Semidiscrete Variational Peierls Framework for Dislocation Core Properties

Vasily V. Bulatov[1] and Efthimios Kaxiras[1,2]
[1]*Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138*
[2]*Department of Physics, Harvard University, Cambridge, Massachusetts 02138*
(Received 12 February 1997)

The classic Peierls theory of dislocations is critically examined and shown to contain a number of inconsistencies. For narrow core dislocations, as in Si, the classic theory leads to gross overestimation of the barrier to dislocation motion. We present a new, semidiscrete theory which corrects the inconsistencies of the classic theory, and gives results remarkably similar to actual atomistic calculations, both qualitatively and quantitatively. Our theory provides a link between accurate nanometer-scale quantum mechanical calculations of the dislocation core energetics to mesoscale continuum descriptions. [S0031-9007(97)03256-0]

PACS numbers: 61.72.Lk, 61.72.Bb, 61.72.Nn, 62.20.Fe

Extended defects, such as dislocations and grain boundaries, are recognized as the principal agents of large-scale behavior of solids, like plasticity, fracture, and the brittle-ductile transition. The challenge for theory is to connect the experimentally observed macroscopic properties of solids to the microscopic structure of extended defects. Continuum elasticity theory has been successfully employed for the description of dislocation properties and dislocation interactions at distances large compared to atomistic scales. At the other extreme, an atomistic description is required for the material specific, discrete atomic core structure of the dislocation, where continuum elasticity breaks down. Peierls first proposed a remarkable hybrid model [1] in which some of the details of the discrete dislocation core are incorporated in an essentially continuum framework. The analytic solution of this model, due to Peierls and Nabarro [2], gave the first meaningful estimate of the lattice resistance to dislocation motion. While extremely useful as a conceptual framework, the Peierls-Nabarro (PN) model becomes increasingly inaccurate for dislocations with narrow cores, as is typically the case in covalently bonded solids [3,4]. The origin of this inaccuracy remains controversial, with the Peierls framework viewed either as having room for improvements, or as being entirely inappropriate in the discrete core limit.

The PN analytical solution is based on a sinusoidal approximation of the nonlinear stress term in terms of the displacement field (the continuous distribution of slip representing the dislocation). Christian and Vitek [5] suggested that the nonlinear stress relation could be obtained from an effective interplanar potential, called the generalized stacking fault (GSF) energy, which can be calculated directly from interatomic force laws. The GSF energy provides a direct link between the PN continuum model of a dislocation and details of interatomic forces in the dislocation core, whereas previous work had been based on misfit stress relations constructed *a priori.* The PN model has now come to represent a combination of the original continuum model and the GSF potential, and its accuracy can be affected by either component. At present, the GSF energies can be calculated very accurately using an *ab initio,* self-consistent quantum mechanical framework [6], which brings to the fore the problem of possible inaccuracies in the continuum model.

In this Letter we address this issue by considering in turn explicit and implicit assumptions present in the PN continuum theory. The limitations of the continuum theory that we address here are as follows: (i) *Lattice discreteness:* The Peierls concept of a dislocation does not incorporate the discrete nature of the crystalline lattice. To correct for this, the PN theory includes a discrete summation of the interface misfit energy over atomic rows when calculating energy and stress [7], which is not based on a variational solution. (ii) *Strain energy:* The elastic strain energy of the dislocation calculated within the PN model can be unrealistically high, especially for solids with a narrow dislocation core. (iii) *Constrained dislocation core:* The neglect of important degrees of freedom, which participate actively in the translation of the real dislocation over the Peierls barrier, is a severe limitation and has the greatest detrimental impact on the description of narrow core dislocations.

We address these problems by developing a variational approach which incorporates the discrete nature of the lattice in a consistent way. Our formulation results in a radically improved description of narrow core dislocations whose behavior matches very closely the behavior of real, atomically discrete, dislocations. In combination with the GSF potential, the new theory permits a realistic treatment of dislocations from first principles, providing an alternative to very large simulations using effective interatomic potentials.

