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The Peierls–Nabarro model revisited

GANG LU, NICHOLAS KIOUSSIS†

Department of Physics, California State University Northridge, Northridge, California 91330-8268, USA

VASILY V. BULATOV

Lawrence Livermore National Laboratory, Livermore, California 94551, USA

and EFTHIMIOS KAXIRAS

Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

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ABSTRACT

We re-examine two important issues within the Peierls–Nabarro model, which are critical in obtaining accurate values for the Peierls stress. The first is related to the sampling scheme (double versus single counting) of the misfit energy across the glide plane and the second is the effect of atomic relaxation on the Peierls stress. We argue that the double-counting scheme is physically more appropriate. An analytical formula is derived for the Peierls stress of dislocations in alternating lattices. The atomic relaxation is shown to play an important role on the Peierls stress for narrow dislocations.

§ 1. INTRODUCTION

The Peierls stress σ_P is the minimum external stress required to move a stationary dislocation irreversibly, without the assistance from lattice vibrations. This fundamental quantity for a dislocation was first estimated by Peierls (1940) and Nabarro (1947) using essentially a continuum model, the so-called Peierls–Nabarro (P–N) model. Owing to the unrealistic sinusoidal force law adopted in the model, the original P–N framework has served more as a conceptual tool for a qualitative understanding of dislocation core properties, rather than providing quantitative estimates of these properties. Recently, there has been renewed interest in applying the P–N model to study the dislocation properties (Joós *et al.* 1994, Juan and Kaxiras 1996, Bulatov and Kaxiras 1997, Joós and Duesbery 1997, Hartford *et al.* 1998, Lu *et al.* 2000). This is motivated by the advance of reliable *ab initio* methods, which allow the accurate determination of the generalized stacking-fault energy (γ energy), that is the interplanar potential energy for sliding one half of the crystal over the other half along the glide plane. To date, the P–N model has come to serve as a link between atomistic and continuum approaches, by providing a means to incorporate information obtained from atomistic (*ab initio* or empirical) calculations directly into continuum models. The resultant approach can then be applied to

† Email: nick.kioussis@csun.edu.

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problems that neither atomistic nor conventional continuum models could handle separately.

Despite the apparent importance of the P–N model, two critical elements within the model have not been well addressed and understood. These are the sampling scheme of the misfit energy across the glide plane and the effect of atomic relaxation on σ_P. The sampling scheme is related to σ_P for different crystal lattices, that is facing lattices (F-type), in which the atoms above and below the glide plane face each other, or alternating lattices (A-type), in which atoms alternate across the glide plane (figure 1). In their original work, Peierls (1940) and Nabarro (1947) summed the misfit energy independently over the top and bottom half-crystals for F-type lattices, the so-called double-counting (DC) scheme. However, their approach yields a variation in the misfit energy and σ_P which have a periodicity of $b/2$, in contrast with the feature of the dislocation barrier, which must in general exhibit the periodicity of the Burgers vector b. This unexpected form of the Peierls energy barrier was attributed in part to the DC approach in the P–N model (Christian and Vitek 1970, Hirth and Lothe 1982). Since then, almost all numerical and analytical work has employed exclusively the single-counting (SC) scheme, in which one sums the misfit energy on only one side of the glide plane, and the misfit energy is expressed as a function of the disregistry (relative displacement) between pairs of atomic rows across the glide plane (Joós *et al.* 1994, Juan and Kaxiras 1996, Joós and Duesbery 1997, Hartford *et al.* 1998). The SC approach is based on the assumption of a nearest-neighbour interaction and on the fact that this scheme gives the correct periodicity. However, as Wang (1996a,b) pointed out recently, the undesired periodicity in the DC scheme is actually due to an erroneous representation of the atomic positions, rather than to the DC scheme itself. In fact, the DC scheme recovers the correct periodicity for both F-type and A-type lattices, after the error of atomic positions is corrected. On the other hand, the accuracy of the nearest-neighbour interaction approximation entering the SC scheme remains questionable. Another shortcoming of the classical P–N model is that it assumes a rigid dislocation translation, where the elastic energy does not change during the process of the dislocation translation.

