

## Peierls Energy of Dislocations: A Critical Assessment

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The normal way to calculate the Peierls energy for dislocations follows the procedure of Peierls and Nabarro, who summed the atomic misfit energy in the glide plane at the position of the atoms. Since the misfit energy is not localized but rather contained in the electron distribution, some averaging must be made. This effect can lead to a considerable lowering of the classic Peierls energy and the resulting Peierls stress. [S0031-9007(99)08545-2]

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The Peierls energy  $E_p$  is the amplitude of the energy variations of a dislocation when its center is shifted by an interatomic distance. In recent time there has been renewed interest in calculating  $E_p$  (and the Peierls stress  $\sigma_p$ ) of dislocations by analytical and numerical methods [1–6]. This was motivated by the fact that recently reliable *ab initio* calculations using the electron density functional theory with the local density approximation became available [7–10] to determine the atomic interaction across the glide plane—the so-called  $\gamma$  surface [11]. Although most of these calculations of  $E_p$  are very sophisticated nearly all of them overlook some very essential details, and, hence, are unable to predict realistic values of  $E_p$  and  $\sigma_p$  which can be compared with experimental values. The most serious shortcomings are as follows:

(i) Most calculations are isotropic or pseudoisotropic, whereas a treatment with full anisotropy is possible and does not require any more computational effort.

(ii) Most calculations are 1D assuming a “constrained path approximation.” It is known, however, that generally the local relative displacement  $\mathbf{u}(x)$  across the glide plane deviates from the direction of the Burgers vector  $\mathbf{b}$  [12] and hence a treatment in 2D is mandatory. This implies that in determining  $\mathbf{u}(x)$ , even for simple dislocations, generally a system of two coupled Peierls integral equations would have to be solved numerically.

(iii) In crystals with fcc Bravais lattices (i.e., also diamond structures) dislocations can dissociate into two Shockley partials which are connected by a stacking fault. Since the Burgers vectors of the two Shockley partials are not parallel a realistic treatment of this important configuration is not possible in 1D.

(iv) In order to obtain the variation of the Peierls energy  $E_p$  with the position of the dislocation, generally the atomic interaction energy is summed over the position of the atoms following the procedure of Peierls [13] and Nabarro [14] (PN). The atomic interaction energy is, however, not localized at the position of the atomic nuclei but contained to a large part in the kinetic, potential, and exchange energy of the electrons. It is therefore physically more realistic to take an average of the energy over an area with the dimension which is characteristic for the electron distribution.

Since methods to overcome objections (i) to (iii) are already in the literature we only briefly summarize the results here. The main purpose of this paper is to use these results in order to show how a realistic averaging procedure will affect the value of the Peierls energy and the Peierls stress.

*The dislocation profile in 2D.*—We consider a straight dislocation with Burgers vector  $\mathbf{b}$  in a crystalline solid. Within the framework of the Peierls model the crystal is bisected along the glide plane and the resulting two semi-infinite half-spaces are treated as linear elastic (anisotropic) continua. They are subjected to surface displacements  $\mathbf{u}(x)$  corresponding to a dislocation where  $x$  is the coordinate perpendicular to the dislocation line. The resulting surface stresses must be balanced by the atomic interaction forces across the glide plane.

The elastic energy  $E_{el}$  in the two half-spaces is given by [3]

$$E_{el} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \partial \mathbf{u}(s) / \partial s \tilde{H}(x-s) \mathbf{u}(x) ds dx. \quad (1)$$

Here  $\tilde{H}$  is the symmetric Stroh tensor of the anisotropic elastic constants, which depends on the orientation of the dislocation line [15,16]. For notational convenience the factor  $1/4\pi$  has been included in  $\tilde{H}$ . For certain high symmetry orientations and for isotropy  $\tilde{H}$  becomes diagonal and in isotropic media it has the components  $(\mu/4\pi)[1/(1-\nu), 1/(1-\nu), 1]$ . Note that  $E_{el}$  can also take into account the opening displacements perpendicular to the glide plane caused by the dislocation.

