Dynamic Emission of Dislocations From a Moving Crack

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The emission of dislocations from a propagating crack in the mode II or III situations is studied by computer simulation. While the crack is moving the steady state number of dislocations is smaller than the saturation number which could be emitted from a stationary crack and such a steady state number decreases with increasing crack velocity. The effect on the emission process of the applied stress, the lattice friction for dislocation motion and the critical stress intensity factor for dislocation emission is studied. The results include also the plastic zone size, the dislocation distribution, the dislocation-free zone, and the instantaneous crack velocity. The average crack velocity does not depend on the applied stress but depends only on the critical stress intensity factor for dislocation emission. When such a factor is zero as assumed in some theories, the crack does not move at all.

Introduction

A recent surge of interest [1–6] in the dislocation-crack interactions stem from the realization that it takes a critical stress intensity factor K_D at the crack tip to emit a dislocation. The importance of this critical factor can be seen from the following: In the BCS theory [7] in which they assumed K_D to be zero, the dislocation distribution in front of the crack at equilibrium resembles an inverted pileup, namely, the density is infinite at the crack tip. As a result the BCS theory cannot explain the existence of a dislocation-free zone recently observed [8, 9] near the crack tip. Another consequence of zero K_D is that the crack tip is completely shielded from the external stress so that the crack cannot propagate as will be shown also later in this study. In fact the steady state velocity of a crack with its plastic zone is related to K_D rather than to the applied K.

While K_D has been estimated for a sharp crack [10] and has been found consistent with the size of the dislocation-free zone [11], the effective value of K_D may depend on crack blunting and the various dislocation activities at the crack tip which may affect the crack tip geometry. It seems advisable to allow K_D to be a variable and to see how K_D may affect the dislocation-crack interactions.

In a previous computer simulation study [12], dislocations are emitted one by one from a stationary crack under load. Each dislocation moves according to a power law of the shear stress exerted on it minus a friction stress. The dislocations must move sufficiently away from the crack tip in order to have the crack tip stress intensity factor exceeding the critical value for dislocation emission. Then a new dislocation will be emitted. This emission process will continue until the plastic zone is saturated. The number of dislocations emitted as a function of time, the rate of emission of dislocations, the strain in the plastic zone, the plastic zone strain rate, the plastic zone size, the dislocation distribution, and the dislocation-free zone during the emission process have all been reported. The present study is an extension of the previous one except that the crack is now moving at a speed which varies with a power (exponent = 3) function of the effective stress intensity factor at the crack tip. The results will include both the behavior of the plastic zone and the speed of crack extension.

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Computation

A semi-infinite crack in the xz plane has its tip at $x = x_c$ parallel to the z axis and extends in the $-x$ direction. The length of the crack, l, is assumed very large so that it remains essentially constant when the crack tip advances. As before [12] the mode of the crack depends on the applied stress σ (σ_{yy} for mode I crack, σ_{xy} for mode II crack and σ_{yz} for mode III crack) and so does the Burgers vector of the dislocations emitted from the crack. The emitted dislocations are all parallel to the crack tip or to the z axis and moving in the x direction. The motion is climb for mode I cracks and slip for mode II and III cracks.

Before any dislocation is emitted, the stress intensity factor K at the crack tip is $\sigma\sqrt{2\pi l}$. The crack velocity is assumed to have a power law relation with the stress intensity factor:

$$v_c = \frac{dx_c}{dt} = bM_c\left(\frac{K}{A\sqrt{2\pi b}}\right)^{\eta} \tag{1}$$

where b is the Burgers vector of dislocations, M_c is the crack mobility which is assumed constant, A is $\mu b/2\pi(1-\nu)$ for edge dislocations and $\mu b/2\pi$ for screw dislocations with μ being the shear modulus and ν the Poisson ratio. In other words, the crack tip position changes with each Δt increment as follows

$$\frac{x_c'}{b} = \frac{x_c}{b} + \left(\frac{K}{A\sqrt{2\pi b}}\right)^{\eta} M_c\Delta t \tag{2}$$

The exponent η is assumed to be 3 in this calculation.