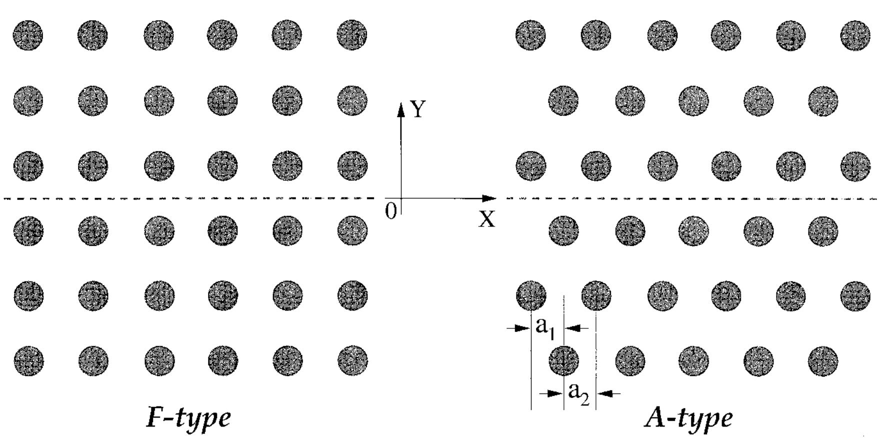

Figure 1. Schematic representation of the facing (F-type) and alternating (A-type) lattices before the introduction of a dislocation: (- - -) glide plane. In A-type lattices, $a_1 \neq a_2$ for unevenly spaced dislocations (general case), and $a_1 = a_2$ for evenly spaced dislocations (30° and 90° dislocations in the fcc lattice).

The purpose of this work is to re-examine these two important issues within the P–N model which are critical in predicting accurate values for σ_P. The DC scheme is shown to be more appropriate than the commonly used SC scheme. Employing the DC scheme, we derive an analytical formula for σ_P and identify for the first time an important degree of freedom entering the P–N model, that is the even versus uneven character of the atomic spacing. Finally, employing the recently developed semi-discrete (SD) variational P–N model (Bulatov and Kaxiras 1997), we investigate the effect of atomic relaxation on σ_P and show that the atomic relaxation can lower σ_P by an order of magnitude for narrow dislocations.

§ 2. Results and discussion

Within the SD variational P–N model, the equilibrium structure of a dislocation is determined by minimizing the dislocation energy functional with respect to the dislocation density or displacement vector (Bulatov and Kaxiras 1997, Lu *et al.* 2000). Because the displacement vector $\boldsymbol{\delta}(x_i)$ is allowed to change during the dislocation translation, the Peierls energy barrier and σ_P can be significantly reduced in comparison with their corresponding values from a rigid translation. The response of the dislocation to an applied stress is achieved by the minimization of the total energy functional (including the stress work) with respect to the dislocation density or displacement vector at a given applied stress. σ_P is then obtained by evaluating the critical value of the applied stress at which the dislocation energy functional fails to be minimized through standard conjugate gradient techniques. This approach of calculating σ_P is more accurate and physically transparent, because it captures the nature of σ_P as the stress at which the displacement field of the dislocation undergoes a discontinuous transition.

In table 1 we list the values of the misfit energy E_{misfit} and σ_P for various complete dislocations in Al, calculated from the SD P–N model using the DC and SC and the *ab initio* determined γ surface (Lu *et al.* 2000). The various dislocations are characterized by the angle θ, which is the angle between the dislocation lines and the common Burgers vector b. It should be pointed out that most of the dislocations in the fcc lattice (A-type lattice) have uneven atomic spacings, except for the 30° and 90° dislocations (see figure 1). Overall we find that the SC scheme consistently underestimates E_{misfit} and overestimates σ_P compared with the DC scheme. Interestingly,

Table 1. Comparison of the misfit energy E_{misfit} and the Peierls stress σ_P for different dislocations in Al, employing the DC and SC schemes. The SD model with the *ab initio* γ surface is used in both calculations.

Dislocation angle	E_{misfit} (eV Å^{-1})		σ_P (MPa)	
(degrees)	DC	SC	DC	SC
0	0.0994	0.0908	256	625
25.3	0.1229	0.1173	6	22
30	0.1221	0.1024	53	369
44.7	0.1370	0.1280	59	135
60	0.1521	0.1356	98	208
85.3	0.1760	0.1630	3	11
90	0.1688	0.1470	3	353

the discrepancy for σ_P between the two schemes becomes more pronounced for the evenly spaced (30° and 90°) dislocations. Thus, while the SC scheme underestimates the misfit energy by at most 15%, it overestimates σ_P by several orders of magnitude. These results demonstrate that the details of atomic spacing (even versus uneven) play an essential role in determining σ_P, which has not been addressed in previous studies.

