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The effect of external dislocations on the crack tip process

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Abstract. We discuss the influence of external dislocations on the crack tip process mainly using the superdislocation pair model. We present a detailed comparison of dislocations emitted from external sources and dislocations emitted from the crack source. The results show that external dislocations play a very significant role in the crack tip process.

1. Introduction

During the last 10 years, interest in the subject of dislocation emission from a crack has increased because direct observations of dislocation behaviour at a crack tip are possible with the help of new techniques such as TEM, but most theories (see, e.g., Dai and Li 1982, Sinclair and Finnis 1983, Majumdar and Burns 1983, Ohr 1985, Li 1986, Pande *et al* 1988) have only discussed the influence of crack-tip-generated dislocations on the crack tip process, and anti-shielding dislocation behaviour at the crack tip has not been understood very well. However, external dislocation sources nearly always exist in a material and, when these sources are sufficiently close to the crack, the stress concentration can cause them to operate even if the crack source does not operate. If the applied stress increases adequately, dislocations will be emitted from both the crack and external sources; this has been observed experimentally (Ohr 1986). It is worth mentioning that, by TEM, Ohr (1987) has indeed observed negative dislocations at the immediate crack tip in stainless steel and, with the etch pit technique, Narita *et al* (1987) have found many dislocation dipoles around a crack tip in NaCl. The existence of negative dislocations at a crack tip has been pointed out by one of the present authors and a co-worker (Lung and Xiong 1983). Although major dislocations may be shielding dislocations emitted from a crack tip (Hmelo *et al* 1983, Chia and Burns 1984), the influence of anti-shielding dislocations on a crack tip process can be appreciable because they are closer to the crack tip owing to the strong attractive force. The aim of the present paper is to discuss the effects of external dislocations on the crack tip process, mainly using a superdislocation pair model.

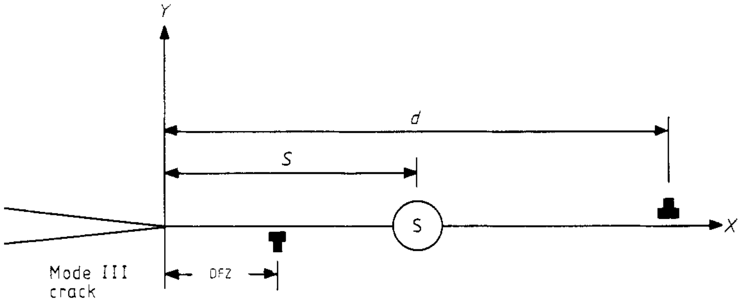

Figure 1. A pair of screw dislocations emitted from an external source labelled S in front of a sharp mode III crack: DFZ, dislocation-free zone.

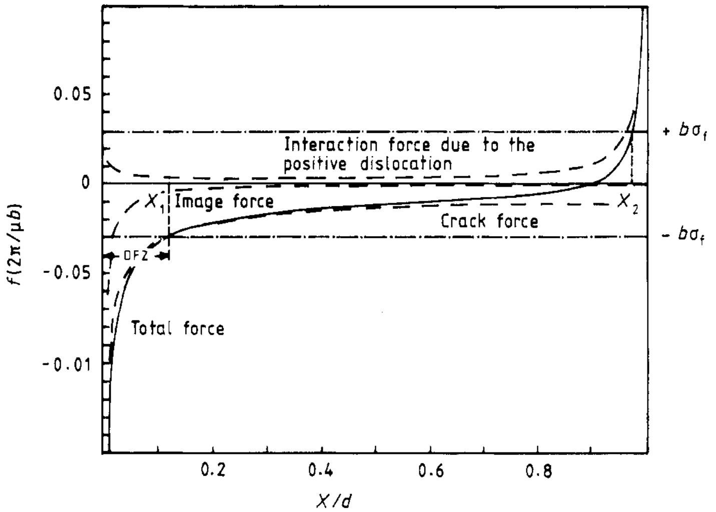

Figure 2. The force on the negative external dislocation near a crack tip of a mode III crack ($d/b = 900$; $2\pi\sigma_f/\mu = 0.03$; $K_{III}\sqrt{2\pi}/\mu\sqrt{b} = 0.3$.