We begin by developing the energy function appropriate for the description of the Peierls dislocation. Consider a misfit distribution $\delta(x)$ in the displacement field across the slip plane in a linear elastic continuum with $\int [d\delta(x)/dx]dx = b$, where b is the Burgers vector. The

dislocation energy functional is given by (the coordinate system is defined in Fig. 1)

$$U_{\rm disl}[\delta(x)] = -K \iint \rho(x)\rho(x') \ln|x - x'|\, dx\, dx' + \int \gamma[\delta(x)]\, dx\,, \quad (1)$$

where $\rho(x) = d\delta(x)/dx$ and K is a certain combination of elastic constants [8]. The first term is the elastic energy which depends on $\delta(x)$ through $\rho(x)$. The second term is the energy cost for the shear displacement jump (the misfit) across the slip interface, with $\gamma(x)$ assumed to depend only on $\delta(x)$, but not on x itself. A variational derivative of the energy functional with respect to $\rho(x)$ gives the PN integrodifferential equation, which can be solved analytically assuming a sinusoidal nonlinear stress term [9]: $d\gamma[\delta(x)]/d\delta(x) = (\pi\gamma_{\rm us}/b)\sin(2\pi\delta/b)$, with $\gamma_{\rm us}$ the amplitude of the misfit energy variation (called the unstable stacking energy by Rice [10]). The analytical solution is

$$\delta(x) = \frac{b}{\pi}\tan^{-1}\left(\frac{x}{\xi}\right), \quad (2)$$

where $2\xi = 2Kb^2/\pi\gamma_{\rm us}$ is the half width of the resulting distribution $\rho(x) = b\xi/\pi(\xi^2 + x^2)$. The optimal shape of the slip distribution $\delta(x)$ in the core results from the competition of the two energy terms in (1). When $\gamma_{\rm us}$ is high, or the elastic moduli are low, the misfit energy dominates and the dislocation becomes narrow in order to minimize the misfit energy [second term in (1)]. In the opposite limit of low $\gamma_{\rm us}$ or high moduli, the dislocation tends to spread out in order to minimize the dominant elastic energy [first term in (1)].

In this formulation, the total energy (1) is invariant with respect to arbitrary translation of the misfit density $\rho(x) \to \rho(x + u)$ and the dislocation is a continuous object. As a consequence, the only effect of the lattice is that the misfit energy and the stress are periodic functions of the misfit δ with the lattice repeat period b. To regain the lattice discreteness, PN constructed a different form of the nonlinear potential where the misfit is not sampled continuously across the slip plane [as in Eq. (2)], but only at the positions of the atomic rows immediately adjacent to the slip plane,

$$U_{\rm misfit}[\{\delta_i\}] = \sum_{i=-\infty}^{\infty} \gamma(\delta(x_i))\, \Delta x\,, \quad (3)$$

where $\delta_i = \delta(x_i)$, with x_i the reference positions and Δx the average spacing of the atomic rows in the lattice. Substituting the continuum solution (2) into (3), it is found that the discrete sum varies periodically as a function of translation u. The amplitude of these periodic variations is identified as the Peierls energy and its maximum derivative with respect to u as the Peierls stress. In addition to several problems addressed earlier in the literature [7,11], this procedure is inconsistent in that two substantially different expressions for the misfit energy, one continuum and one discrete, were used for obtaining the solution (2) and for calculating the lattice resistance. That is, (2) *is not* a variational solution of a total energy functional in which the discrete form is used for the misfit energy term. Also, the shape of the solution $\delta(x)$ is assumed *not to change* during the translation. In the following we show that these two inconsistencies are actually related, leading to gross errors in the description of narrow core dislocations.

We choose to work directly with the total energy functional (1) in which the continuum misfit energy term is replaced by the discrete form (3), providing a more accurate description of the atomic core. In the same spirit, we intend to disregard any details of the displacements across the slip plane other than those related to the positions of the atomic rows, assuming that the displacement across the interface is fully specified by δ_i. Although the elastic energy term is still calculated according to the first term of (1), $\delta(x)$ is now linearly interpolated between the nodal points x_i so that the dislocation density $\rho(x)$ is constant between the nodal points (Fig. 1). Such an explicit discretization of the elastic energy term in Eq. (1) leads to the following expression for the total energy as a function of nodal displacements δ_i,

$$U_{\rm disl}[\{\delta_i\}] = K\sum_{ij}\chi_{ij}\rho_i\rho_j + \Delta x\sum_i \gamma(\delta_i), \quad (4)$$

