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THE PEIERLS DISLOCATION: LINE ENERGY, LINE TENSION, DISSOCIATION AND DEVIATION

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Abstract—Atomic simulations of the dislocation core show that the atomic misfit is often concentrated in the glide plane. Instead of using a step function to describe the displacement as in a classical Volterra dislocation, a better description is obtained by a Peierls dislocation for which the displacement is assumed to have an arctg like shape. The slope in the center is determined by requiring that the total energy must be a minimum. The elastic energy can be expressed in closed form, and with the availability of high speed computing the atomic misfit energy in the glide plane can be calculated by standard numerical integration without any difficulties. When the Peierls model is extended to two dimensions the resulting line energy, line tension and resistance against bow-outs of straight dislocations can be obtained realistically without any adjustable parameters and the way that these quantities are influenced by the interplanar atomic potential can be studied. In addition to undergoing the well-known "dissociation", a mixed dislocation may lower its energy by a "deviation" in which the displacement vector deviates from the direction of the crystallographic Burgers vector even when this runs along a path of lowest misfit energy. © *1997 Acta Metallurgica Inc.*

1. INTRODUCTION

A Volterra dislocation in a continuum is described by a step function-like displacement by a Burgers vector **b**. For a straight dislocation in a linear elastic anisotropic continuum it has the energy per unit length given by

$$E_{el} = \mathbf{b}\tilde{H}\mathbf{b} \ln \frac{R}{r_0}. \quad (1)$$

The prelogarithmic line energy coefficient $\hat{E}_L = \mathbf{b}\tilde{H}\mathbf{b}$ contains the symmetric Stroh tensor $\tilde{H}$ [1–3] which depends on the orientation of the dislocation line only. The components of $\tilde{H}$ can be calculated from the elastic constants as referred to the crystal axes by a computer routine first given by Head *et al.* [4]. (By convention the dislocation axis is along the x_3 axis of a Cartesian system with the x_1 axis in the glide plane and a factor $1/4\pi$ has been incorporated in $\tilde{H}$). For isotropy $\tilde{H}$ is diagonal with components $(\mu/[4\pi(1-\nu)], \mu/[4\pi(1-\nu)], \mu/4\pi)$.

The outer cut-off radius R is determined by the boundary conditions, i.e. by the presence of dislocations of opposite sign or of free surfaces. Eventually an additional term must be added representing the work done to make the surface stress free [5]. The inner cut-off radius r_0 has to be introduced to avoid divergence resulting from the fact that the displacement vector **b** is in the usual convention assumed to be a step function.

In order that equation (1) gives the correct energy, the value of r_0 must be chosen in a way that includes the energy near the dislocation core where linear elasticity theory breaks down. Often an ad hoc value of $r_0 = b$ is assumed, which has the correct order of magnitude but lacks detailed justification. A discussion about the magnitude of r_0 has been given by Saada and Douin [6] in the framework of continuum theory, but clearly a realistic value of r_0 can only be obtained by an atomistic treatment.

A formal way of avoiding the elastic singularity is the so-called "standard core" [7] in which the displacement is distributed homogeneously over a strip of width d (corresponding to a constant density of infinitesimal dislocations). However, little is gained since the appropriate value of d cannot be determined without atomistic considerations.

There are numerous treatments of the dislocation core by atomic simulations as reviewed, for instance, by Duesbery and Richardson [8]. A major problem with these simulations (apart from finding an appropriate interatomic potential) is the limited size of the region that can be treated. When the dislocation core extends over a region d there are elastic stresses associated which decrease as $(d/r)^2$ with distance r. Hence the linear dimension R of the region considered must be $R/d \gg d/b$ in order that for $r > R$ this additional contribution to the elastic energy can be neglected, but computational limitations restrict the value of R. Due to the matching problem between the atomistic region inside and the elastic continuum region outside, it is difficult to obtain a reliable value for the energy that would lead to a value for r_0.

It has already been pointed out by Hirth and Lothe [5] that the core parameter r_0 must depend on orientation to give a consistent description of dislocation interaction. In this paper we derive a relationship between the stiffness of the interplanar potentials and the value of r_0 based on the Peierls model [9]. In order not to cloud the physical concept by geometrical or mathematical complexity, we first give the line energy (characterized by r_0) and the line tension for a simple Peierls dislocation in a simple cubic lattice for various interplanar potentials. We then generalize the result in a straightforward way to dislocations with more general core shapes and with arbitrary orientation in arbitrary glide planes. In particular we will study the conditions under which a dislocation can lower its energy by "dissociation" or "deviation" and investigate how the stiffness of the interplanar potential will influence these effects.

2. THE LINE ENERGY OF A PEIERLS DISLOCATION

When the dislocation has some edge component, the glide plane is well defined. In this case atomistic simulations of the core show [8] that the main atomic distortion is usually spread in the glide plane. As discussed recently [10] the displacement of the atoms above and below the glide plane is continuous and hence can be treated in principle by continuum theory, though possibly nonlinear and nonlocal. Across the glide plane there is a discontinuity and an exchange of nearest neighbours. Therefore this region must be treated atomistically. This is the philosophy of the Peierls–Nabarro model (see Ref. [5]) which gives a reasonably good description of the core structure. Even when the displacement is nonplanar, as for instance in screw dislocations in b.c.c. crystals which show a threefold extension of the core, a treatment in the Peierls–Nabarro model is possible [11]. In the planar model the crystal is treated as two linear elastic half spaces separated by the glide plane. The nonlinear interaction across the glide plane is of atomic nature and hence must be periodic with the lattice periodicity. The requirement that the stresses at the surface of the half spaces must be balanced by the atomic interaction across the glide plane leads to the Peierls integral equation for the unknown relative displacement $\mathbf{u}$. For a pure sinusoidal potential in a simple cubic lattice the solution is

$$\mathbf{u}(x) = \frac{\mathbf{b}}{\pi} \operatorname{arctg} \frac{x}{w} + \frac{\mathbf{b}}{2} \tag{2}$$

where the constant $\mathbf{b}/2$ has been added to satisfy the boundary condition $\mathbf{u}(-\infty) = 0$, $\mathbf{u}(\infty) = b$. For this potential with glide plane separation h the values for the dislocation width are $w = h/[2(1-\nu)]$ for edges and $w = h/2$ for screws [5]. For more complicated interaction potentials (with the exemption of a few very specialized cases [12]) solutions of the Peierls equation are not known.