2. Analysis

We assume that a dislocation source exists in front of a sharp crack (mode III), from which a pair of screw dislocations with opposite Burgers vectors has been emitted. The positive dislocation is blocked by a barrier and the negative dislocation moves along the coplanar slip plane as shown in figure 1.

In terms of the analysis of Li (1981), we obtain the force exerted on the negative external dislocation at X:

$$f = (K_{III}/\sqrt{2\pi X})(-b) + [\mu(-b)/2\pi]\{-(-b)/2X + (\sqrt{d}/\sqrt{X})[-b/(d - X)]\} \qquad (1)$$

where K_{III} is the stress intensity factor at crack tip, μ is the shear modulus and b is the Burgers vector. The first term is due to the applied stress; the second term (or the first term in the braces) is its own image force. Here, we used the image force expression for a free plane for simplicity though we have derived a more rigorous one for a finite-length crack (Zhou and Lung 1988); the third term is due to the positive external dislocation. These three forces are plotted in figure 2. The distances at which the force on the negative

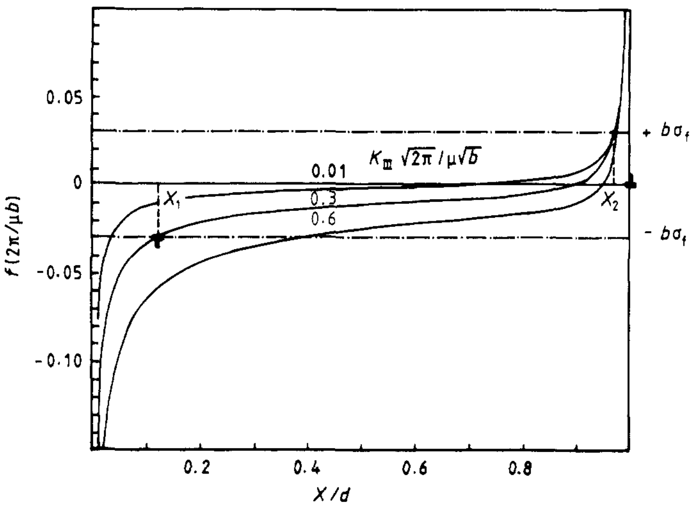

Figure 3. The effect of the crack tip stress intensity on the force exerted on the negative external dislocation ($d/b = 900$; $2\pi\sigma_f/\mu = 0.03$).

external dislocation equals the frictional force are indicated by X_1 and X_2, respectively, and X_1 corresponds to σ_f; X_2 corresponds to $-\sigma_f$ where $\sigma_f > 0$, as shown in figure 2. The value of X_1 can be found from the equation

$$(-b)\sigma_f = K_{III}(-b)/\sqrt{2\pi X} + [\mu(-b)/2\pi]\{-(-b)/2X + (\sqrt{d}/\sqrt{X})[-b/(d-X)]\} \tag{2}$$

which is not very easy to solve. In fact, we are only interested in the X_1 when $X_1 \ll d$ and the X_2 when $X_2 \to d$.

For $X_1 \ll d$, we reduce $d - X_1$ to d; therefore from (2) we obtain

$$\sigma_f \simeq K_{III}/\sqrt{2\pi X_1} + \mu b/4\pi X_1 - (\mu\sqrt{d}/2\pi\sqrt{X_1})(b/d). \tag{3}$$

Let $t = 1/\sqrt{X_1}$; then

$$(\mu b/4\pi)t^2 + (K_{III}/\sqrt{2\pi} - \mu b/2\pi\sqrt{d})t - \sigma_f \simeq 0 \tag{4}$$

whose roots are given by

$$t \simeq (2\pi/\mu b)(-m \pm \sqrt{m^2+n}) \tag{5}$$

where

$$m \equiv K_{III}/\sqrt{2\pi} - \mu b/2\pi\sqrt{d}$$
$$n \equiv (\mu b/\pi)\sigma_f \tag{6}$$

because $\sqrt{m^2+n} > |m|$, and $t > 0$, the reasonable solution is

$$t \simeq (2\pi/\mu b)(-m + \sqrt{m^2+n}) \tag{7}$$

i.e.