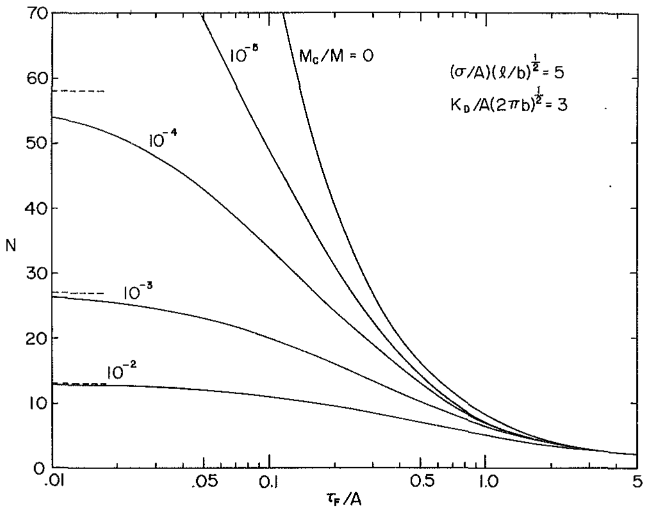

Fig. 1 Steady state number of dislocations emitted from a propagating crack as a function of lattice friction for dislocation motion

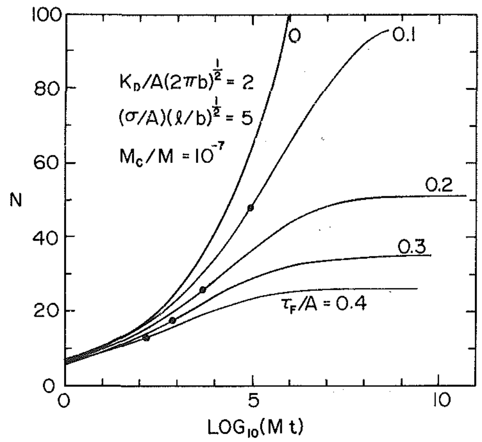

Fig. 2 Emission of dislocations from a propagating crack, effect of lattice friction for dislocation motion

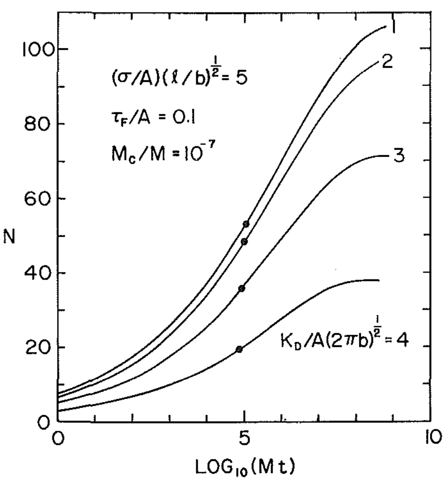

Fig. 3 Emission of dislocations from a propagating crack, effect of the critical stress intensity factor for dislocation emission, the case of small crack mobility

If K exceeds a critical value K_D for dislocation emission, a dislocation will be emitted from the crack tip and will be placed at a position [12] in front of the crack so that it can move away from the tip. In the meantime, the stress intensity factor at the crack tip is modified by the shielding effect of the dislocations:

$$\frac{K}{A\sqrt{2\pi b}} = \frac{\sigma}{A}\sqrt{\frac{l}{b}} - \sum_i \sqrt{\frac{b}{x_i - x_c}} \tag{3}$$

where x_i are the positions of all the emitted dislocations. As a result, the crack velocity depends not only on the applied stress but also on the distribution of dislocations in front of the crack tip. Hence immediately after a dislocation is emitted, the crack may stop its growth momentarily until the emitted dislocation moves away.