Instead of now using a step function as the starting point for characterizing a dislocation, we could use equation (2) as a general description for the displacement in the glide plane and call this a "Peierls dislocation". This avoids the singularity in the center and in addition in most cases gives a more realistic description and does not contain the discontinuities of the standard core [7]. The dislocation with w in equation (2), which seems to be a free parameter, is fixed, however, by the requirement that the total energy must be a minimum. Its value is determined by the competition between the elastic energy which wants to spread the displacement and the atomic interaction which wants to contract it.

The Ansatz equation (2) allows the elastic energy to be calculated in closed form [9, 13]. The resulting stress distribution $\sigma_{i3}(x)$ in the glide plane can be considered to result from the superposition of a distribution $\mathrm{d}\mathbf{u}/\mathrm{d}s$ of infinitesimal dislocations:

$$\boldsymbol{\sigma}(x) = 2\tilde{H} \int_{-\infty}^{+\infty} \frac{\partial \mathbf{u}(s)}{\partial s} \frac{1}{x-s} \, \mathrm{d}s \tag{3a}$$

which leads to

$$\boldsymbol{\sigma}(x) = \begin{pmatrix} \sigma_{13}(x) \\ \sigma_{23}(x) \\ \sigma_{33}(x) \end{pmatrix} = 2\tilde{H}\mathbf{b} \frac{x}{x^2 + w^2}. \tag{3b}$$

The elastic energy of the dislocation in the two semi-infinite half spaces is then

$$E_{\mathrm{el}}(\mathbf{u}) = \frac{1}{2} \int_{-R}^{+R} \boldsymbol{\sigma}(x)\mathbf{u}(x) \, \mathrm{d}x. \tag{4a}$$

Evaluation of integral (12) leads to

$$E_{\mathrm{el}} = \mathbf{b}\tilde{H}\mathbf{b} \ln \frac{R}{2w} \tag{4b}$$

where as before R is some outer cut-off radius determined by the boundary conditions. In addition we have the atomic misfit energy E_{A} in the glide plane which is given by

$$E_{\mathrm{A}} = \int_{-R}^{+R} \gamma[\mathbf{u}(x)] \, \mathrm{d}x \tag{5}$$

where x is the coordinate in the glide plane perpendicular to the dislocation line and $\gamma(\mathbf{u})$ is the interplanar atomic potential or the specific energy of the gamma surface as defined by Vitek [14]. It is the increase in Gibbs free energy when the two half spaces are shifted by a distance $\mathbf{u}$ against each other.

For each lattice plane $\gamma(\mathbf{u})$ can be represented by a Fourier series with the aid of the reciprocal lattice vectors [9]. Since we are interested in a general discussion, we first use a potential for a simple cubic lattice with periodicity b for which the shear modulus μ_0 in the glide plane and the maximum energy γ_0

can be chosen independently. The simplest expression is [15]

$$\gamma = \mu_0 b\left[\frac{1}{(4\pi)^2}\left(1 - \cos\frac{4\pi u}{b}\right) + \frac{g}{8}\left(3 - 4\cos\frac{2\pi u}{b} + \cos\frac{4\pi u}{b}\right)\right] \quad (6)$$

where $g = \gamma_0/\mu_0 b$ is the "stiffness" of the potential. The shape of $\gamma(u)$ is shown in Fig. 1 for values of g between 0.03 and 0.06.

Using equation (5) we can now evaluate the atomic misfit energy E_A. With the magnitude of the displacement u given by equation (2) and introducing $\eta = x/w$ as a variable with $\eta_0 = R/w$, we find

$$E_A = \mu_0 b w[F(\eta_0) + gG(\eta_0)] \quad (7a)$$

where

$$F(\eta_0) = \frac{1}{(4\pi)^2}\int_{-\eta_0}^{\eta_0}\left[1 - \cos\frac{4\pi u(\eta)}{b}\right]d\eta \quad (7b)$$

and

$$G(\eta_0) = \frac{1}{8}\int_{-\eta_0}^{\eta_0}\left(3 - 4\cos\frac{2\pi u(\eta)}{b} + \cos\frac{4\pi u(\eta)}{b}\right)d\eta. \quad (7c)$$

The integrals of equations (7b) and (7c) must be evaluated numerically. For $\eta_0 = R/w \gg 1$ they approach asymptotically limiting values $F_0 = 0.0796$ and $G_0 = 1.571$.

In order to obtain the equilibrium value $\bar{w}$ of the dislocation width we make use of the fact that in equilibrium, when the two half spaces above and below the glide are assumed to be linear elastic, the total atomic misfit energy in the glide plane is independent of the interatomic potential [10] and is given by

$$E_A = \hat{E}_L = \mathbf{b}\tilde{H}\mathbf{b}. \quad (8)$$

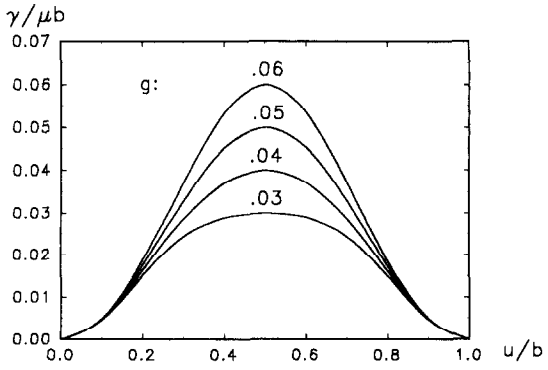

Fig. 1. One dimensional interplanar potential in a simple cubic lattice with stiffness $g = \gamma_0/\mu b$ as parameter.

