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The Peierls–Nabarro model and the mobility of the dislocation line

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ABSTRACT

Within the framework of the Peierls–Nabarro model we present an analytical model for several of the quantities characterizing the mobility of a dislocation line, which covers the whole range of possible values of dislocation width. These quantities include the first-order Peierls stress σ_{1P} (the minimum stress required to move a straight segment of dislocation), the kink profile, the kink pair activation energy H_{kp} and the second-order Peierls stress σ_{2P} (the minimum stress required to move a kink in the dislocation line). These quantities are expressed in terms of fundamental properties of the material, and in particular the relevant generalized stacking-fault surface segment.

§1. INTRODUCTION

The dislocation is a topological line defect which winds its way through the lattice. The singularity in the displacement field that it creates affects the crystal on several length scales in quite a unique way. The study of this defect has therefore to be approached in a number of ways. To gain insight into its varied behaviour it is helpful, in our mind, to have an analytical link between its properties and the fundamental properties of the material. The Peierls (1940)–Nabarro (1947) (PN) model still offers probably the only possible starting point. The insight that this model can provide to dislocation properties has recently been investigated by a number of workers, in particular as to its predictions concerning the core structure, with some degree of success (Joós *et al.* 1994, 1996, Ren *et al.* 1995, 1996, Joós and Duesbery 1997a, Bulatov and Kaxiras 1997, Schoeck 1998, 1999a,b, Ngan 1999). In this paper we explore within the framework of the same model the properties of the kinks. The physical picture that forms the basis of the study is that of a dislocation line acting as an elastic string in a periodic potential (Dorn and Rajnak 1964, Guyot and Dorn 1967).

The model in its present form is obviously limited to dislocations with planar cores, a basic assumption of the PN model. The PN model is however, not in principle limited to planar cores as discussed by Ngan (1999).

The appeal of this formalism is the relatively simple direct link that it provides between the generalized stacking-fault (GSF) surface and the properties of the dislocation line. The formalism is not limited to wide dislocations and their

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corresponding wide kinks but extends to narrow dislocations and kinks. It may serve as a basis for a phenomenological theory of the motion of the dislocation line by focusing on the interconnectiveness of the relevant basic quantities.

§ 2. The Peierls–Nabarro potential and the first-order Peierls stress

With the core assumed spread within a plane known as the glide plane (see figure 1), the equilibrium configuration within the core is obtained by balancing the elastic forces due to deformations in the upper and lower half-planes with the restoring forces at the interface leading to the well known integrodifferential equation. In this paper for simplicity we assume Volterra-type dislocations, that is displacements **f** along the Burgers vector direction **b**. Hence

$$\frac{K}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{y-y'}\frac{df_b(y')}{dy'}\,dy' = F_b(f_b(y)) = -\frac{\partial\gamma}{\partial \mathbf{f}}\cdot\mathbf{b}, \tag{1}$$

where y is the distance from the dislocation line. $\gamma(\mathbf{f})$ is the GSF energy surface. It is generated by cutting the crystal into two halves along the glide plane, displacing the top part with respect to the lower part by **f** and letting the atoms relax perpendicularly to the glide plane. It has been suggested a while ago (Vitek 1968, Christian and Vitek 1970) that the GSF surface would provide a better restoring force than the restoring force predicted by elasticity theory. Recent examples of GSF surfaces were given by Kaxiras and Duesbery (1993), Medvedeva *et al.* (1996), Hartford *et al.* (1998) and Mryasov *et al.* (1998).

With the further assumption that the appropriate cut in the GSF surface can be approximated by a sinusoidal function, the restoring force can be written as