The atomic misfit energy  $E_A$  in the glide plane can be obtained with the aid of the so-called  $\gamma$  surface [11]. It is the 2D energy profile which results when the two crystal halves above and below the glide plane are shifted by a vector  $\mathbf{t}$  in the glide plane, and the atoms are allowed to relax. Whereas previous calculations using central forces, pair potentials, or embedded atom calculation were not very satisfactory, recent *ab initio* calculations using electron density functional calculations with local density approximation are considered to give very reliable results [7–10].

Since the potential must reflect the symmetry in the glide plane it can be represented by a two dimensional

Fourier series with the aid of the reciprocal lattice vectors  $\mathbf{g}_k$ ,

$$\gamma(\mathbf{t}) = \sum_k c_k \exp[2\pi i \mathbf{g}_k \mathbf{t}]. \quad (2)$$

The misfit energy in the glide plane is then obtained as

$$E_A = \int_{-\infty}^{\infty} \gamma(\mathbf{u}(x)) dx. \quad (3)$$

The total energy,

$$E_T = E_{el} + E_A, \quad (4)$$

can be considered as functional of the still unknown displacement  $\mathbf{u}(x)$ , which is subject to the condition that  $E_T$  must be a minimum. Hence the determination of  $\mathbf{u}(x)$  results in a variational problem. The resulting Euler equation leads to

$$2 \int_{-\infty}^{\infty} \partial \mathbf{u}(s) / \partial s \tilde{H}(x-s) ds + \text{grad}[\gamma(\mathbf{u}(x))] = 0, \quad (5)$$

which is a set of two coupled integro-differential equations of Peierls type. Physically this corresponds to balancing the stress components parallel and perpendicular to the dislocation line. Since the elastic response in these two directions is different, the corresponding components of the local displacement vector  $\mathbf{u}(x)$  are not proportional to each other and hence  $\mathbf{u}(x)$  generally deviates from the direction of the crystallographic Burgers vector  $\mathbf{b}$  [12]. A treatment in 1D is therefore not adequate, except possibly for dislocations in pure edge or screw orientation. In stiff potentials, even there the dislocation can take up a component perpendicular to the Burgers vector [17], and then a 2D treatment is necessary.

When the atomic interaction potential in 1D takes the simple form,

$$\gamma(u) = K[1 - \cos(2\pi u/b)], \quad (6)$$

the exact solution of the integral equation in 1D obtained by PN is

$$u = (b/\pi) \arctan(x/w_0) + b/2, \quad (7)$$

where the so-called dislocation width  $w$  has a value of

$$w_0 = \mathbf{b} \tilde{H} \mathbf{b} / 2\pi K. \quad (8)$$

For more general potentials (with the exception of a very special set [18]), analytical solutions are unknown. Then there are two ways to find approximate solutions:

First one can try to solve the PN integral equation (5) numerically, but to our knowledge no solution for a 2D problem has been obtained up to now. The other way is to solve the variational problem by the Ritz method. Here appropriate trial functions for  $\mathbf{u}(x)$  are assumed with free geometrical parameters. The value of these parameters is determined by the condition that the total energy  $E_T$  must be a minimum.

An appropriate set of trial functions is, for instance,

$$\mathbf{u}(x) = \sum_k (\mathbf{b}_k/\pi) \arctan[(x - d_k)/w_k] + \mathbf{b}_0, \quad (9)$$

which corresponds to a set of fractional dislocations with Burgers vector  $\mathbf{b}_k$  and width  $w_k$  situated at  $x = d_k$ . An appropriate choice of  $\mathbf{b}_k$  can be obtained by the inspection of the  $\gamma$  surface. We must have  $\sum \mathbf{b}_k = \mathbf{b}$  and  $\mathbf{b}_0$  must be chosen so that  $\mathbf{u}(-\infty) = 0$  and  $\mathbf{u}(\infty) = \mathbf{b}$ . Using this set of trial functions has the advantage that the elastic energy  $E_{el}$  can be obtained analytically [3], but the misfit energy  $E_A$  must be evaluated numerically.

This method was originally suggested by Leibfried and Dietze [19] and first applied by Seeger and Schoeck [20] to calculate the dissociation width of dislocations in fcc lattices. This method has since been used to obtain the configuration of dissociated dislocation when the  $\gamma$  surface or a selected set of  $\gamma$  values was available [10,21–24].

