A PEIERLS-NABARRO MODEL FOR KINK-PAIR GENERATION IN SCREW DISLOCATIONS AT LOW TEMPERATURES

A.H.W. NGAN
Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong, P.R. China

ABSTRACT

Kink-pair generation in three-fold screw dislocations in the bcc lattice is investigated within the framework of the generalised Peierls-Nabarro model. Using a piece-wise plane strain approximation, the apparent activation energy is predicted to vary with stress in a parabolic manner which is in good agreement with experimental findings.

INTRODUCTION

Most of the current understanding of the behaviour of screw dislocation cores in the bcc lattice is by and large derived from atomistic simulation studies performed in the last three decades or so. These atomistic investigations lead to the current perception that i) ½<111> screw dislocation cores are in general three-fold dissociated with intrinsically high Peierls stress of the order of $10^{-2} \mu$, μ being the shear modulus, ii) their slip behaviour violates Schmid's law, iii) their motion at zero-temperature may follow a path along {101} or a zig-zag path averaging along a twinning or anti-twinning {112} plane, and iv) their motion can be affected by non-glide stress components. At finite temperatures, motion of screw dislocations does not happen in a plane-strain manner but is effected by the generation and nucleation of kink-pairs, and at low deformation temperatures, it is the nucleation of these kink-pairs that forms the rate determining step for slip. The application of atomistic simulation to the investigation of kink-pair generation, however, has so far been very limited, as kink problems are essentially 3-D problems in which the number of atoms to be handled may be too large. In this respect, the most frequently used research tool is still the continuum approach involving the line tension approximation and the phenomenological concept of Peierls potential [1]. The Peierls potential, being the energy potential of the dislocation with respect to its "position", is purely phenomenological because the constraint that must be applied to keep the dislocation at a general non-equilibrium position cannot be clearly defined. Also, the introduction of an inner cut-off radius in the line tension disconnects the whole approach from the vast body of literature on the core behaviour of the dislocation.

In the light of these difficulties, the present work aims at developing a semi-continuum model which combines certain elements of the atomistic and continuum picture of the dislocation kink-pair problem. The model is essentially an extension to the Peierls-Nabarro model, in which the dislocation core is envisaged as comprising of linear elastic regions connected to one another along certain surfaces over which a non-linear misfit force law acts. The misfit force law is readily established as the γ-surface, which can be calculated using atomistic means for specific materials. With the introduction of the misfit surfaces, the elastic field of the dislocation no longer carries any singularities and so the introduction of the dubious inner cut-off is not necessary.

THEORY

The bcc lattice obeys three-fold rotational symmetry about <111> and in the generalised P-N model [2,3], a screw dislocation along this direction is considered to be composed of three 120° elastic wedges with the wedge boundaries along three {101} planes as shown in Fig. 1. The wedges are strained into an anti-plane strain manner so that when they are welded together at the far field, the long-range field of the screw dislocation is established there. At the centre of the dislocation, the total Burgers vector content is partitioned amongst the misfit displacements of the adjacent wedge faces as shown in Fig. 1. The interaction between adjacent wedge faces is characterised by a non-linear force law γ[Φ], where Φ is the misfit displacement. The total energy per unit length E_{tot} of the dislocation is therefore composed of three parts: i) the strain energies of

the wedges, ii) the misfit energy of the three cuts, and iii) the work done by the applied stress τ_a. Each of these energy terms is a functional of the boundary displacement functions $u_{i\pm}$ defined for each wedge relative to the position of the wedge tip. E_{tot} can therefore be expressed as [4]:

$$
\begin{aligned}
E_{tot} =\frac{3\mu}{4\pi} \sum_{i=1}^{3} \int_0^\infty \int_0^\infty \{ &\frac{\eta^{1/2}}{\xi^{3/2}+\eta^{3/2}} \left[u_{i-}{}'(\xi)u_{i+}(\eta)+u_{i+}{}'(\xi)u_{i-}(\eta) \right] - \frac{\eta^{1/2}}{\xi^{3/2}-\eta^{3/2}} \left[u_{i+}{}'(\xi)u_{i+}(\eta)+u_{i-}{}'(\xi)u_{i-}(\eta) \right] \} d\eta d\xi \\
&+\int_0^\infty \gamma \left[\Phi = \Delta_{112}b - u_{1-}(r) - u_{2+}(r) \right] dr + \int_0^\infty \gamma \left[\Phi = (1-\Delta_{112}-\Delta_{311})b - u_{2-}(r) - u_{3+}(r) \right] dr \\
&+\int_0^\infty \gamma \left[\Phi = \Delta_{311}b - u_{3-}(r) - u_{1+}(r) \right] dr + \tau_a \cos(120^\circ - \chi)\int_0^\infty \left[\Delta_{112}b - u_{1-}(r) - u_{2+}(r) \right] dr \\
&+\tau_a \cos\chi\int_0^\infty \left[(1-\Delta_{112}-\Delta_{311})b - u_{2-}(r) - u_{3+}(r) \right] dr + \tau_a \cos(120^\circ + \chi)\int_0^\infty \left[\Delta_{311}b - u_{3-}(r) - u_{1+}(r) \right] dr, \quad (1)
\end{aligned}
$$