$$F_b(f_b(y)) = \tau_{max}\sin\left(\frac{2\pi f_b(y)}{b}\right). \tag{2}$$

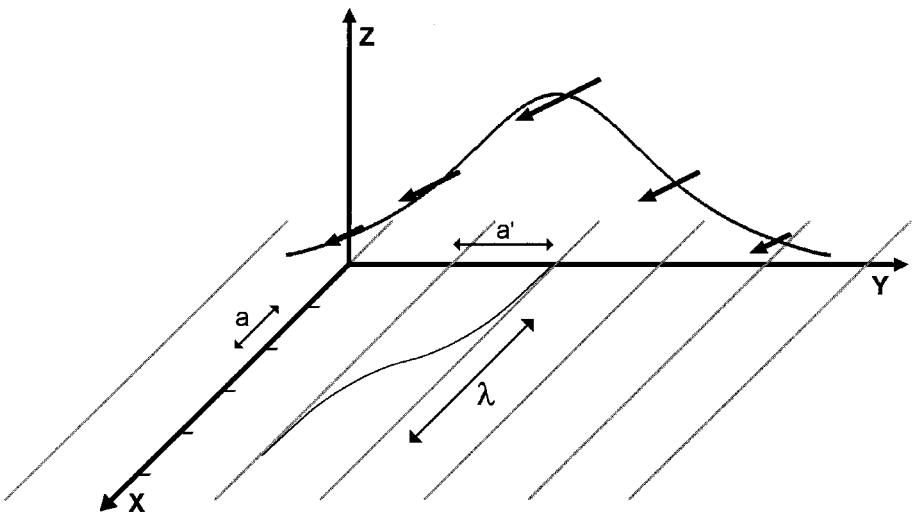

Figure 1. Schematic representation of a glide plane and a dislocation line. The x-y plane is the glide plane, the x axis a minimum-energy dislocation line, and the y axis the glide direction. A dislocation density profile $\partial\mathbf{f}/\partial y$ is shown assumed to be directed along a Burgers vector direction **b**, and a kink of width λ is profiled. The 'atomic plane' periodicities along the dislocation line and glide directions are a and a'.

One parameter determines the magnitude of the sinusoidal restoring force. Traditionally the elastic limit obtained with $f_b/b \ll 1$ has been used but, since the PN model is a model for the core structure, we find that it is more appropriate that F_b be properly represented for the large values of f_b; so the amplitude is being determined by the maximum value of $(\partial\gamma/\partial\mathbf{f})\cdot\mathbf{b}$, τ_{max}. This choice has a much better chance of giving realistic estimates of the core structure as discussed by Joós and Duesbery (1997a). b can be the Burgers vector magnitude for a full or partial dislocation. To satisfy both limits a more complex potential is required, at least two terms in the Fourier expansion of the restoring stress (Schoeck 1997).

The solution to equation (1) with the above approximation is

$$f_b(y) = \frac{b}{\pi}\tan^{-1}\left(\frac{y}{\zeta}\right) + \frac{b}{2}, \tag{3}$$

where $\zeta = Kb/4\pi\tau_{max}$ is the half-width of the dislocation. With a general restoring force, good solutions can be obtained with a linear combination of functions of the form (3) (Joós *et al*. 1994). ζ measures the relative strength of bulk and interface forces. K is equal to the shear modulus for screw dislocations and to $\mu/(1-\nu)$ for pure edge dislocations and takes on a range of intermediate values for other dislocations.

With a solution of the above form the potential barrier that a dislocation has to overcome to move by an atomic site per unit length is given by the potential (Joós and Duesbery 1997a):

$$\begin{aligned} W_{PN}(y) &= \sum_{m=-\infty}^{+\infty} \frac{Kb^2\alpha'}{4\pi^2}\frac{\zeta}{\zeta^2 + (ma' - y)^2} \\ &= \frac{Kb^2}{4\pi}\frac{\sinh(2\pi\zeta/a')}{\cosh(2\pi\zeta/a') - \cos(2\pi y/a')}. \end{aligned} \tag{4}$$

The minimum in $W_{PN}(y)$ is equal to

$$W_{PN}\left(\frac{a'}{2}\right) = \frac{Kb^2}{4\pi}\frac{\sinh(2\pi\zeta/a')}{\cosh(2\pi\zeta/a') + 1}. \tag{5}$$

This is the core energy within the PN model. Rewriting $W_{PN}(y)$ so that the minimum is zero and located at $y = 0$, we obtain

$$W'_{PN}(y) = \frac{W'_0}{4}\frac{1 - \cos(2\pi y/a')}{\cosh(2\pi\zeta/a') + \cos(2\pi y/a')}, \tag{6}$$

where $W'_0 = 4E_{PN}(a'/2)$. The amplitude of this periodic potential is not W'_0 but what we call the PN potential barrier:

$$W_P = \frac{Kb^2}{2\pi}\frac{1}{\sinh(2\pi\zeta/a')}. \tag{7}$$

The periodic part of W_{PN} evolves from a sinusoid to a series of equally spaced δ functions as ζ/a' narrows. In the limit $\zeta/a' > 1$, W'_{PN} is well represented by

$$W'_{PN}(y) = \frac{W_0}{2}\left[1 - \cos\left(\frac{2\pi y}{a'}\right)\right], \tag{8}$$

where $W_0 = (Kb^2/\pi)\exp(-2\pi\zeta/a')$. In the opposite limit $\zeta/a' \to 0$,

$$W'_{PN}(y) = \frac{Kb^2 a'}{4\pi}\,\delta\left(y - \frac{a'}{2}\right). \tag{9}$$