With the treatment given here we can overcome the objections (i) to (iii) raised in the introduction and can realistically describe the dissociation of dislocations.

*The Peierls energy and Peierls stress.*—In Eq. (3) the atomic misfit energy  $E_A$  results from a continuous distribution of energy density  $\gamma$  in the glide plane, and hence  $E_A$  is invariant against a translation of the dislocation center. As pointed out, however, by Peierls [13] and Nabarro [14] in a crystal lattice the misfit energy should depend on the position of the dislocation center within a lattice cell and hence be periodic. They suggested that these energy variations can be obtained by summing the misfit energies at the position of the atom rows parallel to the dislocation, when shifting the 1D displacement profile  $u(x)$  of Eq. (7) rigidly across a lattice cell. They recognized that this implicitly assumes that no change in elastic energy is allowed for. When the atom rows are separated by the period  $a$ , the misfit energy becomes in 2D,

$$E_A = a \sum_n \gamma(\mathbf{u}(na + z)), \quad (10)$$

where  $z$  with  $0 \leq z \leq a$  denotes the position within the lattice cell. This procedure has been followed nearly exclusively in later treatments.

This sampling of the energy at the position of the atoms is, however, not physically realistic. For central forces the interaction energy would be “concentrated” at the position of the atomic nuclei. Within the framework of the electron density functional theory this energy however is largely contained in the potential, kinetic, and nonlocal exchange energy of the electron distribution. When a gradient exists in the displacement of the atoms, this distribution is affected and adjusts continuously to a minimum energy configuration. Therefore the energy must be averaged over an area around the atom position over a distance characteristic for the electron distribution of dimension, let’s say  $t$ .

Thus we obtain for the misfit energy with the averaging procedure,

$$E_A = a \sum_n \Gamma(x_n), \quad (11)$$

where

$$\Gamma(x_n) = (1/2t) \int_{-t}^{+t} \gamma(\mathbf{u}(x_n + t)) dt, \quad (12)$$

and where  $|t| \leq a/2$ .

With  $x_n = na + z$  in Eq. (11) we can make use of the formula of Poisson for sums and have

$$E_A(z) = \sum_k \exp[-2\pi ikz/a] J(k), \quad (13)$$

with

$$J(k) = \int_{-\infty}^{\infty} \Gamma(\mathbf{u}(s)) \exp[2\pi iks/a] ds. \quad (14)$$

When we now assume that  $\gamma(x)$  is symmetric in  $x$ , we obtain the first two terms,

$$E_A(z) = \int_{-\infty}^{\infty} \Gamma(\mathbf{u}(s)) ds + 2 \cos(2\pi z/a) \times \int_{-\infty}^{\infty} \Gamma(\mathbf{u}(s)) \cos(2\pi s/a) ds. \quad (15)$$

When we use the classical PN potential of Eq. (6) with the exact solution for  $u$  of Eq. (7) we find

$$\gamma(x) = 2Kw_0^2/(w_0^2 + x^2) \quad (16)$$

and

$$\Gamma(u(s)) = 2K(w_0 2t) \{ \arctan[(s+t)/w_0] - \arctan[(s-t)/w_0] \}, \quad (17)$$

With the aid of Eq. (17) we can now evaluate the expression for  $E_A$  [Eq. (15)]. Making use of the fact that in equilibrium configuration the first term in Eq. (15) equals  $\mathbf{b}\tilde{\mathbf{H}}\mathbf{b}$  [3], we obtain

$$E_A(z) = \mathbf{b}\tilde{\mathbf{H}}\mathbf{b} [1 + 2F(t) \exp(-2\pi w_0/a) \times \cos(2\pi z/a)]. \quad (18)$$

The influence of the averaging procedure is contained in the function  $F(t)$  which we have evaluated numerically. It can be fitted by the interpolation function,

$$F(t) = \cos[\pi t/a] - 0.08 \sin[2\pi t/a] + 0.03 \sin[4\pi t/a]. \quad (19)$$

The essential contribution results from the first term in Eq. (19). The Peierls energy is now obtained from the variations in the second term in the series for  $E_A$  of Eq. (18) with the maximum amplitude of

$$E_P = 4 \mathbf{b}\tilde{\mathbf{H}}\mathbf{b} F(t) \exp(-2\pi w_0/a). \quad (20)$$