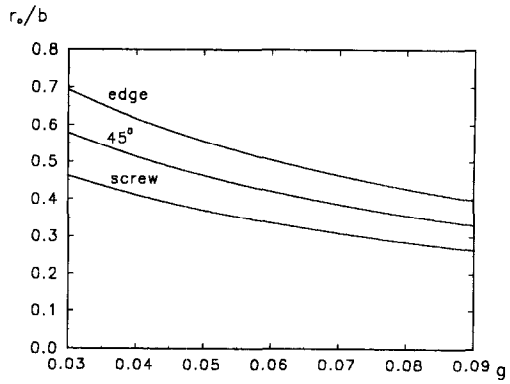

Fig. 2. Effective core radius r_0 of dislocations as a function stiffness g of interplanar potential.

Hence we obtain from equation (7a) for $R \gg b$:

$$\frac{\bar{w}(g, \varphi)}{b} = \frac{\hat{E}_L(\varphi)}{\mu_0 b^2(F_0 + gG_0)} \quad (9a)$$

which for isotropy becomes

$$\frac{\bar{w}(g, \varphi)}{b} = \frac{\cos^2\varphi + \sin^2\varphi/(1 - \nu)}{4\pi(F_0 + gG_0)} \quad (9b)$$

where φ is the angle between dislocation line and the Burgers vector.

Now representing the energy of the dislocation in the form of equation (1) we obtain

$$r_0 = \frac{2\bar{w}(g, \varphi)}{e} \quad (10)$$

where e is Euler's number. In Fig. 2 we have plotted the values of r_0/b with $\nu = 1/3$ for isotropy. For a simple sinusoidal potential as usually used in the Peierls model we have $g \approx 0.05$ and r_0 ranging from $r_0 \approx 0.37$ for screw and $r_0 \approx 0.56$ for edge dislocations.

3. THE LINE TENSION

We have now obtained the line energy for a Peierls dislocation in a linear elastic medium, with stiffness $g = \gamma_0/\mu_0 b$ of the interplanar potential:

$$E_L(g, \varphi) = \hat{E}_L(\varphi)\ln\frac{R}{2\bar{w}(g, \varphi)} + E_A(\varphi) \quad (11)$$

where $\bar{w}(g, \varphi)$ is given by equation (9) and where $E_A(\varphi) = \hat{E}_L(\varphi)$.

The resistance against a bow-out is now described to first order by the line tension [5]

$$T_L = E_L + \frac{\partial^2 E_L}{\partial\varphi^2} \quad (12)$$

which partly results from the resistance against lengthening and partly from the resistance against rotation. For the Peierls dislocation there is also a term resulting from core modification. From equation (11) we obtain

$$T_L = \hat{T}_L \ln \frac{R}{2\bar{w}(g,\varphi)} - \left(\frac{(\hat{E}_L')^2}{\hat{E}_L} + \hat{E}_L''\right) + T_C \quad (13a)$$

with

$$\hat{T}_L = \hat{E}_L + \hat{E}_L'' \quad (13b)$$

and

$$T_C = E_A + E_A'' \quad (13c)$$

where the primes imply differentiation with respect to φ. Here $\hat{T}_L$ is the normal pre-exponential line tension coefficient, T_C the line tension of the core, and the terms in the bracket are due to the change in the core extension. By making use of the relation $E_A(\varphi) = \hat{E}_L(\varphi)$ we finally obtain

$$T_L(\varphi) = \hat{T}_L(\varphi) \ln \frac{R}{2\bar{w}(g,\varphi)} + \hat{E}_L(\varphi) - \frac{(\hat{E}_L'(\varphi))^2}{\hat{E}_L(\varphi)}. \quad (13d)$$

We now consider the change in energy ΔE when forming a small bow-out of maximum height h and length λ with $h \ll \lambda \ll R$ in an otherwise straight dislocation. As first pointed out by Mott and Nabarro [16], this energy depends logarithmically on λ but not on R, for obvious reasons. The bulge can be formed by superimposing an appropriate closed dislocation loop on the straight dislocation. The additional stresses decrease as $1/r^3$ for $r \gg \lambda$ and hence the energy does not diverge. The interaction of the bow-out with the rest of the dislocation also has to be included in ΔE.

This problem has been treated by Püschl *et al.* [17] for arbitrary anisotropy in approximating the bow-out by a set of straight segments and the result has been given as a series expansion up to terms in $(h/\lambda)^2$. However, the contribution of the core could not be evaluated. With the geometry determined by h, s, and l in the configuration of Fig. 3, the increase in line length is $\Delta s = h^2/l$. We refer to the original paper [17] for details and give here the result for a Peierls dislocation by incorporating the line tension for the core of equation (13d). By contracting different terms and replacing the core cut-off ϵ by $2\bar{w}$, the change in energy ΔE per increase in line length Δs is given by

$$\frac{\Delta E}{\Delta s} = \hat{T}_L(\varphi)\left[\ln \frac{l}{\bar{w}(g,\varphi)} - \tfrac{1}{2} + \chi(p)\right] + \tfrac{1}{2}[K(\varphi) + K''(\varphi)] - \frac{[\hat{E}_L'(\varphi)]^2}{\hat{E}_L(\varphi)} \quad (14a)$$