In order to establish which scheme (DC versus SC) is more appropriate and to understand the origin of the different results in table 1, we next take a closer look at the two schemes for A-type lattices (the two schemes are essentially the same for F-type lattices). In the SC scheme, the misfit energy is sampled as a function of the relative displacement between pairs of atomic rows across the glide plane. Therefore the SC model takes into account only the nearest-neighbour interaction across the glide plane, that is the local bonding distortion between pairs of atomic rows. Although this model seems to be applicable to covalently bonded systems, where the bonding across the glide plane is highly localized, it fails to describe metallic systems that have more delocalized electronic states. This also explains why the SC model does not work well for the case of evenly spaced (30° and 90°) dislocations, where the atomic rows below (above) the glide plane are located in the middle of the atomic rows above (below) the glide plane. In this case, it is most ambiguous to define a local atomic pair, and the second-nearest-neighbour interaction is as important as the first nearest-neighbour interaction. The neglect of higher-order interactions in the SC scheme gives rise to a lower misfit energy and to a much higher σ_P. On the other hand, in the DC scheme the misfit energy is defined as a function of the displacement between the original position of an atomic row and its final position after the introduction of a dislocation. Consequently, the misfit energy is summed independently over the top and bottom half-crystals. Two advantages emerge immediately from the DC scheme.

(1) Higher-order interactions are included naturally. In fact the misfit energy results from the overall charge density redistribution due to the displacements of all atoms on both sides of the glide plane, rather than to the local bonding distortion associated with the SC scheme.
(2) The fact that the DC approach samples the misfit energy over twice as many atomic rows as in the SC scheme reduces the error due to the local displacement gradient approximation by a factor of two (Miller and Phillips 1996, Miller *et al.* 1998). This is particularly important for the treatment of narrow dislocations, where the displacement gradients are relatively larger.

Next we present an analytical expression of σ_P for dislocations in A-type lattices, based on the DC scheme. Although this expression is derived using the sinusoidal approximation for the restoring force, it provides insight into the effect of atomic spacing on σ_P and it allows a qualitative understanding of the results in table 1. Generalizing the SC treatment of Joós and Duesbery (1997), the total misfit energy in the DC scheme can be written as the sum of the misfit energy contributions from the two half-crystals:

$$W(u) = \sum_{n=-\infty}^{+\infty} \frac{a_1 + a_2}{2} \left(\gamma[\delta[n(a_1 + a_2) - u]] + \gamma[\delta[n(a_1 + a_2) + a_1 - u]]\right), \qquad (1)$$

where a_1 and a_2 are the alternating spacings between atomic rows across the glide plane (in general $a_1 \neq a_2$), δ represents the displacement of an atomic row relative to its original position, γ is the misfit energy and u is the dislocation translation distance. Assuming a sinusoidal force law for the restoring force $F[\delta(x)] = \tau_{\max} \sin[2\pi\delta(x)/b]$, the misfit energy functional $\gamma[\delta(x)]$ is

$$\gamma[\delta(x)] = \frac{\tau_{\max} b}{2\pi}\left[1 - \cos\left(\frac{2\pi\delta(x)}{b}\right)\right]. \tag{2}$$

The solution of the P–N integrodifferential equation gives $\delta(x) = (b/\pi)\arctan(x/\xi) + b/2$, where ξ is the half-width. Substituting the expressions for $\gamma(x)$ and $\delta(x)$ in equation (1) and introducing $a = a_1 + a_2$ and $u' = u - a_1$, the misfit energy reduces to

$$W(y_1, y_2) = \frac{Kb^2 \sinh(2\pi\Gamma)}{8\pi}\left(\frac{1}{\cosh(2\pi\Gamma) - \cos(2\pi y_1)} + \frac{1}{\cosh(2\pi\Gamma) - \cos(2\pi y_2)}\right), \tag{3}$$