in which the double integral terms represent the strain energy, the γ terms the misfit energy and the τ_a terms the work done against the applied stress τ_a. In this equation, b is the Burgers vector, Δ_{ilj} the fractional Burgers vector content of the ilj cut, and χ the angle between the maximum resolved shear stress plane and the 2l3 cut in Fig. 1. At equilibrium without an applied stress, the core should adopt the symmetrical three-fold configuration for which $\Delta_{112} = \Delta_{311} = {}^1/_3$, and when the core becomes planar along, say, the 2l3 cut under thermal agitation or a large enough τ_a, $\Delta_{112} = \Delta_{311} = 0$. The atomic force law $\gamma[\Phi]$ can be calculated for specific materials using atomistic simulation [5]. The static core configuration under any predefined stress level can then be obtained by minimising E_{tot} in eqn. (1) with respect to u_{ilj} and Δ_{ilj} using a variational technique. For example, the Peierls stress, i.e. the stress required to constrict the three-fold core to the planar configuration, estimated by a Frenkel force law is ~ 0.04 μ when $\chi = 0°$ [6], which is in good agreement with typical values calculated by atomistic simulation or measured by experiments.

At finite temperatures, the dislocation will not move as a rigid line but will have to go through a saddle configuration in the form of a kink-pair illustrated schematically in Fig. 2. In this configuration, the dislocation core changes continuously from the fully dissociated state into the fully recombined state through a kink, and then back to the fully dissociated state through another
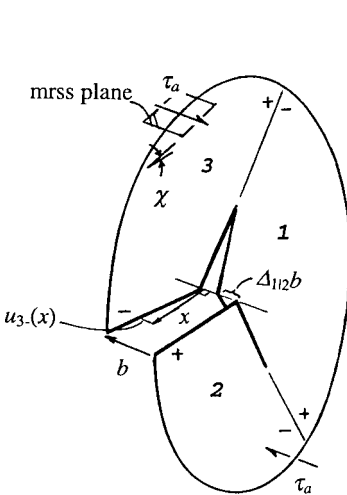

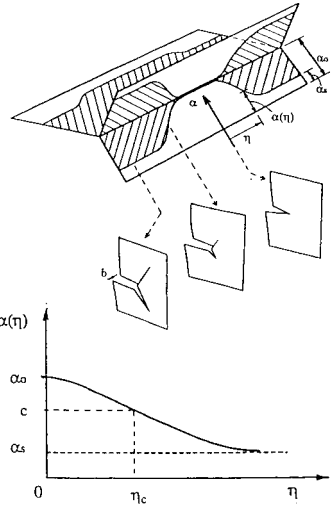Fig. 1 - Three-fold Screw Dislocation Core   Fig. 2 - Double Kink Configuration

kink with opposite sign as shown in Fig. 2. The geometry represents a 3-D elasticity problem and the mathematics can be greatly simplified by invoking the piecewise anti-plane strain approximation, in which we assume that for each section perpendicular to the dislocation line, the local degree of recombination can be characterised by a generalised coordinate α, whose value varies from $\alpha_s \approx 0$ for the fully dissociated state to $\alpha_o \approx 1$ for the fully recombined state. The kink shape is then marked by the function $\alpha(\eta)$, where η is the spatial coordinate along the dislocation line. The section at η is assumed to have a screw direction displacement field u^α in cylindrical coordinates given by

$$u^\alpha(r,\theta,\eta) = u^\Delta(r,\theta) + \alpha(\eta)\,f(r,\theta), \qquad (2)$$