$$X_1 \simeq [(2\pi/\mu b)(-m + \sqrt{m^2+n})]^{-2}. \tag{8}$$

It can be seen that X_1 increases with increasing K_{III} because $dX_1/dK_{III} > 0$ and decreases with increasing σ_f because $dX_1/d\sigma_f < 0$, which are in agreement with the numerical results in figure 3.

Similarly, when $X_2 \to d$, we choose $\sqrt{d}/\sqrt{X_2} \to 1$, $K_{\mathrm{III}}/\sqrt{X_2} \to K_{\mathrm{III}}/\sqrt{d}$ and $\mu b/4\pi X_2 \to \mu b/4\pi d$; therefore the simplified equation for X_2 is given by

$$-\sigma_{\mathrm{f}} \simeq K_{\mathrm{III}}/\sqrt{2\pi d} + \mu b/4\pi d - (\mu b/2\pi)[1/(d - X_2)]. \tag{9}$$

Hence

$$X_2 \simeq d - 2\mu b d/(4\pi d\sigma_{\mathrm{f}} + 2\sqrt{2\pi d}K_{\mathrm{III}} + \mu b). \tag{10}$$

Obviously, equation (10) states that X_2 increases with increase in either K_{III} or σ_{f}, which also fit the numerical results in figure 3. From equation (1) and figure 2, we see that the force on the negative dislocation is dominated by the image force when $X \ll d$; when $X \to d$, then the interaction force due to the positive dislocation dominates. The negative dislocation is attracted towards the crack tip and annihilated by the crack if the distance is less than X_1; it cannot move between X_1 and X_2 because the force is smaller than the lattice friction; it will be attracted towards the positive dislocation if it is placed between X_2 and d. If the applied stress becomes large enough to make $d - X_2$ approach the shortest distance L between nucleated negative and positive external dislocations (for a Frank–Read source, the length of the pinned dislocation segment), it will be stabilised by the lattice friction so that it will not disappear into the external dislocation sources, i.e. the external dislocation pair has been emitted. The critical stress intensity factor at a crack tip required for an external screw dislocation pair emission is then given by

$$K_{\mathrm{III\,pair}} = \sqrt{2\pi(S - L/2)}(-\sigma_f + \mu b/2\pi L). \tag{11}$$

In equation (11), we have neglected the effects of image force on the external dislocation pair emission because these are not important for X_2 larger than ten lattice spacings or so. Generally, any dislocation source will be positioned well beyond this distance (Lin and Thomson 1983).

Since the negative dislocation in the region $X < X_1$ is attracted to the crack tip, negative dislocation annihilation at the crack can occur if K_{III} is sufficiently large that X_1 is larger than r_{c}, the core radius of a dislocation. Thus the condition for the negative dislocation of an external dislocation pair annihilation at a crack is

$$X_1 \geqslant r_{\mathrm{c}}$$

or

$$K_{\mathrm{III}} \geqslant K_{\mathrm{IIIa}}^{-} \tag{12}$$

where

$$K_{\mathrm{IIIa}}^{-} = \sqrt{2\pi r_{\mathrm{c}}}[\![\sigma_f - (\mu/2\pi)\{b/2r_{\mathrm{c}} - (\sqrt{d}/\sqrt{r_{\mathrm{c}}})[b/(d - r_{\mathrm{c}})]\}]\!] \tag{13}$$

where K_{IIIa}^{-} is its critical stress intensity factor obtained from equation (2).

According to Majumdar and Burns (1981), the stress intensity factor at a crack tip due to an emitted external dislocation pair is given by

$$K_{\mathrm{IIId}} = -(\mu/\sqrt{2\pi})(-b/\sqrt{X} + b/\sqrt{d}). \tag{14}$$

The first and second terms are due to the negative and positive dislocations, respectively.

