A Critical Reexamination of the Peierls-Nabarro Model

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We reexamine two essential issues within the Peierls-Nabarro model which are critical in obtaining accurate values for the Peierls stress. The first issue is related to the sampling scheme of the misfit energy across the glide plane and the second one is the effect of relaxation on the Peierls stress. It is shown that most of the current applications of the Peierls-Nabarro model do not treat properly the two issues and therefore are not able to predict reliable values for the Peierls stress. We argue that the double counting scheme for the misfit energy at both sides of the glide plane is physically more reasonable, and it can predict more accurate values for the Peierls stress, especially for dislocations with equal spacing between alternating atomic rows. We also show the importance for allowing atomic relaxation when a dislocation traverses the Peierls barrier, which in turn lowers the Peierls stress for narrow dislocations by an order of magnitude.

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The Peierls stress $\sigma_p$ is the minimum applied external stress required to move a stationary dislocation irreversibly, without the assistance from thermal or quantum lattice vibrations. This fundamental quantity of a lattice dislocation was first estimated by Peierls [1] and Nabarro [2] using essentially a continuum model, which is now referred to as the Peierls-Nabarro (P-N) model. The original P-N model has served more as a conceptual tool for a qualitative understanding of dislocation core properties, rather than providing quantitative estimates of these properties, due to the unrealistic sinusoidal force law adopted in the model. However, there has been renewed interest in the P-N model recently to calculate the Peierls energy and stress \cite{3,4} thanks to the advent of highly accurate \textit{ab initio} total-energy methods based on the density functional theory (DFT). To date, the P-N model serves as a link between atomistic and continuum approaches, by providing a means to incorporate information obtained from the atomistic (\textit{ab initio} or empirical) calculations directly into the continuum model. This resultant approach can then be applied to problems that neither atomistic nor conventional continuum models could handle separately.

After the pioneering work of Peierls and Nabarro, several attempts to improve the original model have been made. For example, the three-dimensional dislocation profile has replaced the one-dimensional constrained path approximation \cite{3,4,5} in the original model. This is particularly important for treating the dissociation of a perfect dislocation into partials. A fully anisotropic treatment of the elastic interaction has been implemented into the model \cite{6}. The above extensions have allowed the study of straight dislocations with arbitrary orientation in an arbitrary glide plane and a medium of arbitrary anisotropy. More recently, an averaging procedure has been proposed to account for the nonlocal nature of the misfit energy \cite{7}. By discretizing the elastic energy, Bulatov and Kaxiras \cite{2} introduced recently a semidiscrete variational model which takes into account the important degrees of freedom which participate actively in the translation of the dislocation over the Peierls barrier.

In spite of the apparent importance and success of the P-N framework, a number of shortcomings still exist in the model. The classic P-N model completely neglects the relaxation of atoms when the dislocation center moves across the Peierls energy barrier, e.g., the dislocation displacement profile stays constant during the translation of the dislocation. Thus two approximate treatments for the total energy are involved in the classical model. Specifically, the variation of the elastic energy with respect to the translation vanishes due to the fact that the elastic energy is the functional of the overall displacement field of the lattice which are not allowed to change during the translation of the dislocation, hence the elastic energy has no contribution to the Peierls stress. On the other hand although the variation of the misfit energy with respect to the dislocation translation exists due to the discrete lattice nature, no relaxation of atoms is allowed to compute the correct (relaxed) lattice potential resulting from the interaction between the moving dislocation and the underlying lattice. In other words, in the classic P-N model the dislocation translates
rigidly through the lattice. How the two approximations affect the description for the dislocation core properties in still an open question, therefore it is one of the purposes in this work to examine the importance of relaxation in determining the Peierls stress and other dislocation core properties for both narrow and intermediate dislocations, such as those in Al.