where $u^\Delta(r,\theta)$ is the screw direction displacement of the stress free, 3-fold symmetrical anti-plane strain state, and $f(r,\theta)$ is the displacement change on going from the $u^\Delta(r,\theta)$ reference state to the fully recombined planar state. In eqn. (2) are implied two approximations. The first is a linearisation approximation, in which the saddle path the core configuration moves along is approximated by the "straight line" joining the starting three-fold and ending two-fold states. The second is the piecewise anti-plane strain approximation as discussed above, which is valid only at the high stress (or low temperature) regime during which the rate-determining step involves kink-pair nucleation. If kink-pair separation is instead the rate-determining step as in the case of the low stress (or high temperature) regime, the two opposite kinks are well-formed and sharp. In this situation, the long-range elastic interaction between the two opposite kinks will dominate and the classical treatment using Volterra fields will be more valid [7].

With the assumptions spelt out in eqn. (2), the different energy contributions of the double kink configuration can be calculated as follows.

i) Self energy E_{self} - Using the stress-free, symmetrical three-fold dissociated state as the reference, the energy change of a partially recombined core given by eqn. (1) may be expressed as $\delta E_{tot} = \delta E_{self} - \tau_a V^*$, where δE_{self} comprises of the strain and misfit energy changes, and the τ_a term in which V^* is the activation volume represents the work done change. It has been shown beforehand [2,3] that the energy per unit length of the equilibrium planar state is higher than the three-fold dissociated state by an amount $\Delta E \sim 0.03\ \mu b^2$. ΔE constitutes the energy barrier that must be overcome before the ground state three-fold configuration can be transformed into the mobile planar state, and in the absence of thermal agitation, this is solely overcome by an applied stress equal to the zero-temperature Peierls stress. Thus in the double kink configuration shown in Fig. 2, a slab situated within the fully recombined planar segment (with $\alpha \sim 1$) would have energy per unit length ΔE higher than one situated well within a ground state segment (with $\alpha \sim 0$), and so it seems reasonable to associate the self-energy δE_{self} of a partially recombined slab with the corresponding α value by a piecewise parabolic relationship:

$$\delta E_{self}(\alpha) \approx \begin{cases} \Delta E\alpha^2/c & \text{for } 0 \leq \alpha \leq c \\ \Delta E - \Delta E(\alpha-1)^2/(1-c) & \text{for } c \leq \alpha \leq 1 \end{cases} \qquad (3)$$

where c is a constant between 0 and 1. Detailed consideration of the strain and misfit energy terms in eqn. (1) using a Rayleigh-Ritz approach to be published elsewhere [4] shows that the lowest energy path can be well approximated by eqn. (3) with c set to 0.2 and ΔE to 0.03 μb^2. With these prescriptions, the total self-energy of the double kink configuration E_{self} is then given by

$$E_{self} = \int_0^\infty \delta E_{self}(\alpha)\,\mathrm{d}\eta \quad . \qquad (4)$$

ii) Interaction energy E_{int} - Provided that $\alpha(\eta)$ is slowly varying, the interaction energy E_{int} between the slabs is given by

$$E_{int} = \sum_{i=1}^{3} \frac{E}{2} \int_0^\infty d\eta \iint_{wedge\,i} \left[\frac{\partial}{\partial \eta} \delta u_\eta^i(r,\theta) \right]^2 r\,dr\,d\theta \qquad (5)$$

where E is the Young's modulus, and $\delta u_\eta^i(r,\theta)$ is the displacement change in polar coordinates of the interior of wedge i when the core goes from the initial three-fold configuration to a general configuration specified by α under the anti-plane strain condition. From eqn. (2), $\delta u_\eta^i(r,\theta) = \alpha(\eta) f_i(r,\theta)$, so that eqn. (5) can be rewritten as

$$E_{int} = \int_0^\infty \frac{[\alpha'(\eta)]^2}{2} \, EP \, d\eta \qquad (5a)$$

where

$$P = \sum_{i=1}^{3} \iint_{wedge\,i} [f_i(r,\theta)]^2 r\,dr\,d\theta. \qquad (6)$$

P can be calculated numerically from eqn. (6) [4] but physically, $\sqrt{P}$ is simply the root-mean-squared change in the displacement on going from the three-fold to the planar configuration multiplied by an effective size of the core, and so $\sqrt{P}$ is of the order of b^2.