To obtain the Peierls stress (PS), the minimum stress required to move a straight segment of dislocation over the potential barrier, we first have to compute the stress associated with the misfit energy variation:

$$\begin{aligned}\sigma(y) &= -\frac{1}{b}\frac{dW_{PN}}{dy} \\ &= \frac{Kb}{2a'}\frac{\sinh(2\pi\zeta/a')\sin(2\pi y/a')}{[\cosh(2\pi\zeta/a') - \cos(2\pi y/a')]^2}.\end{aligned} \tag{10}$$

Maximizing this quantity yields the PS

$$\sigma_P = \sigma(y_M),$$

where

$$y_m = \frac{a'}{2\pi}\cos^{-1}\left(\frac{1}{2}\left\{-\cosh\left(\frac{2\pi\zeta}{a'}\right) + \left[8 + \cosh^2\left(\frac{2\pi\zeta}{a'}\right)\right]^{1/2}\right\}\right). \tag{11}$$

In the range $\zeta/a' < 0.2$, σ_P is well represented by

$$\sigma_P = \frac{3\sqrt{3}}{8}\frac{Kb}{a'}\left(\frac{a'}{2\pi\zeta}\right)^2 \tag{12}$$

and for $\zeta/a' > 0.2$ by the expression

$$\sigma_P = \frac{Kb}{a'}\exp\left(-\frac{2\pi\zeta}{a'}\right)\left[1 + 5\exp\left(-\frac{4\pi\zeta}{a'}\right)\right]. \tag{13}$$

These are the first two terms in the expansion of σ_P in terms of $\exp(-2\pi\zeta/a')$. When $\zeta/a' > 0.5$, this reduces to the well known expression

$$\sigma_P = \frac{Kb}{a'}\exp\left(-\frac{2\pi\zeta}{a'}\right). \tag{14}$$

This model assumes a rigid translation of the dislocation as it moves in the lattice. It is a simplified model and here are a few factors that can affect these results; relaxation of the profile, atomic scale averaging due to the distribution of the electronic cloud around each atom, and departure of the misfit vector **f** from the direction of **b**. Schoeck considered all these effects. Concerning the first, the relaxation seems noticeable but a cancellation effect between the elastic and misfit contributions means that σ_P is not significantly affected (Schoeck 1999a). The averaging due to the spread of the electronic cloud could lower σ_P considerably (Schoeck 1999b). Finally for simple dislocations the displacement does seem to be dominantly along **b**, although rigorously so only for pure edge or pure screw dislocations (Schoeck 1998). What the two-dimensional PN model allows is the study of dissociation processes (Mryasov *et al.* 1998). This model leads to coupled differential equations which have no simple solutions. Equations (12) an (14) have been shown to be good approximants for existing full and partial dislocations in Si and some metals with simple profiles (Joós and Duesbery 1997a). Equation (13) has not been published previously.

§ 3. Kinks

In materials with significant PS, dislocations at finite temperatures do not move by rigid translation, but rather by the nucleation and propagation of kink pairs. A kink pair is created when part of the dislocation line is activated to a neighbouring low-energy channel (see figure 1) over the PN energy barrier W_{PN}. As is well known (Hirth and Lothe 1982), the kink pair mechanism for dislocation motion admits two limiting cases. At high stresses, the rate-controlling mechanism is the nucleation of kink pairs. At low stresses, the periodic potential through which an individual kink must move may be large enough to control the process; this is referred to as the kink migration regime and its resistive stress at 0 K is commonly termed the second-order Peierls stress σ_{2P}.

