Anisotropic Elastic Interactions of a Periodic Dislocation Array

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A method for calculating the anisotropic elastic energy of a dislocation dipole in a periodic cell is derived in which the infinite image summation is absolutely convergent. The core energy of a screw dislocation in Si, extracted from atomistic simulation, is shown to be manifestly system size invariant. Existence of special cell geometry where complete cancellation of elastic interactions occurs is demonstrated.

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Periodic boundary conditions (pbc) are ubiquitous in describing crystalline states theoretically and computationally, its fundamental appeal being that translational invariance of the infinite crystal is naturally preserved. Where long-range fields are present, whether electrostatic as in Coulomb interaction between charges or elastic as in strain-producing dislocations, one encounters an infinite sum of image interactions which is only conditionally convergent. In the case of dislocations, the problem has been solved by summing dislocation walls for edge dislocations [1–3] and performing fast multipole calculations [2] or Ewald-like summations for screw dislocations [4]. However, all the proposed methods are applicable only to isotropic media, leaving the effects of anisotropy without scrutiny.

In this Letter we describe a new method for calculating the elastic energy of a periodic array of dislocation dipoles that is applicable to anisotropic media. By finding the reversible work to create a dislocation dipole from a perfect lattice in a periodic simulation cell, we obtain an expression for the elastic interaction that is manifestly absolutely convergent. Comparing the image interactions thus obtained with the infinite summation previously encountered, we show that the problem of conditional convergence arises from the average stress generated by the array of image dipoles, a mean-field-type elastic energy that has been overlooked heretofore. We extract a self-consistent core energy of the shuffle-set screw dislocation in Si from atomistic calculations and demonstrate its invariance to system size effects, a result which would not be obtained if elastic isotropy had been assumed. Furthermore, we show that an optimum simulation cell geometry (aspect ratio) exists for which there is complete cancellation of the elastic interactions, an effect that also does not arise without accounting for crystal anisotropy.

Consider an atomistic simulation cell for dislocation core energy calculations that is periodic along $\vec{c}_1$, $\vec{c}_2$, and $\vec{c}_3$ directions, and contains a dislocation dipole with Burgers vector $\pm\vec{b}$, as shown in Fig. 1. The dislocation lines are parallel to $\vec{c}_3$ and are separated from each other by $\vec{a}$. The total energy E_{atm}, in excess of that of the perfect periodic lattice, obtained from a fully relaxed atomistic calculation can be separated into core and elastic contributions [5],

$$E_{\text{atm}} = 2E_{\text{core}} + E_{\text{prm}} + E_{\text{img}}\,, \tag{1}$$

where E_{core} is the core energy of each dislocation, E_{prm} represents the linear elastic interaction between the two dislocations in the primary simulation cell, and E_{img} represents the interaction between the primary dipole and all the periodic images. The sums of E_{prm} and E_{img} constitute the elastic interactions, E_{el}. For the sake of simplicity, we assume $\vec{c}_3$ has length unity, so that all the energies are normalized per unit length of dislocation.

For a screw dipole and assuming isotropic elasticity E_{prm} is known [6], $E_{\text{prm}} = \mu b^2/(2\pi)\ln(|\vec{a}|/r_c)$, where μ is the shear modulus and r_c is the core cutoff radius. The problem of extracting E_{core} from E_{atm} therefore reduces to determining E_{img}. Following current practice [5,7] one regards the effect of pbc as introducing an infinite array of image cells (see Fig. 1), and treats E_{img} as the total interaction between the primary dipole and all the image dipoles,

$$E'_{\text{img}} = \frac{1}{2}{\sum_{\vec{R}}}' E_{\text{dd}}(\vec{R})\,, \tag{2}$$

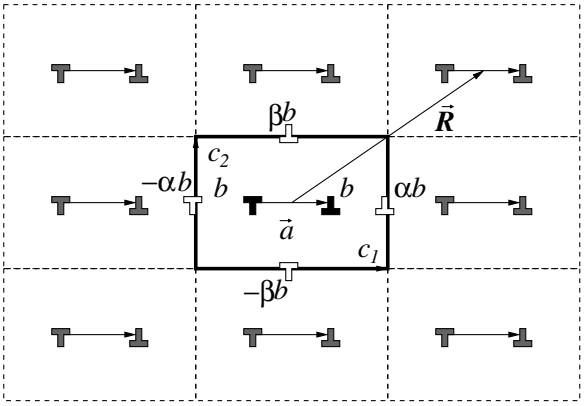

FIG. 1. Schematic of an atomistic simulation cell (solid rectangle) containing a dislocation dipole with Burgers vector $\pm\vec{b}$ and separated by $\vec{a}$ under pbc along $\vec{c}_1$, $\vec{c}_2$, and $\vec{c}_3$ (out of plane). To facilitate calculation of the image energy, we introduce "ghost" dislocations (in white) at the cell boundaries.