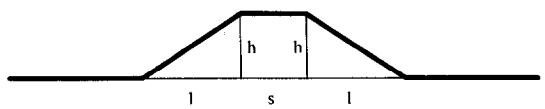

Fig. 3. Configuration of a local bow-out in an otherwise straight dislocation.

where K is the Kirchner integral:

$$K(\varphi) = \int_0^{\pi} [\hat{E}(\varphi + \zeta) - \hat{E}(\varphi)] \frac{\cos^2 \zeta}{\sin \zeta} \, d\zeta \quad (14b)$$

and where with $p = s/l$ we have

$$\chi(p) = (1+p)\ln(1+p) - \tfrac{1}{2}(2+p)\ln(2+p) - \tfrac{1}{2} p \ln p. \quad (14c)$$

For isotropy we have [17]

$$\tfrac{1}{2}[K(\varphi) + K''\varphi] = [E(\pi/2) - E(0)](2\sin^2\varphi - 1). \quad (14d)$$

Then for small bow-outs in an otherwise straight dislocation with $h/l \ll 1$ and $\Delta s = h^2/l$ in an isotropic medium we finally have:

$$\frac{\Delta E}{\Delta s} = \hat{T}_L\left[\ln\left(\frac{l}{2\bar{w}}\right) - \tfrac{1}{2} + \chi(p)\right] + \frac{\mu b^2 \nu}{4\pi(1-\nu)}(2\sin^2\varphi - 1) - \frac{\mu b^2 \nu}{4\pi(1-\nu)} \frac{\sin^2(2\varphi)}{(1 - \nu\cos^2\varphi)} \quad (15a)$$

with

$$\hat{T}_L = \frac{\mu b^2}{4\pi(1-\nu)}[(1+\nu)\cos^2\varphi + (1-2\nu)\sin^2\varphi]. \quad (15b)$$

Note that the stiffness of the potential only affects the value of $\bar{w}$ and changes in shape only affect the value of $\chi(p)$.

4. THE DEVIATION

In the preceding section we have tacitly assumed a constrained path approximation in which the displacement vector is always along the direction of the geometrical Burgers vector of the lattice. When the dislocation has edge and screw components, however, the two can adjust independently to the minimum energy configuration. This occurs because the elastic response of the medium is different for displacements perpendicular and parallel to the dislocation line. Therefore the displacement vector will deviate from the direction of the lattice Burgers vector. We will show the effect using a simple cubic lattice as an example.

When the angle between the dislocation line and the Burgers vector of type b [100] is φ (see Fig. 4) we will assume that for the edge component

$$b_1 = b \sin\varphi\left(\frac{1}{\pi}\operatorname{arctg}\frac{x}{w_1} + \frac{1}{2}\right) \quad (16a)$$

and for the screw component

$$b_3 = b \cos\varphi\left(\frac{1}{\pi}\operatorname{arctg}\frac{x}{w_3} + \frac{1}{2}\right) \quad (16b)$$

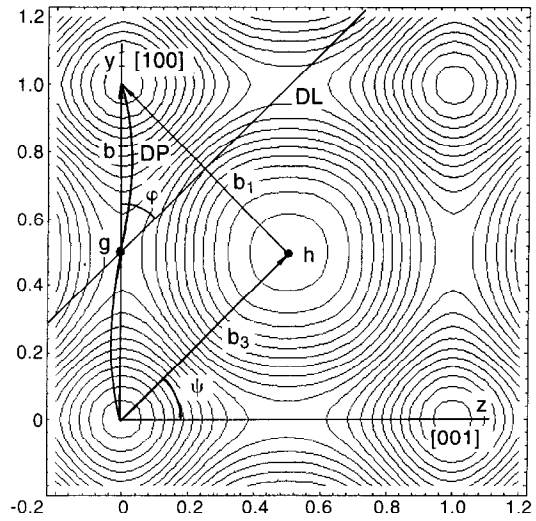

Fig. 4. Deviation path of displacement vector for a mixed dislocation ($\varphi = 45°$) in a simple cubic lattice. (DL = dislocation line, $\mathbf{b}$ = Burger vector, DP = displacement path.)

where w_1 as well as w_3 now adjust to the configuration of minimum energy.

By the procedure used before in the context of equation (4), and choosing $w_3 = aw_1$, we obtain the following expression for the elastic energy:

$$E_{el} = \mathbf{b}\tilde{H}\mathbf{b} \ln \frac{R}{2w_1} + H_{33}b_3^2 \ln \frac{1}{a} + 2H_{13}b_1b_3 \ln \frac{2}{1+a}. \tag{17}$$

For the interplanar potential γ we now need a two dimensional representation which can be made by a Fourier expansion with the aid of the reciprocal lattice vectors [9]. Using an orthogonal system (y, z) along the cube axes in a (001) plane we have for the first four terms:

$$\gamma(y, z) = c_{44}b\left\{c_0 + c_1\left(\cos\frac{2\pi y}{b} + \cos\frac{2\pi z}{b}\right) + c_2\left(\cos\frac{4\pi y}{b} + \cos\frac{4\pi z}{b}\right) + c_3\left(\cos\frac{2\pi(y+z)}{b} + \cos\frac{2\pi(y-z)}{b}\right)\right\}. \tag{18}$$

The coefficients in equation (18) can be obtained from the condition that the shear modulus in the (001) plane is $c_{44} = b\,\partial^2\gamma/\partial y^2 = b\,\partial^2\gamma/\partial z^2$ at $(y, z) = (0, 0)$ and that we have the specific γ values $\gamma(0, 1/2) = \gamma(1/2, 0) = gc_{44}b$ and $\gamma(1/2, 1/2) = hc_{44}b$. This leads to

$$c_0 = \frac{1}{8\pi^2} + \frac{g}{4} + \frac{h}{4}, \quad c_1 = -h/4,$$

$$c_2 = -\frac{1}{16\pi^2} + \frac{g}{8}, \quad c_3 = -\frac{g}{4} + \frac{h}{8}. \tag{19}$$