The second important issue addressed in this paper is more controversial and subtle. It is related to the misfit energy sampling for different crystal lattices, i.e. facing lattice (F-type), in which the atoms just above and below the glide plane face each other, such as the simple cubic lattice or alternating lattices (A-type) in which the atomic sites on the two sides of the glide plane alternatingly distribute as in a closed packing lattice, such as the fcc lattice. In their original work, Peierls, Nabarro and others summed the misfit energy independently over the top and bottom half-crystals for both F and A-type lattices. We will refer to this scheme as the double counting (DC) scheme. However, the DC scheme yields the variations of the misfit energy and the lattice friction which have a periodicity of $b/2$, in contrast with the feature of the dislocation barrier which must in general exhibit the periodicity of $b$. Most people believe the unexpected form of the Peierls energy barrier is attributable to the DC approach in the classic P-N model and since then almost all numerical and analytical work employ exclusively a single counting (SC) scheme, e.g., the scheme in which one sums the misfit energy only on one side of the glide plane as a function of the registry (relative displacement) between pairs of atomic rows. The argument for using the SC approach is based on the assumption of the nearest-neighbor interaction and on the fact that this scheme gives the correct periodicity of $b$. However, as Wang pointed out recently, the undesired periodicity is actually due to an erroneous representation of the atomic positions in the original model rather than the DC scheme itself. In fact, the DC scheme can give the correct periodicity for the both F and A-type lattices after the error of atomic positions is corrected. On the other hand the accuracy of the nearest-neighbor interaction approximation in the SC scheme for the A-type lattice is still questionable. Thus the second aim of this paper is to examine the soundness of the two schemes and compare for the first time the misfit energy and the Peierls stress calculated from these schemes. Finally we present a simple analytical expression for the Peierls stress derived for the A-type lattice based on the DC scheme.

In order to study these subtleties within the P-N model, we employ the semidiscrete variational P-N model, because of its accuracy and expedient [3]. For the study of dislocations in Al (intermediate core width) the $\gamma$ surface is obtained by means of ab initio pseudopotential total-energy calculations [3]. For the case of extremely narrow dislocations, we will resort to a sinusoidal force law for calculating the misfit energy and the Peierls stress. Within the semidiscrete variational approach the equilibrium structure of a dislocation is obtained by minimizing the dislocation energy density functional

$$U_{\text{disl}} = \sum_{i,j} \frac{1}{2} \chi_{ij} [K_e (\rho_i(1) \rho_j(1) + \rho_i(2) \rho_j(2)) + K_s \rho_i(3) \rho_j(3)]$$

$$+ \sum_i \Delta x \gamma_3 (\vec{\delta}_i) - \sum_{i,l} \frac{x_i^2 - x_{i-1}^2}{2} (\rho_i^{(l)} \tau^{(l)}_i)$$

(1)

with respect to the dislocation densities or displacement vectors. Here $\rho_i^{(1)}$, $\rho_i^{(2)}$ and $\rho_i^{(3)}$ are the edge, vertical and screw components of the general interplanar displacement density at the $i$-th nodal point, and $\gamma_3 (\vec{\delta}_i)$ is the three-dimensional misfit potential. The corresponding applied stress components interacting with the $\rho_i^{(1)}$, $\rho_i^{(2)}$ and $\rho_i^{(3)}$, are $\sigma^{(1)} = \sigma_{21}$, $\sigma^{(2)} = \sigma_{22}$ and $\sigma^{(3)} = \sigma_{23}$, respectively. $K_e$ and $K_s$ are the edge and screw pre-logarithmic energy factors. The dislocation density at the $i$-th nodal point is $\rho_i = (\vec{\delta}_i - \vec{\delta}_{i-1})/(x_i - x_{i-1})$, where $\vec{\delta}_i$ and $x_i$ are the displacement vector and the coordinate of the $i$-th nodal point (atomic row), respectively, and $\chi_{ij} = \frac{1}{2} \delta_{ij} \phi_{i,j-1} + \psi_{i,j-1} - \psi_{i-1,j-1} - \psi_{i-1,j-1}$, with $\phi_{i,j} = x_i - x_j$, and $\psi_{i,j} = \frac{1}{2} \phi_{i,j}^2 \ln |\phi_{i,j}|$. Because the displacement vector $\vec{\delta}(x_i)$ is allowed to change during the process of dislocation translation, the Peierls energy barrier can be significantly lowered compared to its corresponding value from a rigid translation. The response of the dislocation to an applied stress is achieved by the minimization of the energy functional with respect to $\rho_i$ at a given value of the applied stress, $\tau_i^{(l)}$. The Peierls stress is then obtained by evaluating the critical value of the applied stress $\tau_i^{(l)}$ at which the dislocation energy functional fails to be minimized with respect to $\rho_i$ through standard conjugate gradient techniques. This approach of calculating the Peierls stress is more accurate and physically transparent because it captures the nature of the Peierls stress as the stress at which the displacement field of the dislocation undergoes a discontinuous transition.

