MOBILITY OF NON-PLANAR SCREW DISLOCATIONS AHEAD OF A MODE III CRACK TIP

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ABSTRACT

The generalised Peierls-Nabarro model is used to study the transformation of screw dislocation cores from the three-fold, non-planar state to the planar, glissile state ahead of a mode III crack tip.

INTRODUCTION

A necessary though not sufficient condition for brittle-to-ductile transition (BDT) to occur is that dislocations can emanate from the crack tip. The problem of dislocation emission from a crack tip has been studied by a number of authors [1-3] who have considered in detail the force required to gradually form a dislocation from zero to unit Burgers vector content and the competition between such mode of dislocation nucleation and crack cleavage. In the incipient process considered by these authors, the dislocation is assumed to have a planar core, and no lattice friction is assumed to exist once the dislocation is fully formed and begins to move away from the crack tip. The omission of friction stress during the incipient process is perhaps not important for close-packed slip systems because the lattice friction can be supposed to be small. However, for the bcc structure for which BDT is particularly important, screw dislocation cores are non-planar and so lattice friction should not be neglected *a priori* in a satisfactory treatment on crack-tip emission.

The present work is therefore an attempt to remedy this deficiency. The dislocation model that we use is the generalised Peierls-Nabarro model [4,5], which is an extended version of the original Peierls-Nabarro model generalised to take into account non-planar core dissociation. In what follows, we will consider the interaction between a mode III crack tip and a three-fold dissociated screw dislocation, which resembles a ½<111> screw dislocation in the bcc lattice. We assume the entire content of the dislocation to emerge from the crack-tip in a fashion similar to what has been considered in ref. [1-3], and we consider in detail here the three-fold dissociation of the dislocation core after its full content has been established but when it is still situated very close to the crack tip. When the dislocation is situated at a distance comparable to its core size from the crack tip, the image effects of the crack should modify significantly the core configuration, and the mobility of the dislocation should be greatly affected.

THEORY

In the generalised Peierls-Nabarro model [4,5], a three-fold screw dislocation is composed by joining together three 120° elastic wedges along surfaces parallel to the dislocation line as shown in Fig. 1. The three wedges are strained into such a way that the long-range field of the dislocation is established at large radial distances from the centre. At small radial distances, the field deviates from the Volterra singular field because of the misfit taken place at the three cut planes. The force law $\gamma(\Phi)$ governing the misfit Φ between adjacent points across the cut plane is non-linear and for specific materials, it can be calculated as the γ-surface using atomistic simulation.

We consider placing a mode III crack tip at a distance x from the dislocation centre so that the crack plane coincides with one of its slip planes, say the 112 plane, as shown in Fig. 1. For a given dislocation core configuration, the energy of the dislocation-crack system is composed of three parts, namely i) the strain energy stored in creating the dislocation ahead of the slit opening of the unloaded crack, ii) the work done against the stress field of the loaded crack-tip as the

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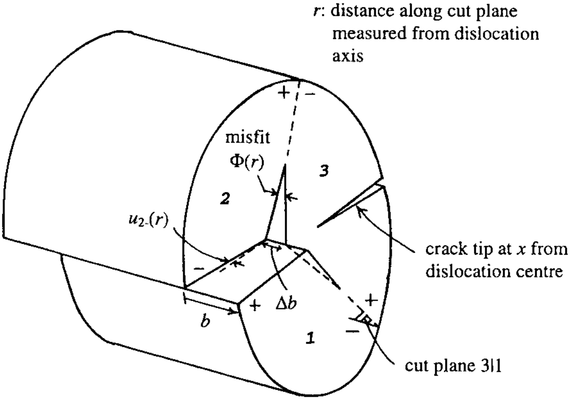

Fig. 1 - Three-fold screw dislocation situated ahead of a mode III crack tip.