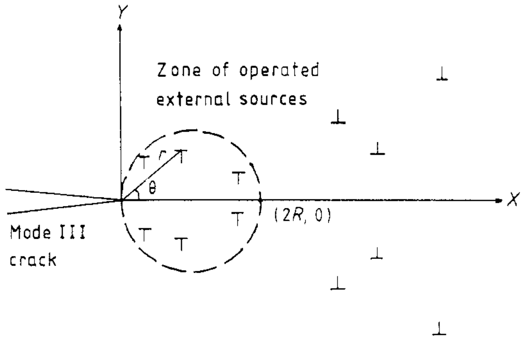

Figure 4. Schematic diagram showing two-dimensional distribution of negative and positive external dislocations near a sharp mode III crack tip.

The stress exerted on the external source for dislocation can be written as

$$\sigma_s = K_{\mathrm{III}}/\sqrt{2\pi S} + \sigma_d \tag{15}$$

where

$$\sigma_d \equiv (\mu\sqrt{X}/2\pi\sqrt{S})[b/(X-S)] - (\mu\sqrt{d}/2\pi\sqrt{S})[b/(d-S)]. \tag{16}$$

The first term in (15) is due to the applied stress; the first and second terms in (16) are due to the negative and positive dislocations, respectively. Because $X < S < d$, we see that $\sigma_d < 0$, i.e. an external dislocation pair shields the external source.

To simulate real materials further, let us consider external sources which may not lie on the crack planes as shown in figure 4. Suppose that only the sources in the circular zone in front of the crack tip will be operated, and the emitted positive dislocations move away from the zone and their shielding effects on the crack tip will be neglected; the negative dislocations are localised in the circle, whose density is assumed roughly to be

$$D^- \simeq g\sqrt{2R}/\sqrt{r} \tag{17}$$

where R is the radius of the circular zone and g is a parameter mainly related to the density of external source and the difference between the resultant stress exerted on it and the critical stress required to operate it. For simplicity, we assume g to be constant.

Then the total number of negative dislocations is given by

$$N^- \simeq \int_{-\pi/2}^{\pi/2}\int_0^{2R\cos\theta} g\frac{\sqrt{2R}}{\sqrt{r}}\, r\,\mathrm{d}r\,\mathrm{d}\theta \tag{18}$$

i.e.

$$N^- \simeq 4.66R^2 g. \tag{19}$$

According to Rice and Thomson (1974), the stress intensity factor at the crack tip due to a negative dislocation located at (r, θ) is given by

$$K_{\mathrm{III}}(r,\theta) = -[\mu(-b)/\sqrt{2\pi r}]\cos(\theta/2). \tag{20}$$

Thus, if we ignore the geometrical change in the shape of the crack tip owing to the negative external dislocation annihilation at the crack, the resultant stress intensity factor due to the negative dislocations is given by

$$K_{\mathrm{IIId}}^{-} \simeq \int_{-\pi/2}^{\pi/2} \int_{0}^{2R\cos\theta} \left(-\frac{\mu(-b)}{\sqrt{2\pi r}}\right) \cos\left(\frac{\theta}{2}\right) g \frac{\sqrt{2R}}{\sqrt{r}}\, r \, \mathrm{d}r \, \mathrm{d}\theta. \tag{21}$$

After some calculation, we have

$$K_{\mathrm{IIId}}^{-} \simeq -2.12\mu bgR\sqrt{R}. \tag{22}$$

Suppose the critical stress for external dislocation source operation to be σ_{op}; then the critical stress intensity factor at the crack tip required for external source operation is

$$K_{\mathrm{IIIs}} = \sigma_{\mathrm{op}}\sqrt{2\pi S}. \tag{23}$$

To compare this with the case of dislocations generated from a crack tip, we choose the critical stress intensity factor for dislocation emission from a crack defined by Ohr (1985), i.e.

$$K_{\mathrm{IIIe}} = \mu b/\sqrt{8\pi r_{\mathrm{c}}} + \sigma_{\mathrm{f}}\sqrt{2\pi r_{\mathrm{c}}}. \tag{24}$$

3. Discussion and conclusions

To obtain a qualitative insight into the problem, we made some crude numerical estimates. Let $r_{\mathrm{c}} = b/2$ and $\sigma_{\mathrm{f}} = \sigma_{\mathrm{op}} = \mu/100$.