In the reference frame of the lattice we have now the displacement (Y, Z) in the y and z direction, respectively (see Fig. 4):

$$Y = b_3 \sin\psi + b_1 \cos\psi \tag{20a}$$

$$Z = b_3 \cos\psi - b_1 \sin\psi. \tag{20b}$$

The interplanar energy is now obtained as before in choosing $\eta = x/w_1$ by numerical integration:

$$E_A = w_1 \int_{\eta_0}^{\eta_0} \gamma[Y(\eta), Z(\eta)]\, d\eta \tag{21}$$

with $\eta_0 = R/w_1$. This integration is easily performed on a modern PC with standard programs. We obtain the two parameters w_1 and a from the equilibrium conditions

$$\mathbf{b}\tilde{H}\mathbf{b} = E_A(w_1, a) \tag{22a}$$

$$\frac{2H_{13}b_1b_3}{1+a} + \frac{H_{33}b_3^2}{a} + \frac{\partial E_A(w_1, a)}{\partial a} = 0. \tag{22b}$$

Here again $\partial E_A/\partial a$ can easily be obtained by performing the differentiation analytically before the numerical integration.

Figure 4 shows the contour plot of the γ-surface of the interplanar potential for a simple cubic lattice with $g = 0.03$ and $h = 0.06$. Whereas for pure edge and pure screw dislocations the displacement is always along a $\langle 001 \rangle$ direction, a deviation exists for $\varphi \neq 0, \pi/2$. The magnitude of the deviation depends on the ratio H_{11}/H_{33} which, for instance, for Cu and Au can come close to 2. The corresponding displacement path for a $\varphi = 45°$ dislocation (with $\psi = \varphi$) is plotted in Fig. 4, which shows that the displacement does not necessarily follow the path of lowest energy in the γ-surface. Though the deviation is clearly marked, the resulting reduction in line energy is small [9], in our case about 1.5%. Deviations may, however, become important for dislocation emission from crack tips [18] when, depending on the type of loading, one of the components is acted upon by a high stress concentration.

5. THE DISSOCIATION

Depending on the profile of the γ-surface, a dislocation can lower its energy by dissociating into a set of partial dislocations. A recent discussion of the various possibilities in various crystal structures has been given by Vitek *et al.* [19]. The best-known dissociation occurs in the (111) plane of an f.c.c. lattice where an $a/2[\bar{1}10]$ dislocation dissociates into two Shockley partials of the type $a/6\langle 211 \rangle$ connected by a stacking fault. This configuration has been studied extensively in the Peierls model [9, 13]. Whereas for singular dislocations the dissociation will

always occur, the treatment in the Peierls model shows that it will only take place when the stacking fault energy is below a critical value.

A generalized splitting of dislocations by a set of discrete singular partial dislocations was discussed by Vitek and Kroupa [20]. We consider here the question of whether in the (110) plane of a b.c.c. lattice a Peierls dislocation of the type $\mathbf{B} = a[001]$ will dissociate according to the reaction $a[001] \Rightarrow a/2[\bar{1}11] + a/2[1\bar{1}1]$ or $\mathbf{B} = \mathbf{b}_1 + \mathbf{b}_2$ into two unit dislocations $\mathbf{b}_1$ and $\mathbf{b}_2$ of Peierls type. According to the energy balance of singular dislocations, **B** will always be stable. As we will find, however, depending on the character of the interplanar potential a dissociation can take place and hence restrict the mobility of **B** onto (110) planes.

The effect will be most pronounced when the **B** dislocation is of edge type along $[1\bar{1}0]$ and we will consider this situation. The coordinate system (y, z) in the lattice and the various components are defined in Fig. 5. When we assume that in the dislocation frame $\mathbf{b}_1 = (q_1, 0, p_1)$ and $\mathbf{b}_2 = (q_1, 0, -p_1)$ are two Peierls dislocations separated by d, the components (Y, Z) of the displacement vector in the lattice frame are given by

$$Y = \frac{p_1}{\pi}\left(\operatorname{arctg}\frac{x}{w} - \operatorname{arctg}\frac{x-d}{w}\right) \tag{23a}$$

$$Z = \frac{q_1}{\pi}\left(\operatorname{arctg}\frac{x}{w} + \operatorname{arctg}\frac{x-d}{w}\right) + \frac{q_1}{2} \tag{23b}$$

where x is the coordinate perpendicular to the dislocation line.

The corresponding elastic energy is [9]

$$E_{el} = \mathbf{B}\tilde{H}\mathbf{B}\ln\frac{R}{2w} - \mathbf{b}_1\tilde{H}\mathbf{b}_2\ln\left(1 + \frac{d^2}{4w^2}\right). \tag{24}$$

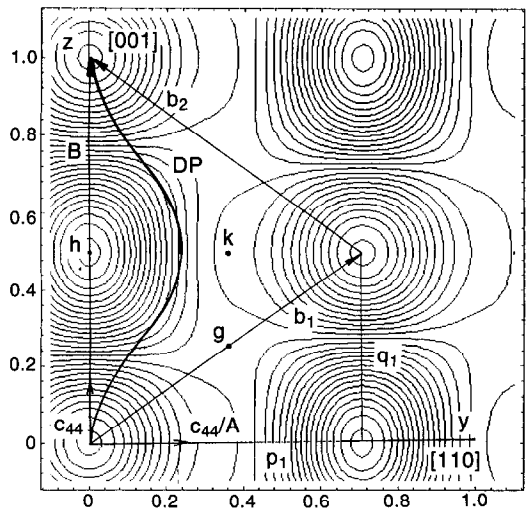

Fig. 5. Displacement path DP of a $\mathbf{B} = a[001]$ dislocation in a (110) plane of a b.c.c. lattice. The values g, h, k, c_{44} and A are fitted for Mo (see text).

