \pm\frac{\hat{b}}{2}$ as $x \to \pm\infty$ and that $\tau_{xy}(x,\, 0) \to 0$ as $x \to \pm\infty$. From these observations, it follows that (7a) is satisfied, regardless of the choice of $b(\eta)$.

For (7b) and (7c), we can use the asymptotic results obtained in the Appendix for $\tau_{xy}(x,\, 0)$ and $\delta(x)$ as $x \to \pm\infty$. Reversing the nondimensionalisation in equations (A3) and (A4) yields

$$\tau_{xy}(x,\, 0) = \frac{\mu}{2\,\pi\,(1-\nu)}\,\left(\hat{b}\,\bar{x}^{-1} - 3\,B_2\,\bar{x}^{-3} + \ldots\right), \tag{9}$$

$$\delta(x) = \pm\frac{\hat{b}}{2} - \frac{2\,B_1}{\pi}\,x^{-1} + \frac{4\,B_3}{3\,\pi}\,\bar{x}^{-3} + \ldots, \tag{10}$$

where

$$B_i = \int_0^{\rho} b(\eta)\,\eta^i\,d\eta.$$

Letting $\xi = x^{-1}$, it follows from these that

$$\tau_{xy}(\xi^{-1},\, 0) \sim f_\tau(\xi), \quad \text{and} \quad \delta(\xi^{-1}) \sim \pm\frac{\hat{b}}{2} + f_\delta(\xi), \tag{11}$$

as $\xi \to 0^{\pm}$, where f_τ and f_δ are obtained from the series in (9) and (10). We note that these are both smooth functions of ξ, and that f_δ is a monotone decreasing function of ξ and therefore invertible.

By letting $\delta = \pm\frac{\hat{b}}{2} + \hat{\delta}$ for some small $\hat{\delta}$, we find in both cases that

$$\tilde{\tau}\,(\delta) = f_\tau\left(f_\delta^{-1}\left(\hat{\delta}\right)\right).$$

Thus, the behaviour of $\tilde{\tau}(\delta)$ in the neighbourhood of $\delta = \frac{\hat{b}}{2}$ is identical to the behaviour of $\tilde{\tau}(\delta)$ in the neighbourhood of $\delta = -\frac{\hat{b}}{2}$ and condition (7b) follows naturally from repeated differentiation.

Also, we note that

$$\tilde{\tau}'\left(\pm\frac{\hat{b}}{2}\right) = \frac{f'_\tau(0)}{f'_\delta(0)}.$$

By differentiating (9) and (10) appropriately, it follows that (7c) is equivalent to

$$\int_0^\rho b(\eta)\,\eta\,d\eta = \frac{\hat{b}^2}{4\,(1-\nu)}. \tag{12}$$

In [8], where $b(\eta) = \frac{\hat{b}}{\rho}$, (7c) yields $\rho = \frac{\hat{b}}{2\,(1-\nu)}$. However, it is also noted in [8] that the Lubarda-Markenscoff approach does not require the development of a strain measure based on the gap between two elastic half-spaces. Hence, it can be argued that (7c), and concomitantly (12), do not need to be satisfied when using the generalised Lubarda-Markenscoff framework.

Regardless of the choice of $b(\eta)$, we have shown that that the associated $\tilde{\tau}(\delta)$ satisfies (7a) and (7b). Thus, any realistic distribution of infinitesimal dislocations along a plane perpendicular to the glide plane is equivalent to a Peierls-Nabarro model where the misalignment force is smooth and periodic in the slip discontinuity. Moreover, it is easy to construct a distribution of infinitesimal dislocations that accords with the Peierls-Nabarro assumption of linear elasticity away from the dislocation by ensuring that (12) holds.

The inverse problem of obtaining $b(\eta)$ from $\tilde{\tau}(\delta)$ is, however, considerably more difficult. As noted above, we have not been able to demonstrate existence or uniqueness of solutions for $\delta(x)$ if $\tilde{\tau}(\delta)$ is given. Moreover, there are further difficulties in going from $\delta(x)$ to $b(\eta)$, which involves solving the integral equation

$$\delta(x) = \frac{1}{\pi}\int_0^\infty b(\eta)\left(\tan^{-1}\frac{x}{\eta} - \frac{x\,\eta}{\eta^2+x^2}\right)d\eta, \quad x>0. \tag{13}$$

Progress can be made by noting that the kernel depends only on $\frac{x}{\eta}$ and thus the substitutions $x = e^X$ and $\eta = e^H$ can be used to obtain a Fourier-style convolution:

$$\delta(e^X) = \frac{1}{\pi}\int_{-\infty}^\infty B(H)\left(\tan^{-1}(e^{X-H}) - \frac{1}{2}\operatorname{sech}(X-H)\right)dH, \quad x>0, \tag{14}$$

where $B(H) = e^H\,b(e^H)$. This will be uniquely invertible to obtain $b(\eta)$, but is also ill-posed, so that small changes to $\delta(x)$ may lead to large changes in $B(H)$

Once $B(H)$ has been found, it is possible to construct $b(\eta)$ directly. However, we have no guarantee that such a $b(\eta)$ will have compact support, or that $b(\eta)$ will be everywhere non-negative. While any non-negative $b(\eta)$ that satisfies (12) will lead to a function $\tilde{\tau}(\delta)$ that satisfies (7), the conditions on $\tilde{\tau}(\delta)$ that lead to sensible results for $b(\eta)$ are left as an open problem.