(i) From (13) and (24), we see that $K_{\mathrm{IIIa}}^{-} < K_{\mathrm{IIIe}}$ if $d > 1.3b$. When $d \geqslant 3.3b$, $K_{\mathrm{IIIa}}^{-} \leqslant 0$. Those results show that negative external dislocation annihilation at a crack is much easier than dislocation emission from the crack tip. In other words, an external dislocation can be annihilated at a crack before a dislocation can be emitted from the crack tip. In fact, for dislocation emission from the crack tip, the applied stress is mainly required to overcome image force F_{i} which is much larger than lattice friction F_{f} at the immediate crack tip (e.g., when $X = r_{\mathrm{c}}$, $F_{\mathrm{i}} \simeq 16F_{\mathrm{f}}$); however, for the negative dislocation in the annihilation of an external dislocation pair at the crack, the applied stress is mainly required to overcome lattice friction. From the viewpoint of energy, we see, when a dislocation whose Burgers vector is normal to the fracture plane is emitted from a crack tip, the energy provided is approximately $\mu b^2 + \gamma b$ whereas, when a negative dislocation corresponding to the above dislocation annihilates at the crack, the net energy change is approximately $\mu b^2 - \gamma b$, which is positive because for many materials the surface energy γ has an order of magnitude of $\mu b/20$. We think that this is one of the reasons that the existence of negative dislocations at the crack tip has not been observed commonly.

(ii) Since $X < d$, we have $K_{\mathrm{IIId}} > 0$ from (14), i.e. the net effect of an external dislocation pair on the crack is anti-shielding. Let $d = 200b$ and $K_{\mathrm{III}} = 0$; then we have $X_1 \simeq 9b$ from (8). In this case, $K_{\mathrm{IIId}} \simeq 48\%\ K_{\mathrm{IIIe}}$. Hence, we think that external dislocations can play a significantly promotive role in dislocation emission. This might be one of the reasons that the measured values of K_{IIIe}, which are about 50 kPa m$^{1/2}$ in LiF (Burns 1986) were much lower than the theoretical values, which are about 230 kPa m$^{1/2}$, evaluated by using the theories of Rice and Thomson (1974) and Chang and Ohr (Ohr 1985).

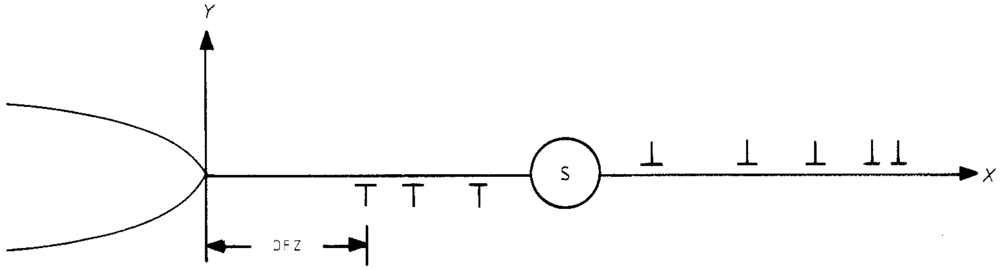

Figure 5. The positive external dislocations and the remaining negative external dislocations are in equilibrium in front of the blunted crack.

(iii) For a Frank–Read source, if $L \geqslant 16b$, we have $K_{\mathrm{III\,pair}} \leqslant 0$ from (11).