Each emitted dislocation moves according to a power law of the effective stress exerted on it, namely, the position of the ith dislocation, x_i, changes with each increment of time Δt as follows:

$$\frac{x_i'}{b} = \frac{x_i}{b} \pm M(\Delta t)\left|\frac{\tau_i \mp \tau_F}{A}\right|^3 \tag{4}$$

where the upper sign is for the forward motion or when $\tau_i > \tau_F$ and the lower sign is for the backward motion or when $\tau_i < -\tau_F$ with τ_F being the frictional stress. The factor M is the mobility of the dislocations and is assumed constant. The dislocation does not move when

$$-\tau_F < \tau_i < \tau_F. \tag{5}$$

The stress exerted on the ith dislocation is given by

$$\tau_i = \sigma\sqrt{\frac{l}{x_i - x_c}} - Ab\left[\frac{1}{2(x_i - x_c)} + \sum_{j \neq i}^{n}\left(\frac{1}{x_i - x_c + \sqrt{(x_i - x_c)(x_j - x_c)}} + \frac{1}{x_j - x_i}\right)\right] \tag{6}$$

where the first term on the right hand side is due to the applied stress modified by the presence of the crack, the second term or the first inside the brackets is due to its own image dislocation distribution, the third term or the first in the summation is due to the image dislocation distribution of all other dislocations and the last term or the second in the summation is due to the other dislocations themselves. These have been explained before [12].

The computation begins with a virgin crack under an applied stress σ without any dislocations. While the crack moves according to equation (1) it emits dislocations whenever the stress intensity factor K given by equation (3) reaches a critical value K_D. In the meantime all the emitted dislocations move according to equation (4) with τ_i given by equation (6). The purpose is to study such dynamic emission process which affects the crack growth in terms of given variables σ, K_D, τ_F and M_c/M.

Results

1. Steady State Dislocation Emission. For a stationary crack, the number of dislocations which can be emitted at saturation is [4]

$$N = \frac{\sigma^2 l - (K_D^2/2\pi)}{2Ab\tau_F} \tag{7}$$

However, for a moving crack, this will be an upper limit for the number which the crack can emit before it reaches a steady state motion, namely, when the whole system, crack and all the dislocations in front of it, moves at the same velocity. The reason is simply that, since the crack moves in the same direction as the dislocations, it detracts from the time allowed for all the dislocations to move away so as to fully exercise its capability of emitting dislocations. In fact the faster the crack moves, the less is the number of dislocations emitted by the crack during the steady state motion. This is shown in Fig. 1 in which the total number of dislocations emitted during the steady state motion is plotted versus the lattice friction for a given applied stress and a given critical stress intensity factor

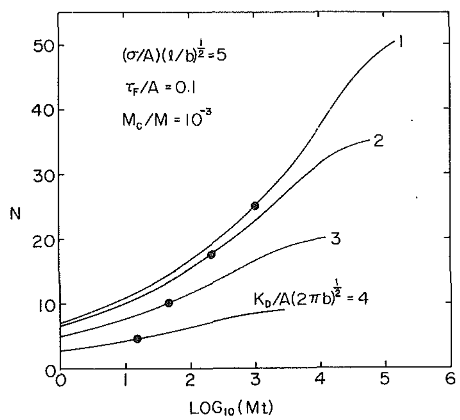

Fig. 4 Emission of dislocations from a propagating crack, effect of the critical stress intensity factor for dislocation emission, the case of large crack mobility

for dislocation emission. The curve marked $M_c/M = 0$ is for a stationary crack and represents equation (7). The asymptotic values indicated by the dotted lines are for zero lattice friction for which there are no saturation values for a stationary crack.

2. Rate of Dislocation Emission. The number of dislocations emitted as a function of time while the crack is propagating is shown in Fig. 2 for the conditions indicated. The behavior is similar to that of a stationary crack [12], namely, it takes many orders of magnitude of time to advance from having a few dislocations emitted to almost "full" emission at the steady state. The time needed for 50 percent emission is a strong function of lattice friction as shown. Unlike the case of the stationary crack, there is a maximum to the steady state number of dislocations which can be emitted even for zero lattice friction when the crack is moving.