5. Discussion and conclusions

In this paper, we have considered generalisations of two different dislocation models, both of which can be used to eliminate the stress singularity at the dislocation core observed in the Volterra model. The Lubarda-Markenscoff model can be justified by atomistic simulations and experimental observations that show a smearing

of the dislocation core along planes that intersect the dislocation [2], while the Peierls-Nabarro model can be viewed as a natural extension of the Frenkel model of crystal shear strength. Our generalisations extend the Lubarda-Markenscoff model to the case where the smearing of the dislocation core is non-uniform, while our generalisation of the Peierls-Nabarro model considers the case where the misalignment force function is periodic, but not necessarily sinusoidal.

The generalised Lubarda-Markenscoff framework promises to be an especially valuable method for describing the core structure of a dislocation as it seeks to describe the displacement distribution throughout the dislocated lattice, not the stresses. Since experimental observations and simulations yield data about atom positions rather than stresses, it follows that this data can be more easily incorporated using the Lubarda-Markenscoff framework than the Peierls-Nabarro framework. For example, [1] used atomistic simulations to investigate $\frac{1}{2}[1\ \bar{1}\ 0]$ edge dislocations in aluminium and copper. One of the results obtained was the Burgers vector distribution along the glide plane, which is equivalent to $\delta'(x)$ in the generalised Lubarda-Markenscoff model presented here. Hence, a simple modification of (14) could be used to construct $b(\eta)$ for this dislocation (although the ill-posedness problems remain). Also, reanalysis of the simulation data might show that $b(\eta)$ can be observed directly by determining the Burgers vector distribution on a line perpendicular to the glide plane.

The work presented here indicates that there will never be a fundamental contradiction between a generalised Lubarda-Markenscoff model and a generalised Peierls-Nabarro model; for any distribution of infinitesimal dislocations along the plane perpendicular to the glide plane, there will be a smooth and periodic misalignment force function that would lead to the same stress and displacement distributions. Hence, the Lubarda-Markenscoff and Peierls-Nabarro approaches are complementary; neither can be as accurate as atomistic modelling, but both are valuable because they can be used to obtain stress and displacement distributions that would be computationally expensive to recover from atomistic models.

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Appendix A. Asymptotic analysis of the stress and slip discontinuity due to a generalised Lubarda-Markenscoff dislocation

We nondimensionalise equations (1) and (4) by introducing the following barred dimensionless variables:

$$\tau_{xy}(x,\,0) = \frac{\mu}{2\,\pi\,(1-\nu)}\,\bar{\tau}(\bar{x}), \qquad x = \rho\,\bar{x}, \qquad \eta = \rho\,\bar{\eta}, \qquad \delta = \rho\,\bar{\delta}, \qquad b(\eta) = \bar{b}(\bar{\eta}).$$

With this transformation and some algebraic rearrangment, equations (1) and

(4) become

$$\bar{\tau}(\bar{x}) = \bar{x}^{-1} \int_0^1 \bar{b}(\bar{\eta}) \, \frac{\bar{x}^4/\bar{\eta}^4 - \bar{x}^2/\bar{\eta}^2}{(\bar{x}^2/\bar{\eta}^2 + 1)^2} \, d\bar{\eta}, \quad \bar{x} \neq 0, \tag{A1}$$

$$\bar{\delta}(\bar{x}) = \frac{1}{\pi} \int_0^1 \bar{b}(\bar{\eta}) \left(\tan^{-1} \frac{\bar{x}}{\bar{\eta}} - \frac{\bar{x}/\bar{\eta}}{\bar{x}^2/\bar{\eta}^2 + 1} \right) d\eta, \quad x \neq 0. \tag{A2}$$

As $X \to \pm\infty$, we note that

$$\frac{X^4 - X^2}{(X^2+1)^2} \sim 1 - 3\,X^{-2} + 5\,X^{-4} - 7\,X^{-6} + \ldots,$$

$$\tan^{-1} X - \frac{X}{1+X^2} \sim \mathrm{sgn}(X)\,\frac{\pi}{2} - 2\,X^{-1} + \frac{4}{3}\,X^{-3} - \frac{6}{5}X^{-5} + \ldots.$$

We can apply these expansions to investigate the case where $\bar{x} \gg 1$ (*i.e.* where $x \gg \rho$) in (A1) and (A2). This yields

$$\bar{\tau}(\bar{x}) = \bar{B}_0\,\bar{x}^{-1} - 3\,\bar{B}_2\,\bar{x}^{-3} + \mathcal{O}\left(\bar{x}^{-5}\right), \tag{A3}$$

$$\bar{\delta}(\bar{x}) = \frac{\bar{B}_0}{2}\,\mathrm{sgn}(\bar{x}) - \frac{2\,\bar{B}_1}{\pi}\,\bar{x}^{-1} + \frac{4\,B_3}{3\,\pi}\,\bar{x}^{-3} + \mathcal{O}\left(\bar{x}^{-5}\right), \tag{A4}$$

where

$$\bar{B}_i = \int_0^1 \bar{b}(\bar{\eta})\,\bar{\eta}^i \, d\bar{\eta}.$$

Except for the leading order term in $\bar{\delta}(\bar{x})$, all of the terms in these series involve odd powers of $\bar{x}$, which is consistent with the fact that $\bar{\tau}\ \bar{\delta}$ are both odd functions.

Reversing the nondimsionalisation leads us to recover (9) and (10).

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