where the summation runs over $\vec{R} = m\vec{c}_1 + n\vec{c}_2$, m and n being integers, and $\vec{R} \neq 0$. $E_{\rm dd}(\vec{R})$ denotes the interaction between the primary dipole and an image dipole at position $\vec{R}$. For screw dislocations in isotropic medium, $E_{\rm dd}(\vec{R}) = \mu b^2/(2\pi)\ln(|\vec{R} + \vec{a}| \cdot |\vec{R} - \vec{a}|/R^2)$ [8]. We denote Eq. (2) as $E'_{\rm img}$ to indicate that this summation is not *absolutely convergent,* since $E_{\rm dd} \sim R^{-2}$ for large R. The cancellation of terms having opposite signs makes the summation *conditionally convergent* [3], its value depending on the ordering of the summand. Similar problems, namely, the Madelung summation [9,10], arising in summing Coulomb interactions of dipole lattices, are typically treated using the Ewald method [11].

In our treatment of the elastic interactions, the issue of conditional convergence does not arise. By evaluating the reversible work to create a dislocation dipole in the periodic cell, we obtain an expression for the elastic interaction energy in terms of the stress field $\sigma(\vec{r})$ in the final configuration,

$$E_{\rm el} = -\frac{1}{2}\int dA_j\, b_i \sigma^0_{ij}(\vec{r}) + \frac{1}{2} S\overline{\sigma}^2 V\,, \qquad (3)$$

where the integral extends over the area enclosed by the dislocation dipole, $\overline{\sigma} = \langle\sigma(\vec{r})\rangle_V$ is the stress averaged over the cell volume V, $\sigma^0(\vec{r}) = \sigma(\vec{r}) - \overline{\sigma}$, and S is the elastic compliance tensor.

Equation (3) is our central result; it follows from the combination of two steps, first creating a perfect lattice under stress $\tilde{\sigma}$ and then creating a dislocation dipole by making a cut on a surface (under stress) and displacing the two sides of the surface relative to each other. In the second step, an internal plastic strain $\epsilon^{\rm p}_{ij} = (b_i A_j + b_j A_i)/2V$ is induced in the cell. Since the total strain is constrained to be zero, the plastic strain is counterbalanced by an internal elastic strain $\epsilon^{\rm e}_{ij} = -\epsilon^{\rm p}_{ij}$. The resulting change in the average stress in the cell is then given by

$$\sigma^{\rm x}_{ij} = \overline{\sigma}_{ij} - \tilde{\sigma}_{ij} = C_{ijkl}\epsilon^{\rm e}_{kl} = -C_{ijkl} b_k A_l/V\,, \qquad (4)$$

where $C = S^{-1}$ is the elastic constant tensor. This leads to the identity $(b_i A_j + b_j A_i)/2 = -S_{ijkl}\sigma^{\rm x}_{kl} V$. The associated work for the two steps is, respectively,

$$\Delta W_1 = \frac{1}{2} S\tilde{\sigma}^2 V = \frac{1}{2} S(\overline{\sigma} - \sigma^{\rm x})^2 V\,, \qquad (5)$$

$$\Delta W_2 = -\int dA_j\, b_i[\tilde{\sigma}_{ij} + \sigma_{ij}(\vec{r})]/2$$
$$= -\frac{1}{2}\int dA_j\, b_i \sigma^0_{ij}(\vec{r}) + \frac{1}{2} S\sigma^{\rm x}(2\overline{\sigma} - \sigma^{\rm x})V\,, \qquad (6)$$

whose summation adds up to Eq. (3). The elastic energy is therefore composed of a defect contribution, which depends only on the stress field variation $\sigma^0(\vec{r})$, and a bulk contribution varying quadratically with the average stress $\overline{\sigma}$.