In Table I, we compare the values of the misfit energy and the Peierls stress for various dislocations in Al, calculated from the DC and SC schemes. The ab initio determined $\gamma$ surface has been implemented into the semidiscrete model to obtain accurate values for the energetics and the Peierls stress. All dislocations considered here are perfect fcc dislocations in (111) plane but with different orientations, e.g., different angles between the dislocation lines and the Burgers vectors. For all dislocations in Al, the atomic rows from the two sides of the glide plane are situated alternatingly from each other. Furthermore it is important to note that, with the exception of the 30° and 90° dislocations, the spacing between alternating atomic rows for all the other dislocations in an fcc lattice is not even. We will refer to the 30° and
90° dislocations as evenly-spaced dislocations. Two conclusions can be drawn from the comparison in Table I. First the SC scheme always underestimates the misfit energy and overestimates the Peierls stress compared to the DC scheme. Second the agreement for the Peierls stress between the two schemes becomes particularly worse for the evenly-spaced (30° and 90°) dislocations. Namely, while the SC scheme underestimates the misfit energy by about 15%, it overestimates the Peierls stress relative to its value from the DC scheme by orders of magnitude. Thus the even versus uneven spacing between atomic rows turns out to be an important issue regarding the Peierls stress, and has not been addressed in previous studies.

In order to establish which scheme is superior over the other and to understand the different results received from two sampling schemes, next we take a closer look at the two schemes for the A-type lattice (the two schemes are essentially the same for the F-type lattice). In the SC scheme, the misfit energy is sampled as a function of the relative displacement between pairs of atomic planes across the glide plane. Therefore, the SC model considers only the nearest-neighbor interaction across the glide plane, e.g., the local bonding distortion between the pair 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, which have more delocalized electronic states. Along the same line of thinking, one can understand why the SC model works particularly worse for the evenly-spaced (30° and 90°) dislocations in which the atomic rows below (above) the glide plane are located right 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-neighbor interaction is as important as the first nearest-neighbor interaction. The neglect of higher nearest-neighbors interactions in the SC scheme gives rise a lower misfit energy and a much higher Peierls stress. On the other hand the DC scheme treats the misfit energy from the top and bottom crystal as separate entities, and 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 can be summed up independently over the top and bottom half-crystals. Two advantages immediately emerge from the DC model: (1) Higher-order interactions are included naturally. In fact the misfit energy is exact, by including the contributions from all atomic rows across the glide plane. In other words the misfit energy is the result from the overall charge density redistribution due to the displacements of all atoms on both sides of the glide plane, rather than 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 method, it reduces the error due to the local displacement gradient approximation by a factor of two. This improvement is particularly important for describing narrow core dislocations where the displacement gradients are relatively larger.

Next we present for the first time a simple and rigorous analytical formula of the Peierls stress for dislocations in A-type lattice based on the DC scheme. Although this formula is derived using the sinusoidal approximation for the restoring force, it will provide insight on the effect of atomic spacing on the Peierls stress and will allow a qualitative understanding of the results in Table I. Following the SC treatment of Joos and Duesbery, the total misfit energy within the DC scheme can be written as the sum of misfit energy contributions from the two half-crystals

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

where \( a_1 \) and \( a_2 \) are the spacings for the atomic rows alternating across the glide plane, which can be different in general. As alluded earlier, \( \delta \) is the displacement field of atomic rows relative their original positions, \( \gamma \) is the misfit potential, and \( u \) is the dislocation translation distance. Introducing \( a = a_1 + a_2 \) and \( u = -(a_1 - u) = u - a_1 \), we have

\[ W(u, u) = \sum_{n=-\infty}^{+\infty} \frac{a}{2} \left\{ \gamma [\delta(na - u)] + \gamma [\delta(na - u')] \right\} = W_1(u) + W_2(u). \]

Assuming a sinusoidal force law for the restoring force \( F(\delta(x)) = \tau_{\text{max}} \sin(2\pi \delta(x))/b \), gives a misfit energy functional \( \gamma(\delta(x)) \) of the form,

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

The solution of the P-N integro-differential equation gives \( \delta(x) = b/\pi \arctan(x/\zeta) + b/2 \), where \( b \) is the Burgers vector of the dislocation and \( \zeta \) is the half-width. Substituting the expressions for \( \gamma(x) \) and \( \delta(x) \) in Eqn. (3) and using the Poisson’s summation formula, the misfit energy reduces to

\[ W(y_1, y_2) = \frac{K b^2 \sinh 2\pi \Gamma}{8\pi} \left( \frac{1}{\cosh 2\pi \Gamma - \cos 2\pi y_1} + \frac{1}{\cosh 2\pi \Gamma - \cos 2\pi y_2} \right), \]
summation formula. It is straightforward however, to calculate the Peierls stress for evenly-spaced dislocations using a similar approach. To get the Peierls stress one needs to calculate the stress associated with the misfit energy variation.