dislocation is created, and iii) the misfit energy which comes from integrating $\gamma(\Phi)$ along the three cut planes with Φ treated as a varying function along each cut. The strain energy term is simply the elastic energy stored in the strained wedges, and can be evaluated from the prescribed boundary displacements of the wedges using standard methods in anti-plane strain elastostatics [6]. The full expression of the dislocation-crack energy E_{tot} per unit length is given by:

$$
\begin{aligned}
E_{tot} = \frac{3\mu}{2\pi} \int_0^\infty \int_0^\infty \{ & \frac{2\eta^2}{(\eta^3 - \xi^3)} \sqrt{\frac{\xi^3 + x^3}{\eta^3 + x^3}}\, u_{3-}'(\xi) u_{3-}(\eta) + \frac{\sqrt{\eta}}{\eta^{3/2} + \xi^{3/2}} \left[u_{2-}'(\xi) u_{2+}(\eta) + u_{2+}'(\xi) u_{2-}(\eta) \right] \\
& + \frac{\sqrt{\eta}}{\eta^{3/2} - \xi^{3/2}} \left[u_{2+}'(\xi) u_{2+}(\eta) + u_{2-}'(\xi) u_{2-}(\eta) \right] \} \, d\eta d\xi + 2\int_0^\infty \gamma[\Phi = \Delta b - u_{3-}(r) - u_{2+}(r)]\, dr \\
& + \int_0^\infty \gamma[\Phi = (1 - 2\Delta) b - 2u_{2-}(r)]\, dr - 2\int_0^\infty \tau_c(r)[u_{3-}(r) + u_{2+}(r)]\, dr + 2\int_0^\infty \frac{K_{III}}{\sqrt{2\pi(r + x)}} u_{2-}(r)\, dr
\end{aligned}
\qquad (1)
$$

where μ is the shear modulus, b the Burgers vector, K_{III} the applied stress intensity factor, $\tau_c(r) = K_{III} \cos(\psi/2+\pi/3)/\sqrt{2\pi\rho}$, $\rho = \sqrt{r^2 + x^2 - rx}$ and $\psi = \tan^{-1}[\sqrt{3}\, r/(2x-r)]$ $(0 \leq \psi \leq \pi)$. In eqn. (1), the double integral term is the strain energy, the terms involving γ the misfit energy and that involving K_{III} the work done against the crack-tip field. $u_{i\pm}(r)$ represents the displacement function of the boundary marked by + or - of wedge i relative to the wedge tip position (see Fig. 1). Δ is the fractional Burgers vector content of the cut 2|3 or 3|1, and can be used as a parameter specifying the degree of recombination of the core into the planar state. In the absence of the crack, the core configuration should be symmetrically three-fold, and Δ will assume the value 1/3. When the core is totally constricted into the planar state, Δ will become 0. To find the stable configuration of the dislocation core under a specific K_{III}, E_{tot} should then be minimised with respect to Δ, u_{3-}, u_{2+} and u_{2-}. The long-range limits of the boundary displacements should match the Volterra solution

$$
u(r,\theta) = \frac{b}{2\pi} \left[\tan^{-1}\left(\frac{\sqrt{2x}\sqrt{A - x - r\cos\theta}}{A - x} \right) - \pi \right]
$$

where $A=\sqrt{r^2+2rx\cos\theta+x^2}$, which requires that as $r/x \to \infty$, $u(r,\theta) \to -b/2$ for all θ. Hence, the free variables in eqn. (1) are subject to the following end conditions

$$u_{3-}(0) = 0,\ u_{3-}(\infty) = b/2,\ u_{2-}(0) = 0,\ u_{2-}(\infty) = (1/2-\Delta)b,\ u_{2+}(0) = 0,\ u_{2+}(\infty) = (\Delta-1/2)b. \quad (2)$$

The variational problems expressed in eqn. (1) and (2) can be solved approximately by the Rayleigh-Ritz method with the following trial functions satisfying the end conditions (2):

$$u_{3-}(x)=\frac{b}{\pi}\tan^{-1}(k_3x),\qquad u_{2-}(x)=(1-2\Delta)\frac{b}{\pi}\tan^{-1}(k_2x),\qquad u_{2+}(x)=(2\Delta-1)\frac{b}{\pi}\tan^{-1}(k_1x)\cdot$$

Here k_i (i = 1,2,3) and Δ are free parameters which are adjusted to obtain minimum values for E_{tot} in eqn. (1).