(iv) From (23) and (24), we see that, if $S < 143b$, then $K_{\mathrm{IIIs}} < K_{\mathrm{IIIe}}$. According to (iii) and (iv), we find that, if an external source is sufficiently close to a crack, it can emit dislocations more easily than the crack, which is in agreement with Hockey's observations for MgO (Thomson 1986), i.e. there are many cases where sources of dislocations operate near the crack position (or near a previous crack position), but only a few where the crack itself may have been the source of the dislocations.

(v) We describe the diameter of the circular zone for operating external sources approximately as the largest distance at which external sources operate while the crack source does not operate, i.e. $2R = 143b$. Then $K_{\mathrm{IIId}}^{-} > K_{\mathrm{IIIe}}$ if the total number of negative dislocations in the circular zone is given by $N^{-} > 5.5$ (i.e. $g > 2.6 \times 10^{15}\ \mathrm{m}^{-2}$) assuming that $b = 3 \times 10^{-10}$ m. Although very crude, this order-of-magnitude calculation suggests that the effect of external dislocations on dislocation emission from the crack tip is very appreciable even if the external negative dislocation density near a crack tip is not very large (the dislocation densities for a recrystallised metal and for a heavily worked metal are roughly $10^{11}\ \mathrm{m}^{-2}$ and $10^{17}\ \mathrm{m}^{-2}$, respectively).

In terms of the discussion above, we can obtain the following physical picture: when $k_{\mathrm{pair}}, k_{\mathrm{a}}, k_{\mathrm{s}} < k < k_{\mathrm{c}}, k_{\mathrm{e}}$ (where k is the local stress intensity factor at the crack tip and k_{c} is the critical stress intensity factor for brittle fracture), external dislocation sources such as a Frank–Read source, which are sufficiently close to the crack tip, are activated to emit dislocation pairs with opposite Burgers vectors. Positive dislocations are repelled away from the crack and blocked by barriers, such as grain boundaries and inclusions, and pile up against the barriers; negative dislocations are attracted strongly towards the crack tip and some of them annihilate at the crack, the crack is therefore blunted and leaves behind a DFZ in front of the crack tip. Because k decreases very little owing to the blunting effect at the crack tip (e.g. elliptical or semi-elliptical (edge) crack under uniform normal remote stress) K_{I} refers to that point of the crack front when its value is greatest. K_{I} decreases monotonically with increasing B/A. K_{I} for $B/A = 1$ is about $2/\pi$ times as large as K_{I} for $B/A = 0$, where A and B represent half the lengths of the short and long axes, respectively, of the crack (Hellan 1984); the net effect of external dislocations on the crack should be shielding so that $k < k_{\mathrm{a}}$ if positive dislocations and remaining portions of negative dislocations reach an equilibrium distribution as sketched in figure 5. On the contrary, the net effect of the dislocation pairs on the external source is to reduce the driving force applied by the crack stress field; finally the process of external source operation and negative dislocation annihilation at the crack both stop. If negative dislocations pile up against barriers in front of the crack tip, the anti-shielding effect is likely to appear. Further understanding is needed to obtain the solution to the whole process. One method which may be used is a computer technique based on the discrete-dislocation model. One shortcoming in previous calculations of the dislocation equilibrium configurations is the assumption that the resultant stress σ exerted on each dislocation equals the constant lattice friction σ_f but in fact, when $-\sigma_f < \sigma < \sigma_f$, equilibrium still exists. Hence if equilibrium equations are established from the viewpoint of energy and satisfy the energy minimisation principle, namely that the total energy associated with the configuration is a minimum, these problems can be avoided and the stable dislocation configuration solution can be obtained. Of course, this complicated problem is intractable, partly because of existence of irreversible frictional forces which lead to the path-dependent energy associated with the configuration and partly because of the existence of dislocation annihilation at the crack which needs to be handled from the atomistic point of view. Because external negative dislocations around a crack tip, which may be closest to the crack tip, will influence dislocation emission from the crack tip by annihilating or forming locked dipoles with negative dislocations, or moving away from the crack tip through the negative dislocation screen with difficulty, we think it necessary to consider their contribution when discussing DFZ formation.

In view of discussion above, we feel that the external dislocations play a very significant role in the crack tip process and should be taken into account adequately.

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