where $\chi_{ij} = \frac{3}{2}\phi_{i,i-1}\phi_{j,j-1} + \psi_{i-1,j-1} + \psi_{i,j} + \psi_{i,j-1} + \psi_{j,i-1}$, with $\phi_{i,j} = x_i - x_j$, $\psi_{i,j} = \frac{1}{2}\phi_{i,j}^2 \ln|\phi_{i,j}|$, and $\rho_i = (\delta_i - \delta_{i-1})/(x_i - x_{i-1})$. Assuming a periodic misfit potential and regularly spaced atomic rows, minimization of (4) with respect to δ_i leads to a dislocation with a definite position in the lattice, identified by the position of the center-of-mass of the slip distribution,

$$\bar{x}_0 = \int x' \frac{\rho_0(x')}{b}\, dx'\,, \quad (5)$$

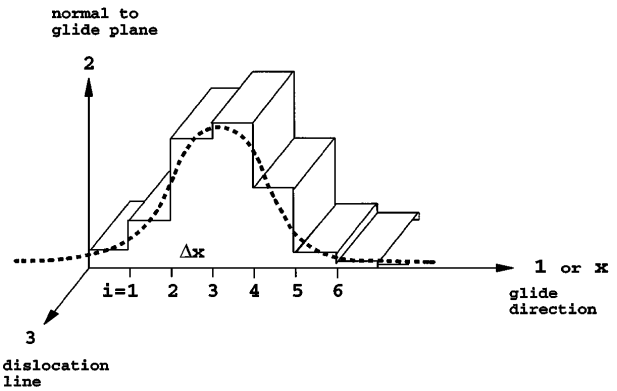

FIG. 1. Two alternative representations of the Peierls dislocation in Cartesian coordinates: the smooth dashed line is the classic PN model and the histogram is the present semidiscrete approach. Notice that axis 2 represents both the normal to glide plane and the magnitude of the dislocation density $\rho(x)$.

where $\rho_0(x)$ is the dislocation density for which (4) reaches its minimum. Because this optimal position is stable with respect to small perturbations of $\rho_0(x)$, the lattice resistance to the dislocation displacement is a natural consequence of the dislocation's resistance to move from its energetically optimal position. The minimum of the total energy function is infinitely degenerate, each optimal solution $\rho_0(x)$ corresponding to a dislocation position between neighboring atomic rows, in the so-called Peierls valleys.

We use Eqs. (4) and (5) to calculate the Peierls barrier by displacing the dislocation position from the minimum $\bar{x}_0$ to a new position x' and optimizing the distribution δ_i anew, with the additional constraint that the center-of-mass position (5) is now fixed at x'. The Peierls barrier is identified as the maximum among the constrained minima in the interval $\bar{x}_0 < x' < \bar{x}_0 + a'$, where a' is the distance between atomic rows in the lattice. The overall effect of letting the dislocation change its shape during translation is that the resulting barrier can be significantly lower than the rigid translation barrier calculated earlier by PN, and the corresponding rates of thermally activated dislocation motion can be significantly higher than in the classic model.

Another characteristic of dislocation mobility is the Peierls stress, defined as the minimum stress required to drive the dislocation from one Peierls valley to the next without thermal activation. In order to calculate the Peierls stress we add a term describing the interaction of the applied stress τ with the nodal displacements δ_i in the total energy expression,

$$U_{\text{int}}[\delta(x), \tau] = -\tau \int x' \rho(x')\, dx' = -\tau \sum_i \frac{x_i^2 - x_{i-1}^2}{2}\, \rho_i\,. \tag{6}$$

The dislocation response to applied stress is obtained by optimization of ρ_i at a given value of τ. An instability is reached when an optimal solution for ρ_i no longer exists, which is manifested numerically by the failure of the minimization procedure to converge. The value of the stress corresponding to the instability is the Peierls stress. This definition is more rigorous than the conventional one which associates the Peierls stress with the maximum slope of dislocation energy obtained by rigid translation. We show below that the present method of calculating the Peierls stress gives results close to exact atomistic calculations, while the conventional approach can lead to unphysical results.