RESULTS AND DISCUSSION

Dislocation Mobility Ahead of Crack-Tip

As an illustration, we present here the results obtained by assuming the following Frenkel sinusoidal γ-force law:

$$\gamma=\frac{\mu b}{4\pi^2}\left[1-\cos\left(\frac{2\pi\Phi}{b}\right)\right]\cdot \quad (3)$$

Fig. 2 shows the relation between the fractional Burgers vector Δ and the applied K_{III} when the dislocation is situated at three different distances x ahead of a loaded crack tip. It can be seen that when K_{III} is zero, the values of Δ are all greater than the three-fold symmetric value 1/3, and with decreasing x, the value of Δ increases. This is due to the image force of the crack surface, which tries to pull the dislocation configuration towards the V-shape. As K_{III} increases from zero, Δ decreases steadily as shown in Fig. 2. However, as soon as Δ decreases to $\sim$ 0.25, the core transforms instantaneously into planar as shown in Fig. 2. It was also found that if the core is stressed to any configuration with $\Delta \gtrsim 0.25$, the configuration will return to the stress-free stable configuration upon removal of stress. However, if the core is stressed to beyond the $\Delta \approx 0.25$ point so that it has become planar, the core will remain in the planar configuration with $\Delta \approx 0$ upon the removal of stress. The condition Δ reaches 0.25 therefore marks an instability point, and the planar state is a metastable state protected by an energy barrier at $\Delta = 0.25$. The instability at $\Delta = 0.25$ can be easily understood from the γ force law expressed in eqn. (3), which shows that the misfit energy attains a maximum when Φ equals $0.5b$. Thus as soon as the opening of 1l2 branch exceeds $0.5b$, there is a net force causing the branch to open further.

The observed instability at $\Delta = 0.25$ is a characteristic behaviour ahead of a crack tip, and no such stability is found to exist in the motion of a dislocation without the presence of the crack. The reason is that the tendency to open up the 1l2 branch after $\Delta = 0.25$ is resisted by the rigidity of the material, and with the presence of the crack, the material trailing the 1l2 branch is slit open and will become much less rigid. The induced strain energy rise as a result of the change in core configuration as branch 1l2 opens up after $\Delta = 0.25$ is therefore too small to offset the associated large drop in misfit energy. The observed instability at $\Delta = 0.25$ is analogous to the conclusion reached by Rice when considering dislocation generation from a mode II crack tip [3]. Rice concluded that as the crack-tip opening reaches $0.5b$, the energy resistance to crack propagation would pass through a maximum value equal to the unstable stacking fault energy. Rice's treatment, however, is based on a J-integral calculation and so it assumes that the field undergoes rigid translation as the dislocation moves out from the crack tip. In our present model, the core configuration changes as the dislocation recombines and so the J-integral method is not valid.

The above results can be compared with predictions obtained by assuming that the dislocation has a Volterra, empty-core field. In Fig. 2, there exists at each value of x a critical K_{III},

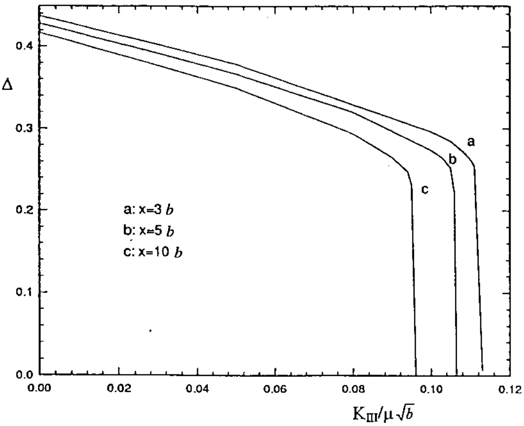

Fig. 2 Relation between equilibrium Δ and applied stress intensity factor K_{III}. x in units of b's.