We note that in a cubic lattice for a dislocation line in a $\langle 110\rangle$ direction there is no interaction between edge and screw component since $H_{13} = 0$. This will simplify the treatment, but here we do not explicitly decompose the elastic terms into their components.

With the displacement vector $\mathbf{u} = (Y, Z)$ in the (110) plane and using first and second order reciprocal lattice vectors, we have six Fourier terms and can therefore fit the two elastic constants c_{44} and $(c_{11} - c_{12})/2 = c_{44}/A$ where A is Zener's anisotropy ratio. We further fit $\gamma(0, 0) = 0$, $\gamma(0, a/2) = hc_{44}b$, $\gamma(a\sqrt{2}/4, a/4) = gc_{44}b$ and $\gamma(a\sqrt{2}/4, a/2) = kc_{44}b$ (see Fig. 5). The resulting potential becomes

$$\begin{aligned}\gamma(Y, Z) = c_{44}b\Bigg\{&c_0 + c_1\cos\frac{4\pi Y}{a\sqrt{2}} + c_2\cos\frac{4\pi Z}{a} \\ &+ c_3\left[\cos\frac{2\pi}{\alpha}\left(\frac{Y}{\sqrt{2}} + Z\right) + \cos\frac{2\pi}{a}\right. \\ &\left.\times\left(\frac{Y}{\sqrt{2}} - Z\right)\right] + c_4\left[\cos\frac{4\pi}{a}\left(\frac{Y}{\sqrt{2}} + Z\right)\right. \\ &\left.+ \cos\frac{4\pi}{a}\left(\frac{Y}{\sqrt{2}} - Z\right)\right] + c_5\left[\cos\frac{2\pi}{a}\right. \\ &\left.\times\left(\frac{3Y}{\sqrt{2}} + Z\right) + \cos\frac{2\pi}{a}\left(\frac{3Y}{\sqrt{2}} - Z\right)\right]\Bigg\}\end{aligned} \tag{25}$$

and with $p = 2\sqrt{2/3}$ we have

$$\begin{aligned}c_0 &= g/4 + 3h/16 + k/4 + p/(32\pi^2) \\ c_1 &= -g/4 + 3h/16 - k/4 + p/(32\pi^2) \\ c_2 &= -g/4 + h/16 + k/4 - p/(32\pi^2) \\ c_3 &= -7h/16 - k/8 + p/(32A\pi^2) \\ c_4 &= g/8 + h/32 - k/8 - p/(64\pi^2) \\ c_5 &= -h/32 + k/8 - p/(32A\pi^2).\end{aligned} \tag{26}$$

In Fig. 5 we show the contours of the Fourier plot of γ fitted for Mo using the results of Vitek, Cserti and Duesbery (unpublished) from which we obtained $g = 0.033$, $h = 0.078$, $k = 0.031$, using $A = 0.91$ and $c_{44} = 121.7$ GPa. The configuration of minimum energy is obtained for a separation of $d \approx 0.9$ with $w \approx 0.7$. The resulting displacement path is also shown in Fig. 5. This result should, however, be considered with caution since it is valid only for this specific situation. The displacement path crosses the γ surface between the points h and k and hence variations in the misfit energy in this region might considerably influence the final configuration.

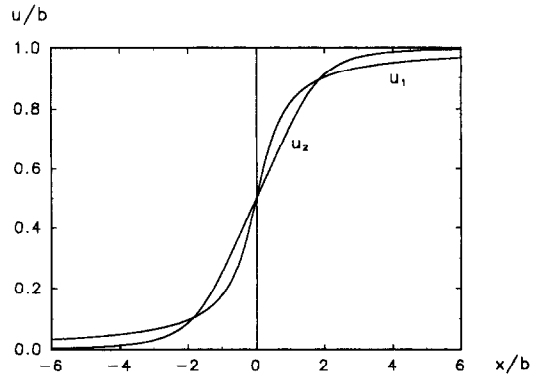

Fig. 6. Displacement $\mathbf{u}_1$ of a Peierls dislocation and $\mathbf{u}_2$ of a narrower dislocation corresponding to the lowest energy for an interplanar potential with $g = 0.03$.

6. THE GENERAL DISLOCATION CORE

The arctg type trial function for the displacement of a Peierls dislocation is very widespread and extends to infinity where it approaches the final value as $1/r$. The question may be asked as to whether for stiff potentials a trial function for the variational problem with a more narrow spread may lead to a lower energy. In the literature displacements have actually been proposed which can be described by a bounded distribution of infinitesimal dislocations [7, 21]. We have therefore studied various distributions of infinitesimal dislocations of the type

$$\rho(x) = \frac{\mathrm{d}u}{\mathrm{d}x} = \frac{p_n}{w^{2n} + x^{2n}} b. \tag{27}$$

For $n = 1$ and $p_1 = w$ we have the dislocation density $\rho(x)$ described by a Lorentz peak which in turn leads by integration to the displacement u_1 of a Peierls dislocation described by equation (2).