When the crack velocity is slow or its mobility is small, the time needed to emit a steady state number of dislocations does not seem to depend much on the critical stress intensity factor K_D for dislocation emission as shown in Fig. 3. This is similar to the case of a stationary crack [12]. However, when the crack velocity is high or its mobility is large, the time needed for saturation seems to depend on K_D as seen in Fig. 4. For larger K_D it seems to take less time to emit a smaller number of dislocations at the steady state.

Also similar to the case of a stationary crack, the time needed to emit the steady state number of dislocations while the crack is moving does not seem to be affected much by the applied stress as seen in Fig. 5. The point on each curve represents 50 percent saturation of the steady state value. When the applied stress increases, the number of dislocations at saturation increases also. Apparently the increased rate of emission is sufficient to keep the saturation time nearly the same.

3. Plastic Zone Size. As before [12] the size of the plastic zone is defined as the distance between the crack tip and the position of the farthest dislocation after n dislocations are emitted and just before the $(n + 1)$th dislocation is about to be emitted. As in the case of a stationary crack, the plastic zone size during the emission process while the crack is moving is proportional to n^2:

$$X_n \propto n^2 \tag{8}$$

In addition, such a relation is independent of lattice friction as found before [12]. Now it is found that such a relation is also independent of the crack mobility M_c as seen in Fig. 6. However, it does depend on the applied stress σ and the critical stress intensity factor for dislocation emission as presented before [12].

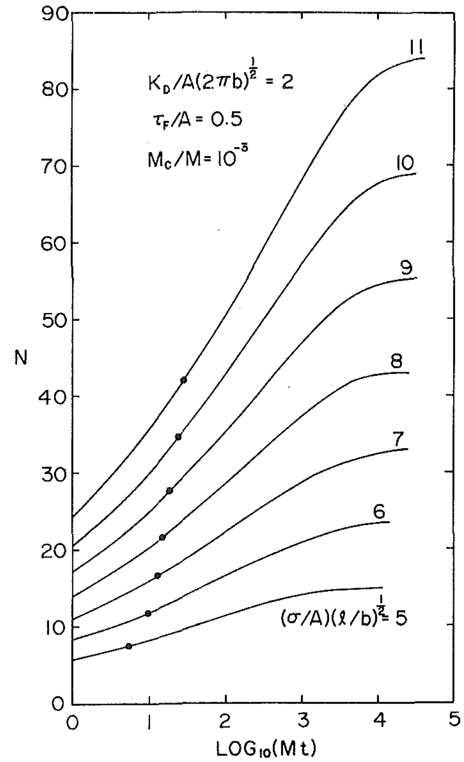

Fig. 5 Emission of dislocations from a propagating crack, effect of external load or the applied stress intensity factor

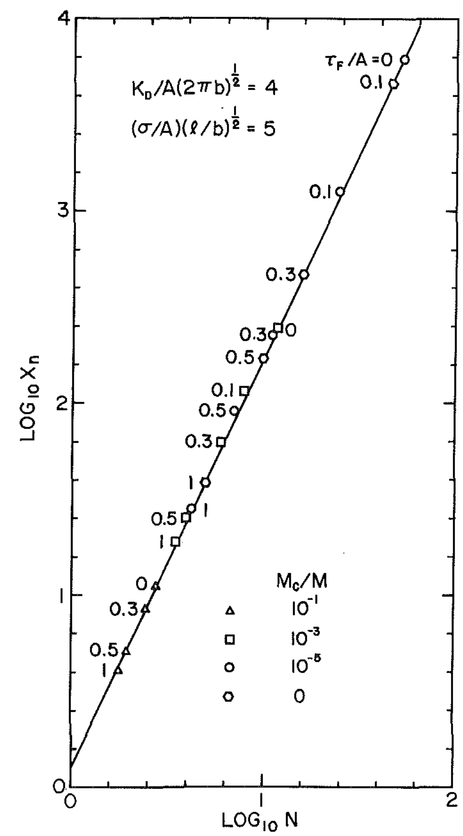

Fig. 6 The relation between plastic zone size and the number of dislocations emitted showing its independence to crack mobility and the lattice friction for dislocation motion