denoted as K_m, at which the core becomes planar and hence mobile. Let us consider the alternative picture in which the dislocation has a Volterra field and possesses a Peierls stress τ_p. τ_p is the homogeneous stress required to convert the core into the planar configuration without the presence of the crack, and using a variational approach similar to the above, it is found to be 0.04μ [6]. In the Volterra model, K_m is the value of $K_{\rm III}$ needed to move the dislocation against τ_p and the image stress, and this is given by

$$\frac{K_m}{\sqrt{2\pi x}} = \tau_p + \frac{\mu b}{4\pi x} \cdot \tag{4}$$

Fig. 3 shows the variation between K_m and x as predicted from eqn. (4) as well as the Peierls-Nabarro model. It can be seen that if the crack-free value of 0.04μ is assumed for τ_p in eqn. (4), the deviation between the Volterra model and the Peierls-Nabarro model is very large. Eqn. (4) will be a good estimate of the Peierls-Nabarro results only when τ_p is decreased to ~ 0.005μ as shown in Fig. 3. Thus, a Peierls-Nabarro dislocation situated in front of a crack tip will experience an effective Peierls stress one order of magnitude lower than if it is situated in a perfect crystal. The crack obviously enhances the mobility of the dislocation by reducing the mechanical rigidity of the material ahead of it.

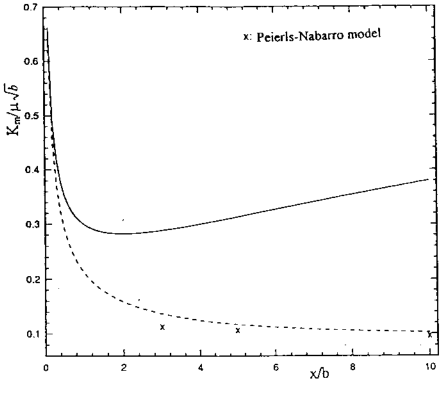

Fig. 3 - Critical stress intensity factor required to move a dislocation K_m.
Solid line - Volterra model with $\tau_p = 0.04\ \mu$.
Dotted line - ditto with $\tau_p = 0.005\mu$.
Crosses - generalised Peierls-Nabarro model.

Crack-tip Shielding

We next consider the shielding at the crack-tip caused by the dislocation field. For the Volterra dislocation, the shielding stress intensity factor K_s is $\mu b/\sqrt{(2\pi x)}$. For the Peierls-Nabarro dislocation, K_s is given by

$$K_s = \mu \sqrt{\frac{6}{\pi x}} \int_0^\infty \sqrt{\frac{x^3}{x^3 + \xi^3}} \; u_{3-}'(\xi)\, d\xi$$

where u_{3-} is the equilibrium boundary displacement, with or without stress, of wedge 3 obtained by minimising the energy functional in eqn. (1) [6]. Fig. 4 shows the variation between K_s and x of the Volterra and the Peierls-Nabarro dislocation when $K_{III} = 0$. It can be seen that at $x \gtrsim 5b$, the Volterra and the Peierls-Nabarro model converge, confirming that at large dislocation distances, the details of the core configuration do not matter. At small dislocation distances, the spreading of the Peierls-Nabarro core reduces the induced crack-tip field as compared with the Volterra core, and so the Peierls-Nabarro K_s is smaller than the Volterra value as shown in Fig. 4 for $x \lesssim 5b$.

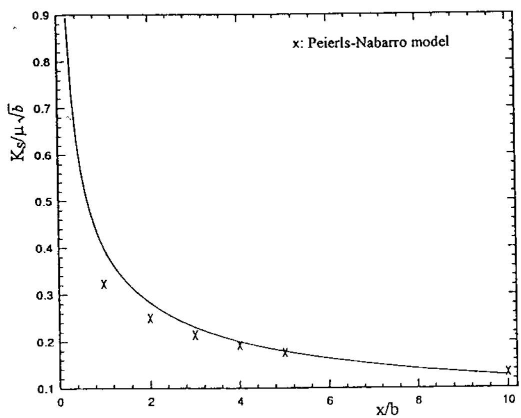

Fig. 4 - Dislocation shielding stress intensity factor K_s.
Curve - Volterra model
Crosses - generalised Peierls-Nabarro model with $K_{III} = 0$.