For $n = 2$ the displacements become narrower and we find that with $p_2 = w^3\sqrt{2}/\pi$:

$$u_2(x) = \frac{b}{2\pi}\left(\operatorname{arctg}\left(1 + \frac{\sqrt{2}x}{w}\right) - \operatorname{arctg}\left(1 - \frac{\sqrt{2}x}{w}\right)\right) + \frac{b}{4\pi}\ln\frac{w^2 + \sqrt{2}wx + x^2}{w^2 - \sqrt{2}w + x^2} + \frac{b}{2}. \tag{28}$$

This seemingly rather complicated expression leads to the simple shape u_2 shown in Fig. 6 together with u_1 corresponding to the Peierls dislocation. As we see, u_2 approaches the limiting values $\pm b/2$ much more rapidly and for $n \to \infty$ would result in the "standard core" [7].

The elastic stress resulting from this distribution $\rho(x)$ can be easily obtained from equation (3a):

$$\sigma_2(x) = 2\tilde{H}b\frac{x^3 + xw^2}{w^4 + x^4}. \tag{29}$$

Using equations (4) and (5) we can calculate the resulting elastic energy EL_2 and atomistic misfit energy EA_2 in a cubic primitive lattice. In analogy to equation (9a), the corresponding equilibrium width $\tilde{w}_2$ is obtained as

$$\tilde{w}_2(g, \varphi) = \frac{\hat{E}(\varphi)}{\mu_0 b^2(0.0184 + 0.8587g)}. \tag{30}$$

In Fig. 7 we have plotted the resulting line energy $E_2 = EL_2 + EA_2$ for the displacement u_2 for screw orientation and for comparison the line energy E_L of equation (11) for the Peierls dislocation. We see that over the total range of stiffness $0.03 \leqslant g \leqslant 0.09$ of the potential, the displacement u_2 leads to in a higher dislocation energy. This result justifies our assumption that the simple Peierls dislocation described by the arctg like displacement of equation (2) may be an adequate trial function even in more complex situations.

We finally consider the general situation where a dislocation of Burgers vector $\mathbf{B}$ splits into a planar set of partial dislocations of Burgers vector $\mathbf{b}_i$ and width w_i situated at $x = d_i$. The total displacement is described by

$$\mathbf{u}(x) = \sum_i \frac{\mathbf{b}_i}{\pi}\operatorname{arctg}\frac{x - d_i}{w_i} + \frac{\mathbf{B}}{2} \tag{31}$$

where with $\mathbf{B} = \Sigma\,\mathbf{b}_i$ the last term ensures the boundary conditions $\mathbf{u}(-\infty) = 0$ and $\mathbf{u}(\infty) = \mathbf{B}$. The elastic energy of this set is given by

$$E_{\mathrm{el}} = \sum_i \mathbf{b}_i\tilde{H}\mathbf{b}_i \ln\frac{R}{2w_i} + 2\sum_{i<k}\mathbf{b}_i\tilde{H}\mathbf{b}_k \ln\frac{R}{w_i + w_k} - \sum_{i<k}\mathbf{b}_i\tilde{H}\mathbf{b}_k \ln\left(1 + \frac{(d_i - d_k)^2}{(w_i + w_k)^2}\right). \tag{32a}$$

By choosing some average dislocation width w_0 and setting $w_i = a_i w_0$ and $\delta_i = d_i/w_0$, this can be transformed into

$$E_{\mathrm{el}} = \mathbf{B}\tilde{H}\mathbf{B} \ln\frac{R}{2w_0} + \sum_i \mathbf{b}_i\tilde{H}\mathbf{b}_i \ln\frac{1}{a_i} + 2\sum_{i<k}\mathbf{b}_i\tilde{H}\mathbf{b}_k$$

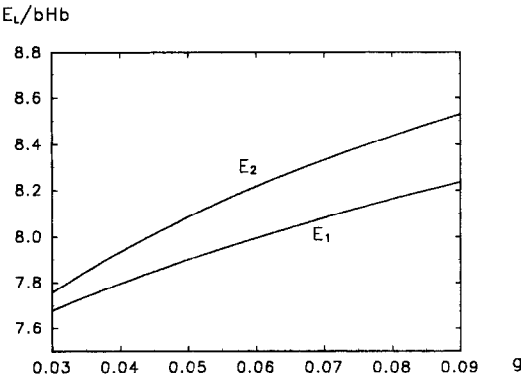

Fig. 7. Line energy (with $R = 10^3 b$) for a Peierls dislocation E_1 and a narrower dislocation E_2 as function of stiffness g of interplanar potential.

$$\times \ln \frac{2}{a_i + a_k} - \sum_{i<k} \mathbf{b}_i \tilde{H} \mathbf{b}_k \ln\left(1 + \frac{(\delta_i - \delta_k)^2}{(a_i + a_k)^2}\right). \quad (32b)$$

Introducing $\eta = x/w_0$ and $\eta_0 = R/w_0$, we obtain the atomistic energy as

$$E_A = w_0 \int_{-\eta_0}^{+\eta_0} \gamma[\mathbf{u}(\eta)]\, d\eta. \quad (33)$$

In the equilibrium configuration (i.e. the configuration of lowest energy), E_A for $\eta_0 \to \infty$ reaches a constant value

$$E_A(\delta_i, \delta_k, a_i, a_k) = \mathbf{B}\tilde{H}\mathbf{B} \quad (34)$$

which relates the equilibrium positions $\bar{d}_i$ and equilibrium widths $\bar{w}_i$ to the properties of the γ-surface.

7. DISCUSSION

From a more fundamental point of view the structure of the dislocation core can be obtained as the solution of a variational problem. The total energy of a dislocation with a planar extension in an anisotropic medium can be expressed as [9]

$$E(\mathbf{u}) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{\partial \mathbf{u}(s)}{\partial s} \frac{\tilde{H}}{x - s} \mathbf{u}(x)\, ds\, dx + \int_{-R}^{+R} \gamma[\mathbf{u}(x)]\, dx \quad (35)$$

where $\mathbf{u}$ is the relative displacement vector across the glide plane. Considering E as a functional of the unknown $\mathbf{u}$, we can obtain $\mathbf{u}$ from the condition that $E(\mathbf{u})$ must be a minimum. The Euler equation of the corresponding variational problem leads to

$$2\tilde{H} \int_{-\infty}^{+\infty} \frac{\partial \mathbf{u}}{\partial s} \frac{1}{x - s}\, ds + \operatorname{grad}_u \gamma(\mathbf{u}) = 0 \quad (36)$$

which is the Peierls–Nabarro differential equation.