iii) Work-done E_w by the applied stress τ_a - The work done term in eqn. (1) as the symmetrical three-fold core recombines into the planar state, within Eshelby's superposition spirit, is equal to the summation over the cuts ilj of the products of the stress component acted on each cut and the area change of the cut δA_{ilj} during the recombination. The work done for a partially recombined section $d\eta$, within the linearisation approximation, is thus given by:

$$\tau_a dV^* = \tau_a \cos(120° - \chi)\alpha(\eta)\delta A_{1l2} d\eta + \tau_a \cos\chi\alpha(\eta)\delta A_{2l3} d\eta + \tau_a \cos(120° + \chi)\alpha(\eta)\delta A_{3l1} d\eta,$$

but because $\delta A_{1l2} \simeq \delta A_{3l1} < 0$ (= $-A_2$, say) and $\delta A_{2l3} > 0$ (= A_1, say), this equals to

$$\tau_a dV^* = \alpha(\eta)\tau_a \cos\chi(\delta A_{2l3} + \delta A_{1l2})d\eta$$
$$= \alpha(\eta)\tau_a \cos\chi \, A^* d\eta$$

where $A^* = A_1 + A_2$ is approximately constant with respect to orientation. Obviously, A^* is of the order of a few b^2. For one half of the kink-pair configuration, the total work done is therefore

$$E_w = \tau_a A^* \cos\chi \int_0^\infty \alpha(\eta) \, d\eta \quad . \qquad (7)$$

The total energy H of the whole kink-pair is

$$H = 2 \times \int_0^\infty \{ [\delta E_{tot}(\alpha) - \delta E_{tot}(\alpha_s)] - \tau_a A^* \cos\chi \, (\alpha - \alpha_s) + EP\alpha'^2/2 \} \, d\eta \qquad (8)$$

where α_s marks the static anti-plane strain configuration under τ_a and is given by $\alpha_s = \tau_a A^* \cos\chi \, c/(2\Delta E)$.

PREDICTIONS

Orientation Dependence of Peierls Stress

The zero-temperature Peierls stress τ_p is the value of τ_a when $\alpha_s = c$ in the anti-plane strain condition, and is given by

$$\tau_p = \frac{2\Delta E}{A^* \cos \chi} \quad . \tag{9}$$

Since $\Delta E \sim 0.03 \ \mu b^2$ and A^* is of the order of a few b^2, within the allowable range $\pm 30°$ for χ, $\tau_p \sim 10^{-2} \ \mu$, which is the order of magnitude observed experimentally. From eqn. (9), τ_p is orientation dependent, showing a minimum at $\chi = 0°$ and maximum at $\chi = \pm 30°$. Such a τ_p-χ relationship is indeed what is observed in Fe and Mo [8]. The magnitude of variation in τ_p from $\chi = 0°$ to $\pm 30°$ estimated by eqn. (9) is $\sim 10^{-3} \ \mu$, which is again in very good agreement with experimental results for Fe and Mo. Generally speaking, for bcc metals which exhibit this type of τ_p- χ relationship, the slip plane would always be {101} irrespective of the stress orientation χ, and this is indeed what is assumed to happen in the present model. In the atomistic simulation performed by Vitek and co-workers [9], this corresponds to the behaviour of the J_2 potential which yields the widest dissociation on {101} planes. If dissociation is of limited extent on {101} planes, there is a general tendency for the core to glide on a {112} plane, and the selection of twinning or anti-twinning {112} is dependent on the stress orientation. The associated τ_p-χ relationship would exhibit a maximum at the χ value at which the slip plane changes from twinning to anti-twinning {112}, and in general, τ_p for twinning slip is lower than that for anti-twinning slip. This twinning/anti-twinning asymmetry in the slip behaviour of bcc materials like Ta, Li-Mg, AgMg and β-CuZn is not predicted by the present model simply because the detailed atomic arrangement along the screw direction is not modelled here.

Critical Kink Shape

At finite temperatures, the critical kink shape can be obtained by extremising H in eqn. (8) with respect to $\alpha(\eta)$. The predicted critical kink height, defined here as $\alpha_o = \alpha(0)$, is found to be

$$\alpha_o = (\sqrt{1-c} + 1) - t [\sqrt{1-c} + (1-c)], \tag{10}$$

where $t = \tau_a/\tau_p$ is a normalised stress. The critical kink height therefore decreases as the applied stress t increases, and this is in qualitative agreement with atomistic calculations [7]. The kink separation may be defined to be the separation $2 \times \eta_c$ between the two points $\eta = \pm\eta_c$ at which $\alpha(\pm\eta_c) = c$ (see Fig. 2), and

$$\eta_c = \sqrt{(1-c)EP/(2\Delta E)} \ \tan^{-1}\left[-\sqrt{c/(1-c)}\right]. \tag{11}$$

The critical kink separation is therefore stress independent, again in qualitative agreement with atomistic simulation [7].