If we view the dislocation line as a string, its energy, for a shape $y(x)$, is simply given at each location within the PN potential by

$$\Gamma(y) = \Gamma_0 + W'_{PN}[y(x)]. \tag{15}$$

Γ_0 is the dislocation line energy and $W'_{PN}(y)$, the potential barrier that the kink has to overcome, has been defined above (see equation (6)).

Γ_0 is dominantly elastic in origin:

$$\Gamma_0 = \frac{Kb^2}{4\pi} \ln\left(\frac{R}{b}\right) = \eta \frac{Kb^2}{4\pi}. \tag{16}$$

R depends on the screening length of the interactions in the material. We define a constant $\eta = \ln(R/b)$ to characterize the screening. Conventionally, for metals with significant screening, η is taken to be $\frac{1}{2}$ whereas, for semiconductors where there is less screening, a value of 1 is used. There is obviously a great deal of uncertainty in this quantity. It is not clear either what contribution the core energy makes to Γ_0. Within the PN model, the core contribution equals $W_{PN}(a'/2)$ (see equation (5)).

The Hamiltonian of a kink can be written as the excess energy resulting from the departure of the dislocation line from its minimum-energy configuration:

$$H = \int_{-\infty}^{\infty} \left\{ \Gamma(y) \left[1 + \left(\frac{dy}{dx}\right)^2 \right]^{1/2} - \Gamma_0 \right\} dx, \tag{17}$$

where y_0 is the equilibrium position of the dislocation. Assuming $(dy/dx)^2$ much smaller than one leads to the simpler form known as the Frenkel–Kontorowa (FK) Hamiltonian when W_{PN} is sinusoidal:

$$H = \int_{-\infty}^{\infty} \left[\frac{1}{2} \Gamma_0 \left(\frac{dy}{dx}\right)^2 + W'_{PN}(y) \right] dx. \tag{18}$$

This is the approximation considered by Joós and Duesbery (1997b). We shall actually solve equation (17). Using Euler's equation, the functional $H(y, x'; y)$ in equation (17) is minimized when

$$1 + \left(\frac{dy}{dx}\right)^2 = \left(\frac{\Gamma(y)}{\Gamma_0}\right)^2. \tag{19}$$

The minimum value of the functional $H(y, y'; x)$ is then

$$H = \frac{1}{\Gamma_0} \int_{-\infty}^{\infty} [\Gamma(y)^2 - \Gamma_0^2]\, dx$$
$$= \Gamma_0 \int_{-\infty}^{\infty} \left(\frac{dy}{dx}\right)^2 dx. \tag{20}$$

For a simple kink, y can be chosen to increase monotonically from 0 to a', so that $dy/dx > 0$ and H can be rewritten entirely in terms of y as

$$H = \int_{y_0}^{y_0 + a'} [\Gamma(y)^2 - \Gamma_0^2]^{1/2}\, dy$$
$$= \Gamma \int_{y_0}^{y_0 + a'} \left(\frac{dy}{dx}\right) dy$$
$$= \frac{\Gamma_0 a'^2}{a} \int_0^1 \frac{d\theta}{dn}\, d\theta, \tag{21}$$

where θ and n are the dimensionless units y/a' and x/a respectively. To obtain the activation energy of a kink pair, one considers the growth of a bulge for which y increases monotonically from a minimum value y_0 to a maximum y_m and then decreases back to the minimum. In the absence of stress its energy is simply twice the kink energy, since y_m, the value at which the integrand above becomes imaginary, is y_0.

Equation (21) shows that the key quantity is $d\theta/dn$ defined by equation (19). It gives the kink profile. Using the PN potential in the expression for the dislocation line energy equation (15), $d\theta/dn$ is given in the dimensionless units by

$$\frac{d\theta}{dn} = \frac{1}{\lambda} \frac{\sin(\pi\theta)}{1 - m \sin^2(\pi\theta)} [1 - (m - g^2) \sin^2(\pi\theta)]^{1/2}, \tag{22}$$

where we have defined a number of quantities: $r = a'/a$ is the ratio of the periodicities in the atomic planes along the dislocation line and perpendicular to it, $\lambda^2 = \Gamma_0 a'^2 [\cosh(2\pi\zeta/a') + 1]/W_0' a^2$, $m = 2/[\cosh(2\pi\zeta/a') + 1]$ and $g = r/2\lambda$. The most important of these quantities is λ related to the kink width. It can be written, in terms of the screening factor η (defined in equation (16)) as

$$\lambda = \eta^{1/2} \frac{r}{2} \frac{\cosh(2\pi\zeta/a') + 1}{[\sinh(2\pi\zeta/a')]^{1/2}}. \tag{23}$$

Equation (22) serves as the starting point for three approximations or models.