One can express $\sigma^0(\vec{r})$ as the summation of variations in the stress due to the individual dislocation dipoles. Denote the stress field of a dipole at $\vec{R}$ by $\sigma^{\rm dipole}_{ij}(\vec{r} - \vec{R})$; this summation is absolutely convergent since the stress difference between two field points decays as R^{-3}. To connect with the existing approach mentioned above, we note that the integral of the stress field of one dipole over the region enclosed by the primary dipole equals to minus the interaction between the two dipoles, so that $E_{\rm prm} = -\frac{1}{2}\int dA_j\, b_i \sigma^{\rm dipole}_{ij}(\vec{r})$ and $E_{\rm dd}(\vec{R}) = -\int dA_j\, b_i \sigma^{\rm dipole}_{ij}(\vec{r} - \vec{R})$. It then follows that $E_{\rm img}$ can be rigorously written as

$$E_{\rm img} = \frac{1}{2}{\sum_{\vec{R}}}' E_{\rm dd}(\vec{R}) + \frac{1}{2} A_j b_i \sigma^{\rm err}_{ij} + \frac{1}{2} S\overline{\sigma}^2 V\,, \qquad (7)$$

where $\sigma^{\rm err}_{ij} = \langle\sum_{\vec{R}} \sigma^{\rm dipole}_{ij}(\vec{r} - \vec{R})\rangle_V$, and the summation here involves the same collection of image dipoles as in the first term of Eq. (7) plus the primary dipole contribution ($\vec{R} = 0$). Equation (7) shows that what is missing in Eq. (2), besides a term describing the bulk stress effect, $\frac{1}{2}S\overline{\sigma}^2 V$, is a dipole correction $\frac{1}{2}A_j b_i \sigma^{\rm err}_{ij}$, which is $-1/2$ of the interaction between the primary dipole and the average stress introduced by the primary and image dipoles. This is similar to that derived by Wolf [12] in treating Coulomb interaction summations in electric dipole lattices. The correction is nonzero only if the primary cell contains a nonzero dipole moment [13]. If one can group every two neighboring cells to form a dislocation quadrupole array [14], its image summation is then free from this dipole correction.

One can show that the dipole correction can be exactly canceled by introducing a set of specially chosen "ghost" dislocations to interact with all the dipoles. This is analogous to the fictitious charges introduced in [15] to cancel the dipole correction in the lattice of electric dipoles. As shown in Fig. 1, ghost dislocation with Burgers vector $\alpha\vec{b}$ can be placed at $\vec{c}_1/2$, $-\alpha\vec{b}$ at $-\vec{c}_1/2$, $\beta\vec{b}$ at $\vec{c}_2/2$, and $-\beta\vec{b}$ at $-\vec{c}_2/2$, with α, β satisfying $\vec{a} = \alpha\vec{c}_1 + \beta\vec{c}_2$. In this way $E_{\rm img}$ becomes

$$E_{\rm img} = \frac{1}{2}{\sum_{\vec{R}}}'[E_{\rm dd}(\vec{R}) - E_{\rm dg}(\vec{R})] - \frac{1}{2}E_{\rm dg}(0) + \frac{1}{2} S\overline{\sigma}^2 V\,, \qquad (8)$$

where $E_{\rm dg}(\vec{R})$ represents the interaction energy between a dislocation dipole (at offset $\vec{R}$) and the ghost dislocations. The summation in Eq. (8) is absolutely convergent because the ghost dislocations have exactly the same dipole moment as the primary dipole, so that $E_{\rm dd}(\vec{R}) - E_{\rm dg}(\vec{R}) \sim R^{-3}$ for large R. Since Eq. (8) does not depend on the explicit form of dislocation interactions, our method is applicable to dislocations of any character in a general anisotropic elastic medium.