Activation Energy

The minimised value of H from eqn. (8) is found to be

$$H = (1 - t)^2 \left[\sqrt{2(\Delta E)cEP} + 2\Delta E\eta_c /(1-c)\right] \quad . \tag{12}$$

The apparent activation energy is therefore predicted to vary parabolically with the applied shear stress t. Fig. 3 shows the experimental data of activation energy vs stress for potassium and high purity iron. It can be seen that the experimental data for both Fe and K fall on the same relationship $\sqrt{(H/\mu b^3)} \approx (0.30 \pm 0.03) \times (1-t)$, where $t = \tau_a /\tau_p$. Furthermore, for the case of Fe, this relationship also holds for two different tensile orientations as indicated. The Table shows the experimental values of $\sqrt{(H(\tau_a=0)/\mu b^3)}$ for a few other bcc metals, which indicate clearly that the parameter falls in a narrow range around 0.30 ± 0.03. The constancy of the relationship $\sqrt{(H/\mu b^3)} \approx 0.3 \times (1-t)$ is a strong verification for the present model, which predicts the same relation as expressed in eqn. (12) if one takes the expected values $\Delta E \sim 0.03 \ \mu b^2$, $c \sim 0.2$ and $EP \sim 0.1 \ \mu b^4$.

Fig. 3 also shows the atomistic simulation results for K by Duesbury [7], which significantly overestimate the kink energy at the intermediate to large stress regime.
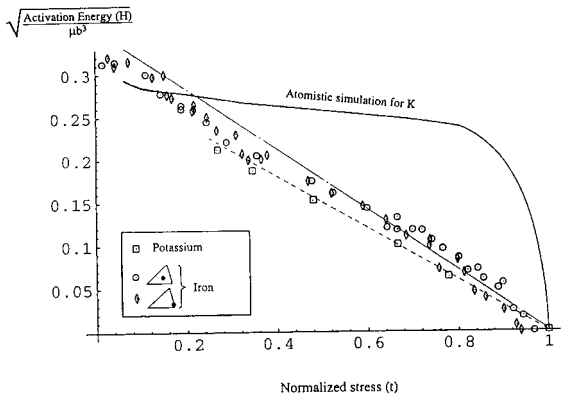

Fig. 3 - Activation Energy vs Normalised Applied Stress

[Ref. for K: Basinski, Duesbury and Murty (1981); for Fe: Aono, Kuramoto and Kitajima (1981).]

Table - Experimental Values of Zero-stress Activation Energies

	Cr	Ta	V	Mo	W	Nb
$\sqrt{(H(\tau_a=0)/\mu b^3)}$	0.25-0.30	0.28-0.31	0.34	0.30	0.28	0.30
References	← experimental data quoted in Dorn and Rajnak (1964) →					Conrad and Hayes (1963)

CONCLUSIONS

The movement of 1/2<111> screw dislocations in Fe-like bcc metals can be modelled within the framework of the generalised Peierls-Nabarro model. The apparent activation energy is predicted to vary with stress in a parabolic manner, in good agreement with experimental findings for iron and potassium.

ACKNOWLEDGMENT

REFERENCES

1. See, e.g. T. Suzuki, H. Koizumi and H.O.K. Kirchner, Acta Metall. Mater., **43**, 2177 (1995) and references therein.
2. A.H.W. Ngan, Phil. Mag. Lett., **72**, p. 207 (1995).
3. A.H.W. Ngan, J. Mech. Phys. Solids, **45**, p. 903 (1997).
4. A.H.W. Ngan, to appear in Phil. Mag. A.
5. M.S. Duesbury, and V. Vitek, Acta Mater., **46**, 1481 (1998).
6. A.H.W. Ngan in *Strength Theory: Application, Development & Prospects for 21st Century*, edited by M.H. Yu and S.C. Fan (Science Press, Beijing China 1998), p. 151-156.
7. M.S. Duesbury, Acta Metall., **31**, 1747 (1983).
8. T. Suzuki, S. Takeuchi and H.Yoshinaga, *Dislocation Dynamics and Plasticity*, Springer-Verlag Berlin Heidelberg, 1991, Chp. 6.
9. V. Vitek, Crystal Lattice Defects, **5**, 1 (1974).