4. Dislocation Distribution. The dislocation distribution in front of a moving crack as they are being emitted is also similar to that of the stationary crack, namely, it begins by concentrating near the tip and gradually spreading out more

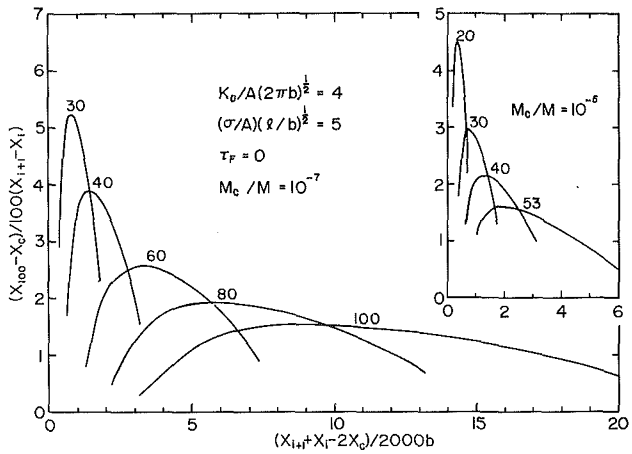

Fig. 7 The dynamic distribution of dislocations emitted from a propagating crack

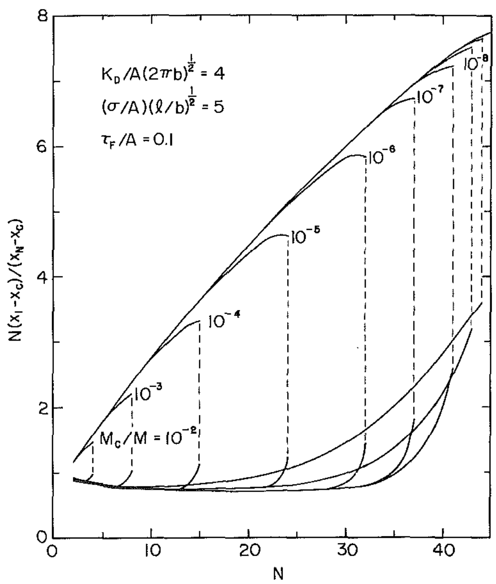

Fig. 8 The dislocation-free zone in front of a propagating crack during dislocation emission and after unloading

homogeneously throughout the plastic zone as shown in Fig. 7. At all the stages of the emission process it is obvious that a dislocation-free zone exists under the given conditions. For a larger crack mobility (insert in Fig. 7) the steady state number of dislocations is smaller but the behavior is similar.

5. Dislocation-Free Zone. The dislocation-free zone as indicated by the ratio of the distance of the nearest dislocation from the crack tip to the average spacing between dislocations is shown in Fig. 8 where such ratio is plotted as a function of the number of dislocations emitted. It is seen that such a ratio increases during dislocation emission and finally reaches a steady state value at saturation. This saturation value increases with decreasing crack mobility and is the largest for a stationary crack. Upon unloading, all the dislocations one by one disappear into the crack. It is seen also in Fig. 8 that the dislocation-free zone during the retraction process is much smaller than that during the emission of dislocations.