We apply our method to extract the core energy of a shuffle-set screw dislocation in Si from atomistic calculations [16] using the Stillinger-Weber (SW) [17] potential. Figure 2(a) shows the variation of the total energy per unit dislocation length (E_{atm}) with cell dimension $\vec{c}_1$, while $\vec{c}_2$ is fixed at 3[111]. For a given simulation cell, we calculate the corresponding elastic energy $E_{\text{prm}} + E_{\text{img}}$ through Eq. (8) and use sextic anisotropic elasticity theory for individual dislocation interaction energies [18]. The anisotropic elasticity results, Eq. (3), are seen to fall on a straight line with a slope that agrees with the atomistic result to within 0.5%. This agreement between atomistic and anisotropic linear elasticity results is significant because there are no adjustable parameters in either calculation, in contrast to previous studies [3,5]. The difference between the two gives the core energy $E_{\text{core}} = 0.526 \pm 0.002$ eV/Å, at $r_c = b = 3.84$ Å, which is manifestly independent of $\vec{c}_1$. A previous calculation using first principles method and isotropic elasticity theory [5] has given $E_{\text{core}} = 0.56 \pm 0.21$ eV/Å using the same r_c. First principles method is supposed to be more accurate than empirical potentials in obtaining the atomistic energy, while anisotropic elasticity is more accurate than isotropic elasticity in estimating the image energy. In view of this and considering the large error bar in the previous work, one cannot conclude much at this stage.

In Fig. 2(b) we directly compare the two sides of Eq. (1) by fixing $\vec{c}_1$ at $4[11\bar{2}]$ and varying $\vec{c}_2$ from 2 to 10[111]. The atomistic result agrees very well with the sum of anisotropic elasticity results plus $2E_{\text{core}}$ obtained from Fig. 2(a), except at the smallest $\vec{c}_2$ (2[111]) , where the dislocation cores overlap with their own image and linear elasticity is expected to break down. This is a direct confirmation of Eq. (1) as the proper way to define the core energy of a dislocation.

To bring out the effects of elastic anisotropy, we repeat our calculation by assuming elastic isotropy [20]. The results, shown in Fig. 2(a), also follow a linear variation with a slope that is now 14% larger than the atomistic calculation. One could try "improving" the isotropic elasticity estimate by replacing the shear modulus μ by an energy prefactor K [4], with K taken from an anisotropic expression of screw dislocation self-energies [20], but the resulting slope is still too large by 8%. Alternatively one could treat μ as a free parameter [3,5] to obtain a best fit with atomistic data. Such a procedure leads to a core energy of $E_{\text{core}} = 0.532 \pm 0.002$ eV/Å.

We have also performed similar calculations for edge dislocations in a bcc metal Mo [21], and find similar behavior as in Fig. 2(a). The core energy predicted by anisotropic elasticity is $E_{\text{core}} = 0.324 \pm 0.002$ eV/Å, at $r_c = b = 2.7256$ Å. On the other hand, using μ as a free parameter, isotropic elasticity gives $E_{\text{core}} = 0.382 \pm 0.002$ eV/Å, significantly different from anisotropic results. Thus dislocation core energies obtained under the assumption of elastic isotropy can be in appreciable error even when the energy prefactor is fitted to atomistic data.

While we have emphasized that proper atomistic calculations should give results independent of system size, a question of practical interest is whether there exists an optimum cell geometry for which the elastic interactions are minimized. Consider a simulation cell [Fig. 3(a)] containing an edge dislocation dipole at separation $\vec{a} = \vec{c}_2/2$ which can only glide along $\vec{c}_1$. The system energy is then a periodic function of their relative displacement x along the $\vec{c}_1$ direction, the energy barrier being a result of an

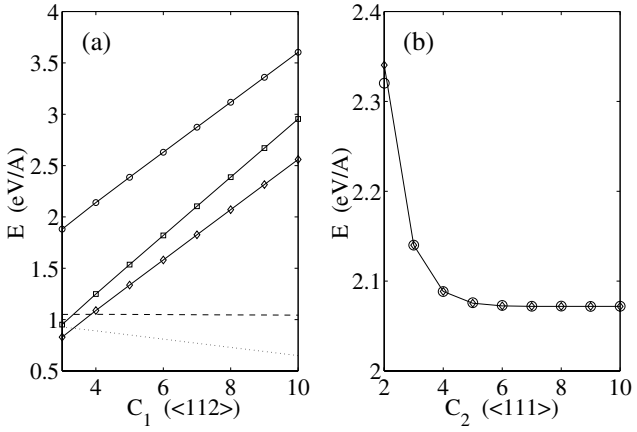

FIG. 2. (a) Variation of atomistic (○) E_{atm} and linear elastic (anisotropic ◇ and isotropic □) E_{el} energies of a shuffle-set screw dislocation dipole in a pbc cell of Si [16] with $\vec{c}_1$ at $\vec{c}_2 = 3[111]$. Predictions of $2E_{\text{core}}$ are shown in dashed and dotted lines, respectively. (b) Variation of E_{atm} with $\vec{c}_2$ at $\vec{c}_1 = 4[11\bar{2}]$. Atomistic simulation results are shown as ○, while anisotropic elastic results for E_{el} plus $2E_{\text{core}}$ obtained from (a) are shown as ◇.