(i) *Model A*. In this model, both m and g are assumed to be negligible. This is the approximation made in the FK model. It is the wide-kink limit.

(ii) *Model B*. In this model, m is neglected, but g is kept. This is what is obtained when solving the full Hamiltonian given by equation (17) with a sinusoidal potential. It is very similar to model A except that it does not assume that $[1 + (dy/dy)^2]^{1/2}$ can be replaced by $1 + \frac{1}{2}(dy/dx)^2$.

(iii) *Model C*. This model uses the full form in equation (22) with the PN potential (20).

We shall now see what properties for the kinks they each predict.

3.1. *Kink width*

Solving for θ as a function of n in equation (22) would yield the kink solutions. A simple kink solution as sketched in figure 1 is obtained for instance with a solution with the boundary conditions $\theta = 0$ at $n = -\infty$, and $\theta = 1$ at $n = \infty$, and by symmetry at $n = 0$, $\theta = \frac{1}{2}$.

Before considering the specific form of the profile, we can easily calculate a width for the kink. A convenient definition of the kink width is

$$w = \left(\frac{d\theta}{dn}\right)^{-1}_{\theta=1/2}. \tag{24}$$

$dn/d\theta$ measured in the middle of the kink gives the maximum slope in the kink profile. The straight line defined by that slope and passing at the centre of the kink cuts the nearest-neighbour potential wells in which the asymptotic parts of the dislocation line lie at points apart by $wa\,\Delta\theta$ sites. Since $\Delta\theta = 1$, $dn/d\theta$ is the width in number of sites.

In the limit $\zeta > a'$ (model A), $m \to 0$, $g \to 0$, this is equal to λ, which itself tends to

$$w = \lambda \approx \frac{r}{2}\left(\frac{\eta}{2}\right)^{1/2} \exp\left(\frac{\pi\zeta}{A}\right). \tag{25}$$

We see the exponential growth of the kink width with ζ.

Model B, which more rigorously takes into account the change in length of the dislocation as the kink is created, yields a narrowed width

$$w = \frac{\lambda}{(1+g^2)^{1/2}}. \tag{26}$$

Model C, which replaces the sinusoidal potential in model B by the full PN potential predicts a width

$$w = \lambda\,\frac{1-m}{(1-m+g^2)^{1/2}}. \tag{27}$$

Model C is the only model which allows investigation of kinks in narrow dislocations. In the limit $\zeta \to 0$,

$$w \to \pi\eta r\left(\frac{\zeta}{a'}\right) = \frac{\pi\eta\zeta}{a}, \tag{28}$$

an approximate form surprisingly valid up to $\zeta/a' = 0.5$ for $\eta \approx 1$.

3.2. *Kink profile*

The kink profile for model A is the well known sine–Gordon soliton. Equation (22) with $m = g = 0$ is

$$\frac{d\theta}{\sin(\pi\theta)} = \frac{dn}{\lambda}. \tag{29}$$

Integrated it yields the single-kink solution usually written as

$$\theta = \frac{1}{\pi}\cos^{-1}\left[\tanh\left(\frac{\pi n}{\lambda}\right)\right]. \tag{30}$$

Alternative forms are

$$\theta = \frac{2}{\pi}\tan^{-1}\left[\exp\left(\frac{\pi n}{\lambda}\right)\right] = \frac{1}{\pi}\sin^{-1}\left[\operatorname{sech}\left(\frac{\pi n}{\lambda}\right)\right]. \tag{31}$$

Model B yields a form very similar to the last above

$$\theta = \frac{1}{\pi}\sin^{-1}\left(\frac{1}{\cosh^2(\pi n/\lambda) + g^2\sinh^2(\pi n/\lambda)}\right)^{1/2}. \tag{32}$$

The expression for the profile of the kink in model C is considerably more involved but n as a function of θ can be expressed in terms of elementary functions, transcendental and algebraic.

As ζ/a' approaches 0, θ becomes a step function. For all values of θ except $\frac{1}{2}$, $d\theta/dn$ is zero.