Physically it corresponds to the condition that the elastic forces in the glide plane are balanced by the atomic interaction across the glide plane. Note that equation (36) has vector form and we have a set of two coupled integro-differential equations for the two components in the glide plane. We note here that in the literature practically all treatments of the core structure with the aid of the Peierls equation are one dimensional and either consider the edge or the screw component to be isolated [22, 23] or consider a constrained path approximation [24].

The only known solution of the Peierls equation results from a simple sinusoidal potential and leads to the Peierls dislocation. Instead of trying to solve the Peierls equation for more complex potentials by numerical methods we might as well solve the variational problem by the Ritz method. The first use of this method was made by Leibfried and Dietze [25] and Seeger and Schoeck [13]. Here an appropriate trial function is assumed with adjustable geometrical parameters which are determined by minimizing the energy. Since the Peierls dislocation as a trial function is at least the solution for one special potential, and since we have shown that displacement shapes that are narrower than the arctg type lead to higher energies, we can expect that the minimum obtained by the superposition of Peierls dislocations is close to the absolute minimum. Due to the existence of this minimum, small deviations in the exact shape will not influence the energy very much.

In our treatment we have assumed that the displacement vector $\mathbf{u}$ is in the glide plane. The expression for the energy in equation (35), however, also allows displacements u_2 perpendicular to the glide plane, which of course will be localized close to the core. If the dependence of γ on these displacements were known, such modifications could be included in the variational calculations.

In replacing the singular Volterra dislocation by a Peierls dislocation with an arctg type displacement we are able to describe the dislocation core more realistically and give an absolute value for the dislocation energy which includes the atomistic energy in the glide plane. In a simple cubic lattice with shear modulus μ_0 and maximum stacking energy γ_0, the width of the dislocation in equilibrium is given by

$$\bar{w} = \mathbf{b}\tilde{H}\mathbf{b}/(0.0796\mu_0 b + 1.571\gamma_0). \quad (37)$$

Of fundamental importance is the fact that in an otherwise linear elastic solid the atomic misfit energy of a dislocation of arbitrary shape with total Burgers vector $\mathbf{B}$ in equilibrium has a constant value $E_A = \mathbf{B}\tilde{H}\mathbf{B}$. This is independent of the shape of the γ-surface and also independent of the number of geometrical parameters used to describe the dislocation [10]. The interplanar potential only influences the elastic energy of the dislocation by modifying the shape of the core but not its energy.

For more complex γ-surface the dislocation can lower its energy by dissociation or deviation. This can be described by a set of partial Peierls dislocations. In a deviation which can occur in dislocations of mixed type the displacement vector does not follow the path of the crystallographic Burgers vector even when this lies along an energy trough of the γ-surface. Since the specific elastic energy of the edge component is larger than that of the screw component, it will have a wider core and hence the two components no longer increase proportionally to each other. The reduction in energy obtained by a deviation is usually small, but it may be important for the emission of dislocations from the crack tip when one of the components is acted upon by a high stress concentration [18].

The best starting point when considering a possible dissociation of $\mathbf{B}$ is to inspect the γ-surface in relation to the position and height of the minima, maxima,

and saddle points. Here even the direction and magnitude of the fractional dislocation can be subjected to a variational treatment. In this case the procedure to find the configuration of lowest energy will become more complex. Nevertheless, the advantage of a treatment on the energy level is especially apparent here. For the overall shape it is essentially the position and height of these extrema that controls the configuration of the core. The local gradient which is the starting point for a treatment on the force level is the derivative of the γ-function for which even the exact position and the exact values of these extrema are somewhat uncertain. In addition, on the energy level mixed dislocations are easily described, whereas on the force level we have to assume either a constrained displacement path unless we consider the two force components which lead to two coupled integral equations.

The other method of obtaining the core structure of dislocation is by atomic simulation, which has now reached a certain level of standardization [26]. However, we believe that our method, at least at present, is potentially more powerful than these simulations when planar spreading is observed. One condition is that the γ-surface for the corresponding lattice plane has been determined from atomistic considerations. The essential features of γ may then be represented analytically by a Fourier series with the aid of the reciprocal lattice vectors [9] where the coefficients depend on these values. It is then possible to study the influence of the elastic constants on the one hand and the influence of the atomic misfit on the other hand independently of each other. It is, for instance, well known that small amounts of alloying elements may drastically change the stacking fault energy with only a very minor influence on the elastic constants. This problem can easily be handled with the variational method but eludes a treatment by atomic simulation—at least at present.

The outcome of the atomic simulation depends on the interatomic potential used [26]. Since these potentials are derived from equilibrium configurations there is considerable uncertainty as to whether they can be used for configurations far from equilibrium. There are some geometric features that are not very sensitive to the choice of the potentials, but the value obtained for the energy of a dislocated configuration and comparison between different configurations based on atomic simulations is extremely uncertain. For instance, even for the simple configuration of an unbounded stacking fault in the (111) plane of a f.c.c. lattice the EAM method grossly underestimates the value of γ_{st} [27]. In some cases even the position of the minima in the γ-surface depends on the choice of the potential (for a review see Ref. [19]). Hopefully, *ab initio* calculations based on density functional theory will become more readily available [28, 29].

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