The final modification we have introduced concerns the degrees of freedom available for relaxation as the dislocation moves through the lattice. The preceding discussion involved only one component of the interplanar misfit, i.e., all δ_i were assumed to be along the Burgers vector. Atomistic simulations suggest that lateral and even vertical displacement of atomic rows across the slip plane are important degrees of freedom during dislocation translation, which make it possible to avoid close encounters of sliding atoms. For example, in Si the coupling of in-plane and vertical displacements is much greater for the closely spaced atomic planes [12]. In order to account for such effects we generalize the total energy function and the stress interaction term in a manner analogous to that of Eq. (4),

$$U_{\text{disl}}[\{\vec{\delta}_i\}] = \sum_{i,j} \chi_{ij}[K_e(\rho_i^{(1)}\rho_j^{(1)} + \rho_i^{(2)}\rho_j^{(2)}) + K_s \rho_i^{(3)}\rho_j^{(3)}] + \sum_i \Delta x\, \gamma_3(\vec{\delta}_i) - \sum_{i,l} \frac{x_i^2 - x_{i-1}^2}{2}\, (\rho_i^{(l)}\tau^{(l)}). \tag{7}$$

Here $\rho_i^{(1)}$, $\rho_i^{(2)}$, and $\rho_i^{(3)}$ are the edge, vertical, and screw components of the general interplanar displacement density, $\tau^{(1)} = \sigma_{21}$, $\tau^{(2)} = \sigma_{22}$, and $\tau^{(3)} = \sigma_{23}$ are the corresponding stress components interacting with $\rho_i^{(1)}$, $\rho_i^{(2)}$, and $\rho_i^{(3)}$, respectively, and K_e and K_s are the edge and screw factors [8].

Equation (7) makes use of the fact that there are no elastic cross-interactions between the three displacement components. At the same time, the nonlinear misfit potential is now a function of all three components of the nodal displacements, $\gamma_3(\vec{\delta}_i)$. Previous attempts at including shear-tension coupling include potentials constructed *a priori* [13,14], or calculated atomistically for an fcc [100] plane using an interatomic force law [15]. We complete the formulation of the new approach by calculating, for the first time from first principles (DFT/LDA), the shear-tension potential for a {111} glide plane in Si. The details of the latter calculation are as in Ref. [12]. In addition, in order to examine critically the accuracy of the new semidiscrete theory, we calculate the same misfit potential using the empirical model of Stillinger and Weber (SW), for which exact atomistic calculations of the Peierls resistance are possible. In the following we establish the applicability of the new theory to narrow core dislocations, by comparing its predictions to exact atomistic results using the SW interatomic potential. Then, the DFT/LDA misfit potential is used for more accurate predictions of dislocation properties in the {111} glide plane is Si.

The 3D misfit potential $\gamma_3(\vec{\delta})$ is obtained by sampling 90 different combinations of displacements $\delta^{(1)}, \delta^{(2)}, \delta^{(3)}$, and fitting the results by properly symmetrized basis functions. We use Eq. (7) together with the misfit potential $\gamma_3(\vec{\delta})$ to calculate the lattice resistance to motion of dislocations in the {111} glide plane of Si. To examine the relative importance of the various new elements of the theory introduced here, we will consider a sequence of models in which the new elements are included in turn. The results of each model, all based on the SW misfit potential, are compared to the results of direct atomistic calculations using the same empirical model. Here we concentrate on one particular example, the $a/2 < 110 > \{111\}$ glide screw dislocation in Si, for which the classic PN theory

TABLE I. Peierls stress of glide screw dislocation in Si when the various improvements to the classic PN model are included in turn, denoted by models A–E; the result of the atomistic calculation is 0.021 eV/Å^3.

Feature/model	A	B	C	D	E
Displacement along $\vec{b}$	✓	✓	✓	✓	✓
Relaxation of dislocation shape		✓	✓	✓	✓
Discrete sampling of misfit energy		✓	✓	✓	✓
Lateral in-plane displacements			✓		✓
Vertical displacements				✓	✓
Peierls stress (in eV/Å^3)	10.3 (9.0)	1.07 (0.95)	0.320 (0.196)	0.230 (0.205)	0.078 (0.065)

gives a particularly poor description, with an unrealistically high value of 9.0 eV/Å^3 for the Peierls stress [3]. For comparison, the value we obtained by direct atomistic calculations is 0.021 eV/Å^3, almost 3 orders of magnitude lower. Comparison of the models that include successive elements of the new theory are presented in Table I. Also shown in this table are the corresponding values (in parentheses) obtained from the theory using the DFT/LDA values for the misfit potential $\gamma_3(\vec{\delta})$.