3.3. *Kink energy and kink pair activation energy*

In the absence of stress, which is the situation discussed here, the kink-pair activation energy E_{kp} is simply twice the single-kink energy E_k since the maximum value of the bulge reaches the next minimum-energy Peierls valley.

We shall use the reduced units $\Gamma_0 a'^2/a$ in the derivations distinguishing the energies with a prime. So, using equations (21) and (22), the kink energy $E_k = E_k'(\Gamma_0 a'^2/a)$ is given by

$$E_k' = \frac{1}{\lambda}\int_0^1 \frac{\sin(\pi\theta)}{1 - m\sin^2(\pi\theta)}\left[1 - (m - g^2)\sin^2(\pi\theta)\right]^{1/2} d\theta. \tag{33}$$

Model A has the trivial well known value of the FK model (Joós 1982, Joós and Duesbery 1997b):

$$E_k' = \frac{1}{\lambda}\int_0^1 \sin(\pi\theta)\, d\theta = \frac{2}{\pi\lambda}. \tag{34}$$

Model B introduces the effect of $r = a'/a$. In model A, it is as if the distance between neighbouring PN potential wells a' is zero:

$$E_k' = \frac{1}{\lambda}\int_0^1 \sin(\pi\theta)\left[1 + g^2\sin^2(\pi\theta)\right]^{1/2} d\theta, \tag{35}$$

which with the change in variable $u = \cos(\pi\theta)$ gives

$$E_k' = \frac{1}{\pi\lambda}\int_{-1}^1 du\left[(1 + g^2) - g^2u^2\right]^{1/2}. \tag{36}$$

This integral is equal to

$$E_k' = \frac{1}{\lambda\pi}\left(1 + (1 + g^2)\frac{\tan^{-1} g}{g}\right). \tag{37}$$

This case has been considered by Dorn and Rajnak (1964) previously.

Model C yields

$$E_k' = \frac{2}{\lambda\pi}\frac{1}{m}\left[\frac{g}{(1-m)^{1/2}}\tan^{-1}\left(\frac{g}{(1-m)^{1/2}}\right) + (m-g^2)^{1/2}\tanh^{-1}[(m-g^2)^{1/2}]\right]. \tag{38}$$

We always have $m/g^2 > 2\eta$. Since we expect $\eta \geqslant \frac{1}{2}$, usually $m - g^2 > 0$, and hence the choice of $\tanh^{-1}$ in the above equation. In the limit $\zeta/a' \gg 1$, we recover the result of model A while, in the limit $\zeta/a' \to 0$, E_k' tends to

$$E_k' = \frac{1}{\eta r}. \tag{39}$$

The excess energy in the dislocation line due to the kink is therefore simply in this limit (for $\zeta/a' < 2a'$)

$$E_k = \frac{\Gamma_0 a'}{\eta} = \frac{Kb^2}{4\pi}a', \tag{40}$$

an additional average misfit energy corresponding to a length a'. Note that

$$\int_0^{a'} W_{PN}(y)\,dy = \frac{Kb^2}{4\pi}a'. \tag{41}$$

3.4. *Kink migration energy and stress*

To calculate the kink migration energy E_M, we start from the expression for the kink energy in equation (20):

$$H = \frac{\Gamma_0 a'^2}{a}\int_{-\infty}^{\infty}\left(\frac{d\theta}{dn}\right)^2 dn \tag{42}$$

and rewrite it using the solution for the profile θ. For model A ($g = 0$) and model B, and in units of $\Gamma_0 a'^2/a$, $H' = H/(\Gamma_0 a'^2/a)$, we have for the single-kink energy

$$H' = \frac{1+g^2}{\lambda^2}\int_{-\infty}^{\infty}\frac{\cosh^2(\pi n/\lambda)}{[\cosh^2(\pi n/\lambda) + g^2\sinh^2(\pi n/\lambda)]^2}\,dn. \tag{43}$$

Viewed as a string with a continuous mass the kink can be displaced in the lattice without any change in energy. To obtain the energy barrier to motion, the lattice periodicity has to be included. Equation (43) then becomes

$$H' = \frac{1+g^2}{\lambda^2}\sum_{n=-\infty}^{\infty}\frac{\cosh^2(\pi n/\lambda)}{[\cosh^2(\pi n/\lambda) + g^2\sinh^2(\pi n/\lambda)]^2}. \tag{44}$$