6. Crack Motion. Crack propagation is not expected to be smooth during the period of dislocation emission although it is expected at the steady state. The instantaneous crack velocity is shown in Fig. 9 for the conditions indicated. Before any dislocation is emitted, the crack moves at a log v_c = -2.903 using the units in the figure. Counting as $t = 0$ the time when the first dislocation is emitted, the instantaneous

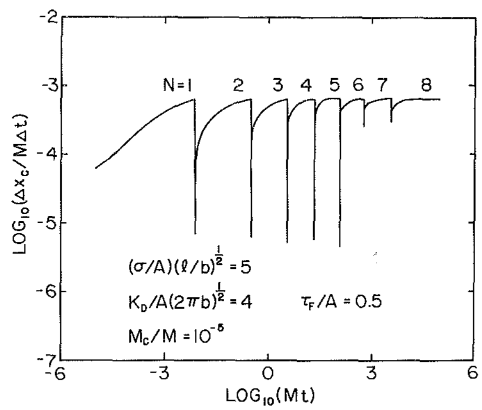

Fig. 9 The instantaneous crack velocity before and after each dislocation emission

crack velocity begins with a small value due to a dislocation-shielded stress intensity factor. As shown, the crack velocity increases when the emitted dislocation moves away. It will reach a value of log $v_c = -3.194$ (when $K = K_D$) before a second dislocation is emitted. The crack velocity drops precipitously at the time each dislocation is emitted and then gradually recovers while all the emitted dislocations are moving away. The velocity will reach a value corresponding to $K = K_D$ before a new dislocation is emitted. The waiting time between successive emissions increases with the number of dislocations already emitted (see Fig. 9). when all the dislocations are emitted at the steady state, the final velocity could reach that corresponding to $K = K_D$.

Because of the velocity drops after each dislocation emission, the overall crack velocity is smaller than that corresponding to $K = K_D$ during the emission period and approaches such a velocity only near the end of or after the emission period. This is shown in Fig. 10. The initial velocity of the crack before dislocation emission should be

$$\frac{\Delta x_c}{\Delta t} = 0.00125\ bM \tag{9}$$

with K due to the applied stress only. Then when the first dislocation is emitted, K drops and so does the crack velocity. During the emission period K fluctuates between K_D and values below K_D but stays longer near K_D when more dislocations are emitted. The situation of $K_D = A\sqrt{2\pi b}$ is probably due to the initial location of the emitted dislocations. The zero K_D situation is the BCS condition [7] and the crack should not propagate at all during or even after the emission process. There is no steady state crack motion for the BCS condition.

That the average crack speed is close to that corresponding to $K = K_D$ is not affected by crack mobility as shown in Fig. 11 in which such mobility varies from 10^{-2}M to 10^{-9}M, even though the steady state number of dislocations in the plastic zone varies from 5 to 44.

Discussion

The present study illustrates clearly the competitive nature of brittle fracture between crack propagation and dislocation emission. It shows also the importance of the critical stress intensity factor for dislocation emission which controls not only the dislocation emission process but also the speed of crack extension. It seems unreasonable to assume that such a critical factor is zero because then there will be no driving force for crack propagation.

Whatever is the relation between the crack velocity and the effective stress intensity factor at the crack tip, the steady state crack velocity with dislocation emission is always that corresponding to K_D, the critical stress intensity factor for

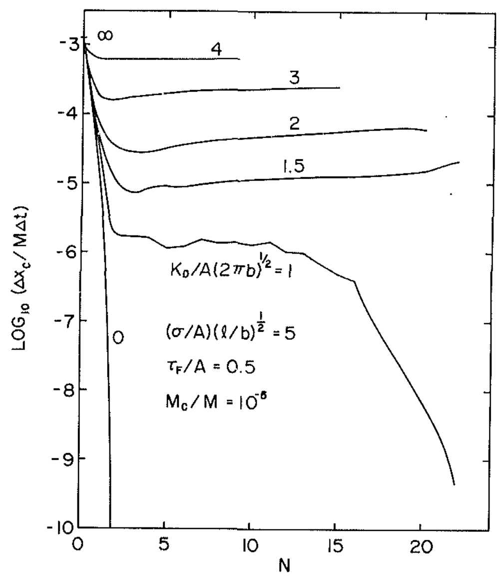

Fig. 10 Average crack velocity between dislocation emissions as a function of the number of dislocations emitted, effect of K_D