\[
\sigma(y_1, y_2) = \frac{1}{b} \frac{dW}{du} = -\frac{Kb \sin 2\pi \Gamma}{4a} \left( \frac{\sin 2\pi y_1}{(\cosh 2\pi \Gamma - \cos 2\pi y_1)^2} + \frac{\sin 2\pi y_2}{(\cosh 2\pi \Gamma - \cos 2\pi y_2)^2} \right).
\]

Letting \( t = a_1 / a \) and \( t \neq \frac{1}{2} \),

\[
\sigma(y_1, t) = -\frac{Kb \sin 2\pi \Gamma}{2a \cosh 2\pi \Gamma} \frac{\sin 2\pi y_1}{(\cosh 2\pi \Gamma - \cos 2\pi y_1)^2} + \frac{\sin 2\pi (y_1 - t)}{(\cosh 2\pi \Gamma - \cos 2\pi (y_1 - t))^2}.
\]

For all dislocations studied in Al, we find \( \Gamma = \frac{\pi}{a} > 1 \) and this should hold also for not very narrow dislocations. In this limit, Eqn. (7) reduces to

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

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

\[
\sigma_p = \frac{Kb}{a} e^{-2\pi \zeta / a} |\cos(\pi t)|.
\]

For comparison we present below also the formula derived by Joos and Duesbery using the SC model [Eqn. (24) in Ref. 4]

\[
\sigma_p = \frac{Kb}{a} \frac{e^{-2\pi \zeta / a}}{a t}.
\]

Here \( at = a \). Two results are evident from the simple analytical expression derived above. First, Eqn. (8) shows that the DC scheme gives the correct periodicity \( a \). Second, the value of the Peierls stress 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 non-evenly spaced dislocations in the fcc lattice, \( t = 2/3 \), thus we find that the SC scheme predicts a Peierls stress which is twice as large as that obtained from the DC scheme using the sinusoidal force law. For the evenly-spaced dislocations, it can be easily shown that

\[
\sigma_p = \frac{2Kb}{a} e^{-4\pi \zeta / a},
\]

and the ratio \( m(\zeta) \) of the Peierls stress from the SC (\( \sigma_p^{SC} \)) to the DC (\( \sigma_p^{DC} \)) scheme is

\[
m(\zeta) = \frac{\sigma^{SC}_p}{\sigma^{DC}_p} = \frac{1}{2} e^{2\pi \zeta / a}.
\]

This equation shows that for the evenly spaced dislocations (30° and 90°), the SC scheme predicts a much higher Peierls stress than the DC scheme. It also demonstrates that \( m(\zeta) \) increases exponentially with \( \zeta \), yielding a larger \( m(\zeta) \) ratio for the 90° dislocation compared to that for the 30°, due to the larger half-width of the 90° dislocation. Although this simple formula gives the correct qualitative trend for \( \sigma_p \), it is rather limited in predicting reliable Peierls stress for real materials because of the sinusoidal force law employed in its derivation. For example one problem associated with the sinusoidal force law is that it yields no dissociation into partials, which can result in several orders of magnitude difference in the \( \sigma_p \) if the dissociation is allowed. It needs to be emphasized that in order to test the reliability of different models, one needs to compare to direct atomistic calculations. The semidiscrete model with the DC scheme has been found to be able to predict reliable values for the \( \sigma_p \) for both covalent and metallic systems, e.g., in good agreement with the direct atomistic simulation results using the same interatomic potentials.

We next examine the effect of atomic relaxation on the Peierls stress for different types of dislocations in Al. In Table II, we list the \( \sigma_p \) for different dislocations using three different approaches. All the three methods are based on the DC scheme. The first (SD+DFT) and second (SD+sin) methods employ the semidiscrete model but with different restoring forces. Namely the SD+DFT method uses a restoring force obtained from density functional calculations, whereas the second method (SD+sin) uses a sinusoidal force law, but with the \( \tau_{max} \) in Eqn. (4) adjusted to give the same value for the dislocation half-width (\( \zeta \)) as in the SD+DFT calculations. The third method uses the analytical expressions (Eqns. (9) and (11)) for the \( \sigma_p \) using the same \( \zeta \) as for the first two methods. Therefore the comparison between the (SD+DFT) and (SD+sin) methods provides information for the effect of sinusoidal approximation on \( \sigma_p \) (both schemes include relaxation), while the comparison between the second and third methods illustrates the effect of atomic relaxation. It is interesting to note that the relaxation effect is small for all dislocations in Al, whereas the approximation of the sinusoidal restoring force is not good, as we addressed earlier.