To simulate the motion of the kink, we replace n by $n - \alpha$. α indicates the location of the kink. With this substitution, $H'(\alpha)$ becomes an even periodic function of period 1, whose cosine series has the form

$$H'(\alpha) = \frac{a_0}{2} + \sum_{m=1}^{\infty} a_m \cos(2\pi m\alpha), \tag{45}$$

where

$$a_m = 2\int_0^1 \sum_{n=-\infty}^{+\infty} \frac{1+g^2}{\lambda^2} \frac{\cosh^2[\pi(n-\alpha)/\lambda]\cos(2\pi m\alpha)}{\{\cosh^2[\pi(n-\alpha)/\lambda] + g^2\sinh^2[\pi(n-\alpha)/\lambda]\}^2}. \tag{46}$$

With the change in variable $t = \alpha - n$, this becomes

$$a_m = \frac{2(1+g^2)}{\lambda^2}\int_{-\infty}^{\infty} \frac{\cosh^2(\pi t/\lambda)\cos(2\pi m\alpha)}{[\cosh^2(\pi t/\lambda) + g^2\sinh^2(\pi t/\lambda)]^2}\,dt, \tag{47}$$

which equals, recalling that $g = r/2\lambda$,

$$a_m = \frac{2m}{\sinh(m\pi\lambda)}\left\{\cosh\left[2m\lambda\tan^{-1}\left(\frac{r}{2\lambda}\right)\right] + \left[1+\left(\frac{r}{2\lambda}\right)^2\right]\frac{\sinh[2m\lambda\tan^{-1}(r/2\lambda)]}{mr}\right\}. \tag{48}$$

This reduces to the FK model value (Joós and Duesbery 1997b) in the limit $g = r/2\lambda \to 0$, or more precisely $r \to 0$, with

$$a_m = \frac{4m}{\sinh(m\pi\lambda)}. \tag{49}$$

The migration energy E'_M is the difference between the maximum- and minimum-energy configurations, $\alpha = 0$ and $\frac{1}{2}$ respectively, that is

$$E'_M = 2\sum_{m,\text{odd}}^{\infty} a_m. \tag{50}$$

This is expected to be equal in most cases to $2a_1$, that is

$$E'_M = \frac{4}{\sinh(\lambda)}\left\{\cosh\left[2\lambda\tan^{-1}\left(\frac{r}{2\lambda}\right)\right] + \left[1+\left(\frac{r}{2\lambda}\right)^2\right]\frac{\sinh[2\lambda\tan^{-1}(r/2\lambda)]}{r}\right\}. \tag{51}$$

When $\lambda > 1$, $2\lambda\tan^{-1}(r/2\lambda) \approx r$ (for $r < 2$), and $\sinh(\pi\lambda) \approx \exp(\pi\lambda)/2$,

$$E_M = 8\left(\cosh r + \frac{\sinh r}{r}\right)\exp(-\pi\lambda)\,\Gamma_0\,\frac{a'^2}{a}. \tag{52}$$

We have multiplied by $\Gamma_0 a'^2$ to restore the units of energy. When $\lambda < 0.5$, the departure from this form is significant.

The stress corresponding to this migration energy is

$$\sigma_{2P} = \frac{1}{a'2}\left(\frac{\partial H(\alpha)}{\partial\alpha}\right)_{\max} = 2\pi\sum_{m=1}^{\infty} m a_m\,\frac{\Gamma_0}{a}. \tag{53}$$

$H(\alpha)$ departs from a sinusoidal form near $\lambda = 1$. Down to that value, σ_{2P} is adequately given by the leading term in equation (53):

$$\sigma_{2P} = 8\pi\left(\cosh r + \frac{\sinh r}{r}\right)\exp(-\pi\lambda)\left(\frac{\Gamma_0}{a}\right). \tag{54}$$

$r = a'/a$ has a significant effect on the pre-factor. Comparison between the discrete model with relaxation and the rigid translation approximation used here revealed for

the FK model ($r = 0$) good agreement between the two calculations (Joós and Duesbery 1997b).