Implications for Brittle/Ductile Behaviour

From Fig. 2, a dislocation situated closer to the crack tip would require a larger K_{III} (= K_m) to mobilise it. This is due to the image stress, which would tend to retract the spreading on the slip plane co-planar with the crack plane, and to widen the spreading on slip planes inclining to the crack plane. An applied $K_{III} = K_m$ is required to overcome the image stress to make the core planar for motion. It is evident from Fig. 2 that K_m tends to ~ 0.12 $\mu\sqrt{b}$ as x approaches zero. Thus, if K_{III} is larger than ~ 0.12 $\mu\sqrt{b}$, all dislocations ahead of the crack tip including the one that has been freshly emitted from the crack tip would be planar. The limiting K_m ~ 0.12 $\mu\sqrt{b}$ therefore represents a critical stress intensity factor K_{mc} such that if the applied K_{III} is higher than or equal to this value, then all dislocations ahead of the crack tip would be mobile. If the applied K_{III} is lower than K_{mc}, then a non-planar zone would exist ahead of the crack tip, the size of which would increase as the difference (K_{mc} - K_{III}) increases. A dislocation situated outside this non-planar zone would have planar core and is mobile, but a dislocation existing within the zone would have non-planar core and would require thermal activation before it can move away from the crack tip.

The next question to be asked concerns the competition between dislocation mobility, nucleation and cleavage. Rice [3] has concluded that the critical K_{III} for dislocation nucleation directly from crack tip is $K_e = \sqrt{(2\mu\gamma_{us})}$ where γ_{us} is the unstable stacking fault energy. Taking γ_{us} to be the maximum value of the γ-force law in eqn. (3), $\gamma_{us} = \mu b/(2\pi^2)$, and so $K_e \approx 0.3\ \mu\sqrt{b}$ for a mode III crack. K_e is therefore of similar magnitude but higher than K_{mc} for motion, implying that nucleation from crack-tip would be slightly more difficult than subsequent motion. Thus, if dislocations can be nucleated from the crack-tip, they can move away from it and so crack-tip emission is nucleation rather than mobility controlled. Because nucleation must precede motion, whether the material is brittle or ductile still depends on the competition between nucleation and cleavage as Rice has suggested, and mobility is not a concern. It should be noted, however, that this is quite a fortuitous result, and only comes about because of the enhancement in mobility offered by the crack opening. If the intrinsic value $\tau_p = 0.04\mu$ were to be believed for motion ahead of the crack-tip, Fig. 3 shows that K_m at $x \approx b$ is roughly 0.3 $\mu\sqrt{b}$, implying that mobility would have been considered as difficult as nucleation.

Future Work

In the bcc lattice, motion of non-screw dislocations presents no problems and so one has a valid reason to focus on screw dislocations. The present analysis assumes that the crack plane is parallel to a slip plane and the crack front is parallel to the <111> Burgers vector direction. This is a rather exceptional situation and as future work one may attempt to investigate the more general condition in which the crack plane is inclined with respect to the glide plane. Insofar as the crack front is parallel to the Burgers vector, the problem is still anti-plane strain as only the mode III component will interact with the screw dislocation. If the crack front is not parallel to the Burgers vector, the core recombination problem is a three dimensional one and analytical formulation becomes very difficult.

CONCLUSIONS

The core dissociation of a three-fold screw dislocation ahead of a mode III crack tip has been studied within the framework of the generalised Peierls-Nabarro model. The image effects of the crack cause extensive dissociation of the dislocation core on slip planes that are inclined with respect to the crack plane. Core spreading reduces the degree of overshielding at the crack tip by the dislocation field when the dislocation is situated near the crack tip. The presence of the crack also enhances significantly the mobility of the dislocation. The presence of the crack slit opening reduces the rigidity of the material ahead of the crack tip, thus makes recombination of the dislocation core into the planar, mobile configuration by stress much easier. Emission of dislocations from crack-tip is therefore nucleation rather than mobility controlled.

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REFERENCES

1. J. Weertman, Phil. Mag. *A*, **43**, 1103 (1981).

2. G. Schoeck, Phil. Mag. *A*, **63**, 111 (1991).

3. J.R. Rice, J. Mech. Phys. Solids, **40**, 239 (1992).

4. A.H.W. Ngan, Phil. Mag. Lett., **72**, 207 (1995).

5. A.H.W. Ngan, J. Mech. Phys. Solids, **45**, 903 (1997).

6. A.H.W. Ngan and H.F. Zhang, to appear in Mech. Mater.