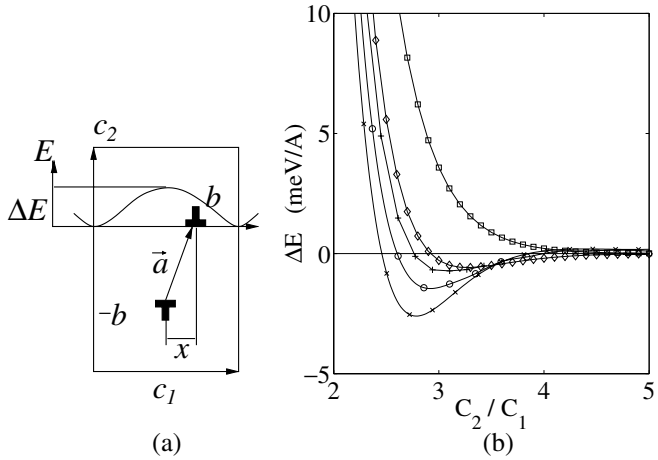

FIG. 3. (a) Schematic of the total energy variation with relative displacement x, ΔE being the maximum. (b) Variation of ΔE with cell aspect ratio c_2/c_1 for edge dislocations in Mo [21]. Anisotropic elasticity predicts $\Delta E = 0$ at $c_2/c_1 = 2.918$ (◇). Isotropic elasticity predicts a monotonic decrease of ΔE with increasing c_2/c_1 (□). Atomistic simulations with $c_1 = 15$, 20, and 30[111] are shown as ×, ○, and +, respectively.

oscillatory image stress field superimposed on any applied external stress. Linear elastic considerations show that the energy variation has extrema at $x = 0$ and $x = c_1/2$, so that $\Delta E = E(x = 0) - E(x = c_1/2)$, a function only of the cell aspect ratio, is an appropriate measure of the internal dislocation interaction. For dislocation mobility simulations [23] a minimum value ΔE is desirable for obtaining an accurate relation between the dislocation velocity and the applied stress.

Results for the energy barrier determined separately by isotropic and anisotropic elasticity calculations are compared in Fig. 3(b). One sees the former clearly decreases monotonically with increasing aspect ratio without becoming negative, whereas the latter vanishes at the value of $c_2/c_1 = 2.918$. Also shown in Fig. 3(b) are direct atomistic simulation results for the energy barrier for three cell sizes, showing a converging behavior toward the elasticity result.

The vanishing of the energy barrier at the special aspect ratio implies a complete cancellation among the primary and image interactions, thus allowing unhindered dislocation glide in the pbc simulation cell. Direct atomistic simulations confirm that ΔE indeed is greatly reduced at a cell geometry close to the predicted c_2/c_1. For example, at $\vec{c}_1 = 20[111]$ and $\vec{c}_2 = 64[\bar{1}01]$, simulation gives $\Delta E = 0.091$ meV/Å, corresponding to a maximum internal stress of about 0.3 MPa. In contrast, typical stresses applied in mobility simulations are in the range of 10–1000 MPa [23].

It may appear that the atomistic results in Fig. 3(b) indicate a significant size dependence. Indeed, a contributing factor could be the higher order (e.g., $\sim 1/r$) terms in the elastic interactions. On the other hand, it should be noted that the energy scale in this figure is about 2 orders of magnitude smaller than typical values for migration barriers for dislocations, so the effect here is rather small. Nevertheless we believe the existence of special geometries, arising from elastic anisotropy, for which $\Delta E = 0$ is quite general, and it is indeed confirmed by our results for a screw dislocation in Mo.

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[21] We use a simulation cell with $\vec{c}_1$, $\vec{c}_2$, $\vec{c}_3$ along $[111]$, $[\bar{1}01]$, $[1\bar{2}1]$ directions, respectively, $\vec{a} = \vec{c}_2/2$ and $\vec{b} = \pm[111]/2$. The dislocation dipole is created by removing a layer of atoms followed by relaxing the configuration to zero stress using the Finnis-Sinclair [22] potential.

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