3.5. *Effect of stress*

When a constant stress σ is applied in the glide plane, it exerts a force σb per unit length on the dislocation line, which adds a $-\sigma bx$ potential energy term to the dislocation energy. The stress displaces the position of the dislocation line to a new equilibrium position y_0. This will have a significant effect on the kink pair activation energy, which now can be written as

$$H_{kp} = \int_{-\infty}^{\infty} \left\{ \Gamma(y) \left[1 + \left(\frac{dy}{dx} \right)^2 \right]^{1/2} - \Gamma(y_0) - \sigma b (y - y_0) \right\} dx. \tag{55}$$

The energy minimization can be carried out in a similar way to previously. Equation (19) needs simply to be rewritten with Γ_0 replaced by $\Gamma(y_0) + \sigma b(y - y_0)$, yielding

$$H_{kp} = 2 \int_{y_0}^{y_M} \{ \Gamma(y)^2 - [\Gamma(y_0) + \sigma b (y - y_0)]^2 \}^{1/2} dy. \tag{56}$$

Analytical integration with the inclusion of the stress becomes difficult. The only obvious result is that, with the application of stress, H_{kp} decreases monotonically with increasing σ down to zero at $\sigma = \sigma_P$ (Dorn and Rajnak 1964, Guyot and Dorn 1967, Duesbery and Joós 1996). Indeed, y_0 is obtained by minimizing H_{kp} with $dy/dx = 0$, or

$$\sigma b = \left(\frac{\partial \Gamma}{\partial y} \right)_{y = y_0}, \tag{57}$$

and y_m is determined by the point where the integrand in equation (56) becomes imaginary. At σ_P, $\partial\Gamma/\partial y$ is a maximum; therefore $\Gamma(y) - \Gamma(y_0) - \sigma b(y - y_0)$ changes sign at y_0 and hence also the integrand. So $y_0 = y_m$, and $H_{kp} = 0$.

With a sinusoidal $\Gamma(y)$,

$$y_0 = \frac{a'}{2\pi} \sin^{-1} \left(\frac{\sigma}{\sigma_P} \right) \tag{58}$$

and

$$\Gamma(y_0) = \Gamma_0 + \frac{W_0}{2} \left\{ 1 - \left[1 - \left(\frac{\sigma}{\sigma_P} \right)^2 \right]^{1/2} \right\}. \tag{59}$$

To leading order, equation (56) can be written as

$$H_{kp} = \frac{1}{2^{1/2} \lambda \pi} \frac{\Gamma_0 a'^2}{a} \int_{u_0}^{u_m} [\cos u_0 - \cos u - \sin u_0 (u - u_0)]^{1/2} du \tag{60}$$

where $u = 2\pi y/a'$, $\sin u_0 = \sigma/\sigma_P$ and u_m is the maximum value of u defined as the point where the integrand becomes imaginary. It is clear that, when $\sigma = \sigma_P$, $u_0 = u_m = \pi/2$ and $H_{kp} = 0$. Seeger (1984) discussed the dynamics of the kinks for this latter case.

§4. Discussion

To be able to start from a GSF barrier for atomic planes $\gamma(f)$, to generate the 'washboard-like' potential field W_{PN} felt by the dislocation line and then to extract

some fundamental properties for its motion is a satisfying feeling. It is certainly a credit to the PN model that this is possible, but at this stage it can only be done on the one-dimensional version of the model and not the more realistic two-dimensional version. In this simplified version, all quantities are related to an elastic constant K which characterizes the response of the lattice to deformations along the Burgers vector direction, and τ_{max} which gives a measure of the intensity of restoring forces at the interface. It gives the trends expected in the two-dimensional model. If dissociations occur, the one-dimensional model would be applied to the individual partials, and not the full dislocation, as was done for partials in Si (Joós *et al.* 1994, Joós and Duesbery 1997a). It is quite remarkable that down to $\zeta/a' = 0$ there is no singular behaviour. There are two limits. First the wide-dislocation limit (large ζ/a') where the kink width λ grows exponentially as $\exp(\pi\zeta/a')$ and the PN barrier energy W_P and kink-pair activation energy E_{kp} decrease exponentially at the same rate $\exp(-\pi\zeta/a')$ as expected. At the other limit where atomistic effects will be important, and ζ/a', and consequently λ also, approach zero, it is nevertheless interesting to note that, in spite of the divergence of W_P, the kink pair activation reaches a limiting value related to the misfit energy gain in creating the kink.

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