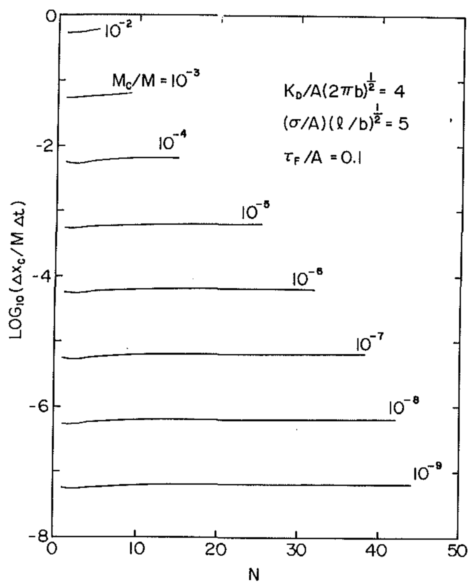

Fig. 11 Average crack velocity between dislocation emissions as a function of the number of dislocations emitted, effect of crack mobility

dislocation emission. Below K_D, no dislocation is emitted and the crack propagates on its own. Above K_D, the emitted dislocations (the more of them the larger the applied stress intensity factor) will reduce the effective K at the tip to a value somewhat below K_D so that the crack velocity cannot exceed that corresponding to K_D. In this respect, K_D is an important parameter separating ductile (small K_D) from brittle (large K_D) materials, as suggested by Rice and Thomson [10]. However, K_D can be altered by microstructural modification.

If K_D is increased but the crack velocity corresponding to K_D remains the same, the plastic zone is smaller and so is the toughness. On the other hand, if K_D remains the same but the crack velocity corresponding to K_D decreases, the plastic zone is larger and so is the toughness. By properly adjusting these two parameters, it is possible to obtain or approach the desirable fracture behavior.

Summary and Conclusions

1. The steady state number of dislocations which can be maintained in front of a propagating crack and moving with the crack at the same speed decreases with increasing crack velocity and with increasing lattice friction τ_F for dislocation motion. It increases with the applied stress σ (or the applied stress intensity factor) and decreases with the critical stress intensity factor K_D for dislocation emission.

2. Starting with a virgin crack without dislocations, an applied stress intensity factor will propagate the crack and, if it exceeds K_D, will at the same time emitting dislocations. The rate of dislocation emission is fast in the beginning and then slows down when more dislocations are emitted until a steady state number is emitted. Then the rate of emission is zero. The time needed to emit the steady state number (or one half of that number) depends strongly on the lattice friction for dislocation motion (shorter for larger friction) and weakly on the applied stress (longer for larger stress). At low crack speeds, the time needed to emit the steady state number of dislocations is independent of K_D. But at high crack speeds it increases with decreasing K_D.

3. The plastic zone size is proportional to the square of the number of dislocations emitted, before or at the steady state. Such a relation is independent of τ_F and the crack speed.

4. The dislocation-free zone always exists unless K_D is zero. Then the crack ceases to propagate and the situation reduces to the case analyzed by BCS [7]. Otherwise the dislocation-free zone grows with increasing number of dislocations emitted but decreases with increasing crack velocity. Unlike the case of a stationary crack, the dislocation-free zone decreases upon unloading when the crack propagates forward into the plastic zone.

5. As in the case of a stationary crack, the dislocation distribution is initially concentrated near the crack tip and gradually spreads out when more dislocations are emitted. The steady state distribution is similar to the equilibrium distribution in front of a stationary crack.

6. The crack stops propagating right after each dislocation emission but accelerates when the dislocation moves away from the tip of the crack. This acceleration continues but decreases in magnitude until another dislocation is emitted. The final crack velocity approaches that corresponding to K_D. The time for crack extension between dislocation emissions increases with the number of dislocations emitted. As a result, the crack extends more and faster when the plastic zone is near saturation. The average crack speed during the emission process is only slightly less than the steady state speed which corresponds to that of K_D.

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