Recently Schoeck claimed that the relaxation effect on the Peierls stress can be canceled out by the opposite contributions from the misfit energy and the elastic energy. Thus we need to clarify the cause of the negligible relaxation effect in Al, i.e., whether it is due to the small Peierls energy barrier or the cancellation effect. We have carried out two sets of calculations based on the DC scheme and a sinusoidal force law, but \( \tau_{max} \) is chosen large enough (1.2 ev/Å³) to produce narrow dislocations (\( \zeta \) less than 0.5 Å) in the Al lattice. The first set of calculations employs the semidiscrete model which allows relaxation while the second set is based on the an-
alytical formula $\sigma_p = \frac{3\sqrt{3}}{2} r_{\text{max}} a / K b$ derived for narrow dislocations \cite{4} (no relaxation is included). Note for very narrow dislocation the misfit energy is localized within one lattice spacing and hence the details of the misfit energy sampling (DC vs SC) is not relevant. Listed in Table III are the results of the $\sigma_p$ for different dislocations from these two sets of calculations. One can see that the relaxation effect is significant (more than one order of magnitude) and no canceling effect is observed.

In summary we have examined two essential issues within the Peierls-Nabarro model which are critical to obtain accurate values for the Peierls stress. The first issue concerns the sampling scheme for the misfit energy. We have shown that the DC scheme is more appropriate for determining the Peierls stress, especially for evenly-spaced dislocations, although most work in the literature has done otherwise. An analytical formula is derived to help understanding the results received from the numerical calculations. The second issue addressed in this work is the effect of relaxation for various dislocations. We have demonstrated the importance of relaxation in obtaining reliable Peierls stress for narrow dislocations. Comparison of the Peierls stress using \textit{ab initio} and the sinusoidal restoring force illustrates the failure of the sinusoidal approximation.

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\begin{thebibliography}{99}
\bibitem{8} G. Lu, N. Kioussis, V. Bulatov and E. Kaxiras (submitted to Philos. Mag. A).
\end{thebibliography}
TABLE I. Comparison of the misfit energy (ev/Å) and Peierls stress (mev/Å³) employing the DC and SC schemes. The semidiscrete model with the ab initio $\gamma$ surface is used for the calculations.

<table>
<thead>
<tr>
<th>Angle</th>
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<th>SC</th>
<th>DC</th>
<th>SC</th>
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<tr>
<td>0°</td>
<td>0.0994</td>
<td>0.0908</td>
<td>1.60</td>
<td>3.90</td>
</tr>
<tr>
<td>25.3°</td>
<td>0.1229</td>
<td>0.1173</td>
<td>0.04</td>
<td>0.14</td>
</tr>
<tr>
<td>30°</td>
<td>0.1221</td>
<td>0.1024</td>
<td>0.33</td>
<td>3.40</td>
</tr>
<tr>
<td>44.7°</td>
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</tr>
<tr>
<td>55.3°</td>
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<td>0.1356</td>
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<td>1.30</td>
</tr>
<tr>
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<td>0.1706</td>
<td>0.1630</td>
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</tr>
<tr>
<td>85.3°</td>
<td>0.1688</td>
<td>0.1470</td>
<td>0.02</td>
<td>2.20</td>
</tr>
</tbody>
</table>

TABLE II. The Peierls stress (mev/Å³) for dislocations in Al determined through three different approaches. The DC scheme is used in the semidiscrete model (SD) and the analytical formula calculations. For the same dislocation all the three methods use the same core width in order to give a fair comparison.

<table>
<thead>
<tr>
<th>Angle</th>
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<th>SD+sin</th>
<th>Formula</th>
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<tbody>
<tr>
<td>0°</td>
<td>1.60</td>
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<td>66.6°</td>
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<td>0.03</td>
<td>0.05</td>
</tr>
</tbody>
</table>

TABLE III. The Peierls stress (ev/Å) for dislocations in Al lattice calculated from the semidiscrete model (SD) and the analytical formula derived only for narrow dislocations (see text). The same sinusoidal restoring force with the magnitude $\tau_{max} = 1.2$ ev/Å³ is used for both methods. The core widths for all the dislocations studied here are less than 0.5 Å.

<table>
<thead>
<tr>
<th>Angle</th>
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