The classic PN theory (model A), with all new elements of the theory excluded reproduces the high value of the Peierls stress 10.3 eV/Å^3 (close to 9.0 eV/Å^3 cited above [16]). When all new elements of the new theory are included (model E), the value of the Peierls stress becomes 0.078 eV/Å^3, within a factor of 4 of the atomistic result. A similar reduction in the Peierls stress is observed from the DFT/LDA calculations. This is an impressive improvement over the classic model. In another example, the Peierls stress for the practically important partial dislocations is in even closer agreement with atomistic results: 0.138 eV/Å^3 compared to the atomistic result of 0.108 eV/Å^3, for the 90° partial dislocation.

Equally important is the fact that the present model reproduces the atomistic structure of the dislocation very well. With the definition of the dislocation position given in Eq. (5), the lowest energy position $\bar{x}_0$ of the dislocation falls midway between two widely spaced neighboring atomic rows, i.e., in the middle of the Peierls valley. When stress is applied, the optimal position shifts until the dislocation becomes unstable and breaks into two 30° partial dislocations at the critical stress of 0.078 eV/Å^3. The partial dislocations move away from each other but then stop at a short distance since the applied stress is below the Peierls stress of the 30° partial dislocations (0.228 eV/Å^3). Precisely the same behavior is obtained by atomistic calculations, the only difference being that the dissociation stress is lower.

In summary, we have developed a semidiscrete variational theory of the Peierls dislocation. The new approach overcomes several key deficiencies of the classic PN theory and extends the range of applicability of the continuum approach to narrow core dislocations. While our model does not reproduce exactly the results of atomistic calculations, it is a very significant improvement over the classic PN model. The approach presented here provides the necessary connection between the large-scale dislocation processes and the details of interatomic interaction in the dislocation core. Although an analytic solution is no longer feasible, the model is numerically expedient and can be extended to deal with various complex dislocation processes, such as cross slip, dislocation intersections, and nonplanar cores.

This work was supported by the Harvard Materials Research Science and Engineering Center which is funded by the National Science Foundation. V. V. B. acknowledges partial support from the MIT Center for Materials Science and Engineering. The authors wish to thank M. S. Duesbery, R. Phillips, E. Tadmor, and R. Miller for their valuable comments.

[1] R. E. Peierls, Proc. Phys. Soc. **52**, 23 (1940).
[2] F. R. N. Nabarro, Proc. Phys. Soc. **59**, 256 (1947).
[3] B. Joos, Q. Ren, and M. S. Duesbery, Phys. Rev. B **50**, 5890 (1994).
[4] R. Miller and R. Phillips, Philos. Mag. A **73**, 803 (1996).
[5] J. W. Christian and V. Vitek, Rep. Prog. Phys. **33**, 307 (1970).
[6] E. Kaxiras and M. S. Duesbery, Phys. Rev. Lett. **70**, 3752 (1993).
[7] J. P. Hirth and J. Lothe, *Theory of Dislocations* (Wiley, New York, 1982).
[8] For a screw dislocation $K = K_s = \mu/4\pi$, while for an edge dislocation $K = K_e = \mu/4\pi(1 + \nu)$, where μ is the shear modulus and ν is Poisson's ratio.
[9] J. Frenkel, Z. Phys. **37**, 572 (1926).
[10] J. R. Rice, J. Mech. Phys. Solids **40**, 239 (1992).
[11] B. Joos and M. S. Duesbery, Phys. Rev. Lett. **78**, 266 (1997).
[12] Y. M. Juan and E. Kaxiras, Philos. Mag. A **74**, 1367 (1996).
[13] Y. Sun, G. E. Beltz, and J. R. Rice, Mater. Sci. Eng. A **170**, 67 (1993).
[14] A. Needlemann, Ultramicroscopy **40**, 203 (1992).
[15] G. Bozzolo, J. Ferrante, and J. R. Smith, Scr. Metall. **25**, 1927 (1991).
[16] The value of 9.0 /Å^3 cited in [3] was calculated using the DFT/LDA GSF energies reported in Ref. [6].