where

$$y_1 = \frac{u}{a}, \quad y_2 = \frac{u'}{a} = \frac{u - a_1}{a} = y_1 - \frac{a_1}{a}, \quad \Gamma = \frac{\xi}{a},$$

$$K = \left(\frac{\mu}{2\pi}\right)\left[\frac{(\sin^2\theta)}{(1-\nu)} + \cos^2\theta\right]$$

for isotropic solids. $\mu = 28.8$ GPa and $\nu = 0.344$ are the shear modulus and Poisson's ratio respectively for Al. It should be pointed out that equation (3) is valid only for unevenly spaced dislocations, because of the requirement imposed by the Poisson summation formula. It is straightforward, however, to calculate the Peierls stress for evenly spaced dislocations using a similar approach. Introducing the dimensionless quantity $t = a_1/a \neq \frac{1}{2}$, the stress associated with the variation in the misfit energy is

$$\sigma(y_1, t) = -\frac{Kb\sinh(2\pi\Gamma)}{4a} \times \left(\frac{\sin(2\pi y_1)}{[\cosh(2\pi\Gamma) - \cos(2\pi y_1)]^2} + \frac{\sin[2\pi(y_1 - t)]}{\{\cosh(2\pi\Gamma) - \cos[2\pi(y_1 - t)]\}^2}\right). \tag{4}$$

For all dislocations in Al, $\Gamma = \xi/a > 1$ and hence equation (4) reduces to

$$\sigma(y_1, t) = -\frac{Kb\cos(\pi t)}{2a\cosh(2\pi\Gamma)}\sin(2\pi y_1 - \pi t). \tag{5}$$

For a given t, the maximum value of $\sigma(y_1, t)$ yields the Peierls stress

$$\sigma_{\mathrm{P}} = \frac{Kb}{a}\exp\left(\frac{-2\pi\xi}{a}\right)|\cos(\pi t)|. \tag{6}$$

For comparison, we also present the following expression for σ_{P} (equation (24) in the paper by Joós and Duesbery (1997)) employing the SC model:

$$\sigma_{\mathrm{P}}^{\mathrm{SC}} = \frac{Kb}{a'}\exp\left(\frac{-2\pi\xi}{a'}\right). \tag{7}$$

Here $a' = a$. Two important results are evident from the expression derived here. First, equation (5) shows that the DC scheme gives the correct periodicity a. Second, the value of σ_{P} calculated from the DC scheme is always smaller than that from the

SC scheme. Both these analytical results are consistent with our numerical results listed in table 1. For the unevenly spaced dislocations in the fcc lattice, $t = \frac{2}{3}$, and the Peierls stress predicted from the SC scheme is twice that from the DC scheme. For the evenly spaced dislocations the DC scheme gives

$$\sigma_{\mathrm{P}}^{\mathrm{DC}} = \frac{2Kb}{a} \exp\left(-\frac{4\pi\xi}{a}\right). \tag{8}$$

Thus the ratio $m(\xi)$ of the σ_{P} values from the SC ($\sigma_{\mathrm{P}}^{\mathrm{SC}}$) to the DC ($\sigma_{\mathrm{P}}^{\mathrm{DC}}$) scheme for evenly spaced dislocations is

$$m(\xi) = \frac{\sigma_{\mathrm{P}}^{\mathrm{SC}}}{\sigma_{\mathrm{P}}^{\mathrm{DC}}} = \frac{1}{2} \exp\left(\frac{2\pi\xi}{a}\right). \tag{9}$$

This equation clearly shows that the SC scheme predicts a much higher Peierls stress than the DC scheme for the evenly spaced dislocations (30° and 90°). It also demonstrates that $m(\xi)$ increases exponentially with increasing ξ, yielding a larger $m(\xi)$ ratio for the 90° dislocation than for the 30°, owing to the larger ξ of the 90° dislocation (Lu *et al.* 2000). It should be pointed out, however, in order to test the reliability of the various approximations entering the different models, one needs to check with direct atomistic simulation results. The SD model with the DC scheme has been shown to predict values for σ_{P} in both Al and Si, in excellent agreement with direct atomistic simulations using the same interatomic potentials (Bulatov and Kaxiras 1997, Lu *et al.* 2000).