For  $t \rightarrow 0$  the function for  $\Gamma$  of Eq. (12) degenerates into a  $\delta$  function and with  $F(0) = 1$  we have for  $E_P$  the (corrected) result of PN. For  $t = a/2$  we average

over the whole period and with  $F(a/2) = 0$  we also have  $E_P = 0$  which is the result for a continuous energy distribution.

The resulting Peierls stress is obtained as the maximum force  $\sigma b = \partial E_A / \partial z$  exerted on the dislocation,

$$\sigma_p = 4\pi \mathbf{b}\tilde{\mathbf{H}}\mathbf{b} F(t) / (ab) \exp[-2\pi w_0/a] \quad (21)$$

and depends on the value of  $t$  in the same way as  $E_P$ .

In the preceding sections we have shown how a realistic fully anisotropic determination of the displacement path  $\mathbf{u}(x)$  in 2D is possible when *ab initio* calculations electron density functional theory (DFT) of the  $\gamma$  surface are available. More complex is the calculation of the Peierls energy  $E_P$  and the resulting Peierls stress  $\sigma_p$ . Their values depend sensitively on the distance  $t$  over which the energy must be averaged to account for the nonlocal distribution in energy density. A series development of Eq. (12) shows that  $\Gamma(x+z) = \Gamma(x) + (z^2/2)\partial^2\Gamma(x)/\partial x^2$ , and hence the averaging will mainly affect the result in regions where  $\gamma(x)$  has a strong curvature, i.e., mainly in the inner region of the dislocation core. A finite value of  $t$  will always reduce the energy variations.

It should be mentioned that the need for some averaging was already proposed by Dietze [24] in 1952. He constructed a 2D interplanar potential—today called  $\gamma$  surface—in various crystal planes assuming an atomic interaction by short-ranged central forces. At a close distance one has to consider, however, the finite extension of the atoms, and he proposed a force distribution by a weighted average with a sharp maximum at the position of the nuclei.

It is difficult to assess a value of  $t$  from physical arguments. For central forces the energy would be concentrated at the position of the atoms; however, the situation is different considering the energy of the electron distribution. For free electrons  $t$  should be of the order of the Thomas-Fermi radius but the rearrangement in the displacement gradient also affects the valence electrons. The model assumes that we can separate the energy in an atomic part in the glide plane and in an elastic part in the surrounding half-spaces. This concept is adequate to describe the global features of the dislocation, and it is successful in studying the dissociation of dislocations into partial dislocations [10,21–24]. However, when it comes to accounting for the energy density in a displacement gradient, the artificial separation into atomic misfit and elastic energy cannot be maintained, and the solution of the problem is beyond the scope of the model. Therefore the value of  $t$  can be fixed only by intuitive reasoning, but before its value is known a comparison between theoretical and experimental values of  $E_P$  and  $\sigma_p$  is rather arbitrary.

Recently Bulatov and Kaxiras [1] tried a different way to resolve the problem of connecting the discrete atomic structure in the glide plane with the surrounding elastic continuum. They discretized the elastic energy

by representing the displacement path with a linear spline function between the positions of the atoms. This corresponds to a sequence of closely spaced fractional dislocations with a standard linear core [25] and local Burgers vector  $b_n = u(x_n) - u(x_{n-1})$ . By minimizing the total energy they can determine the set of  $\{b_n\}$ . In this way they are able to account for changes in the displacement profile during the shifting, but the problem of assigning a value of misfit energy to an area where a displacement gradient exists is not resolved.

The summing procedure of PN implicitly assumes that the displacement profile stays constant, and hence the elastic energy does not change during the shifting of the dislocation centers within a lattice cell. It can, however, be shown that changes in configuration do take place. The resulting changes in misfit energy and elastic energy are of opposite sign with the effect that they nearly cancel each other. These results will be published in a follow-up paper.

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