Finally, we employ the SD P–N model to examine the effect of atomic relaxation on σ_{P}. In this model, the dislocation profile $\delta(x)$ is allowed to change during the translation of the dislocation centre, in contrast with the original P–N model and most recent work. In table 2 we list the values of σ_{P} for different dislocations in Al, using three different approaches, all based on the DC sampling scheme. The first (SD + density functional theory (DFT)) and second (SD + sin) methods employ the SD scheme but with different restoring forces, that is the SD + DFT method uses a restoring force calculated from DFT, whereas the second method (SD + sin) uses a sinusoidal force law, but with $\tau_{\max}$ in equation (2) adjusted to give the same half-width ξ as in the SD + DFT method. The third method uses the analytical

Table 2. The Peierls stress (σ_{P}) for dislocations in Al employing three different approaches and the DC scheme. The SD + DFT method uses the SD scheme and a restoring force calculated from DFT, whereas the SD + sin method uses the SD scheme with a sinusoidal force law. The third method uses the analytical equations (6) and (8). For any given dislocation all three approaches use the same value for ξ.

Dislocation angle	σ_{P} (MPa)		
(degrees)	SD + DFT	SD + sin	Equations (6) and (8)
0	256	104	159
30	53	3	6
44.7	59	6	10
55.3	85	11	19
60	98	14	22
66.6	64	5	8

Table 3. The Peierls stress (σ_P) calculated from the SD + sin method which uses the SD model and a sinusoidal force law, and equation (10) for narrow dislocations. The same sinusoidal restoring force with $\tau_{max} = 192\,GPa$ is used in both calculations.

Dislocation angle (degrees)	σ_P (GPa)	
	SD + sin	Equation (10)
0	192	2884
30	144	2948
60	176	2067
90	112	2195

expressions (equations (6) and (8)) for σ_P, based on the sinusoidal approximation, with the same ξ as in the two previous methods. Thus, comparison between the first (SD + DFT) and second (SD + sin) methods tests the accuracy of the sinusoidal approximation, while comparison between the second and third methods demonstrates the importance of atomic relaxation. It is interesting to note that the relaxation effect is small for all dislocations in Al, whereas the sinusoidal approximation turns out to be quite rough, as expected.

The negligible relaxation effect found in Al can be due to either a small Peierls energy barrier or the cancellation effect recently proposed by Schoeck (1999), where the changes in misfit energy and elastic energy due to atomic relaxation are of opposite sign, thus nearly cancelling each other. In order to clarify the origin of the negligible relaxation effect, we have carried out two sets of calculations based on the DC scheme and the sinusoidal force law, but with τ_{max} now chosen large enough (192 GPa) to give narrow dislocations $\xi < 0.5\,\text{Å}$. The first calculation employs the SD method which allows atomic relaxation and the second uses the analytical expression

$$\sigma_P = \frac{3\sqrt{3}}{2}\frac{\tau_{max}^2 a}{Kb}, \tag{10}$$

derived for narrow dislocations (Joós and Duesbery 1997). For $\xi \ll a$, the misfit energy is localized within one lattice spacing and hence the details of the misfit energy sampling (DC versus SC) are not relevant. In table 3 we list the values of σ_P for different dislocations from the two sets of calculations. One can see that the relaxation effect *is* significant (more than one order of magnitude) and there is no cancellation effect, indicating that the negligible relaxation effect in Al is due to its small Peierls energy barrier, resolving the issue recently raised by Schoeck (1999).

§ 3. Summary

In summary, we have revisited two critical issues in the P–N model which are essential for accurate predictions of σ_P. We have examined the sampling schemes for the misfit energy and have shown that, although most of the work in the literature has been employing the SC scheme, the DC scheme is more appropriate for the determination of σ_P, especially for the case of evenly spaced dislocations. An analytical expression of σ_P is derived for dislocations in A-type lattices, which demonstrates for the first time the effect of atomic spacing (even versus uneven) on σ_P. Finally, we have shown the importance of atomic relaxation in predicting accurate Peierls stress for narrow dislocations. It should be pointed out that, despite recent advances in the P–N model (Bulatov and Kaxiras 1991, Hartford *et al.* 1998, Lu *et al.* 2000), one needs to be cautious in using such an approach to determine the lattice resistance for soft materials, such as fcc metals with a low Peierls stress. Instead, the P–N model can be used to predict the relative trend of intrinsic resistance, say, from one fcc alloy to another.

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