DYNAMIC EMISSION OF DISLOCATIONS FROM A CRACK TIP - A COMPUTER SIMULATION

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INTRODUCTION

A computer simulation of dislocation emission from a crack tip in the Mode II or III situation is presented. A semi-infinite crack is assumed to lie betweeen $x=-\ell$ and $x=0$ in the xz plane. The emitted dislocations are assumed all straight and parallel to the crack tip (z axis) each having the same Burgers vector b. Let the applied stress be σ (σ_{xy} for mode II and σ_{yz} for mode III). Before dislocation emission, the stress intensity factor is $\sigma\sqrt{(2\pi\ell)}$ at the crack tip. If this factor exceeds a critical value K_D, a dislocation will be emitted from the crack tip. Interacting with the crack and the applied stress, this dislocation experiences the following stress (τ_{xy} for mode II and τ_{yz} for mode III) at a distance x:

$$\tau = \sigma \sqrt{(\frac{\ell}{x})} - \frac{Ab}{2x} \qquad (1)$$

for $\ell >> x$, where A is $\mu/2\pi(1-\nu)$ for mode II and $\mu/2\pi$ for mode III with μ being the shear modulus. If this stress exceeds the lattice friction τ_F, the dislocation will move; otherwise it will not. In view of Eq. (1) (see Fig. 3 of reference 1), the space in front of the crack can be divided into four regions separated by the following distances:

$$x_1 = [\sigma\sqrt{\ell} - \sqrt{(\sigma^2\ell + 2Ab\tau_F)}]^2/4\tau_F^2 \qquad (2)$$

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$$x_2 = [\sigma\sqrt{\ell} - \sqrt{(\sigma^2\ell - 2Ab\tau_F)}]^2/4\pi\tau_F^2 \quad (3)$$

and $$x_3 = [\sigma\sqrt{\ell} + \sqrt{(\sigma^2\ell - 2Ab\tau_F)}]^2/4\pi\tau_F^2 \quad (4)$$

The dislocation will be attracted toward the crack for $x < x_1$, will not be able to move between x_1 and x_2, will move away from the crack between x_2 and x_3 and will not be able to move for $x > x_3$. In this computation, the dislocation is placed just beyond x_2 so that it will move away from the crack. This is done for each subsequent dislocation after it is emitted from the crack although the position is no longer given by Eq. (3).

When there are n dislocations in front of the crack, the stress at the ith dislocation is τ_i (see formula in references 1 or 2). If τ_i exceeds τ_F in absolute value, the dislocation moves with a velocity proportional to a power function of the effective stress. In other words, after a small time interval Δt, the new position of the ith dislocation is

$$\frac{x_i'}{b} = \frac{x_i}{b} \pm M(\Delta t)\left|\frac{\tau_i \mp \tau_F}{A}\right|^m \quad (5)$$

where the first sign is for the forward motion and the second for the backward motion. In Eq. (5) M is the mobility and m is the power law exponent (assigned to be 3); both are assumed constant for the entire calculation. To keep the dislocation sequence as they are emitted one by one from the crack tip, the computer is instructed to search for the largest velocity and the smallest spacing and from these to select a proper time interval.

At any time the stress intensity factor at the crack tip is K:

$$\frac{K}{\sqrt{(2\pi)}} = \sigma\sqrt{\ell} - Ab\sum_{i=1}^{n}\frac{1}{\sqrt{x_i}} \quad (6)$$

This factor is calculated after each set of dislocation movement and if it exceeds a critical value K_D for dislocation emission, a new dislocation is emitted from the tip of the crack. This dislocation is placed in a region just beyond the immobility zone as described earlier so that it can move forward. The emission process will continue until a maximum

number is emitted which depends on σ and K_D as follows:

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

The situation reduces to the equilibrium distribution as reported before (2) when τ_i for each dislocation is equal to τ_F. However, the dynamic distribution at the time when all the dislocations stop moving may be somewhat different because the latter condition is

$$-\tau_F < \tau_i < \tau_F. \quad (8)$$

In the simulations in which the crack moves forward also, the crack velocity is assumed to be a power function of K.

RESULTS

The following summarizes the results of such calculations:

(1) The rate of dislocation emission always decreases with time for a given σ, K_D and τ_F. After a certain number of dislocations is emitted, the rate of emission increases with increasing σ, decreasing K_D and decreasing τ_F. The time needed to emit the maximum number of dislocations (or one half of the maximum number) depends strongly on the lattice friction τ_F, weakly on the applied stress σ and is almost independent of K_D. For example, about a factor of hundred increase in time is needed when τ_F decreases from 0.1A to 0.05A, or from 0.3A to 0.1A or from A to 0.3A. In other words, a total of six order of magnitude increase in time between τ_F=A and τ_F=0.05A. This is indeed amazing since the maximum number of dislocations increases by only about one order of magnitude. For the same order of increase of the maximum number of dislocations such as due to a factor of 3 increase in applied stress, the time needed for emitting all dislocations (or one half the maximum number of dislocations) increases by less than an order of magnitude. Similarly within the range of parameters studied, the time needed for emitting the maximum number of dislocations (or one half of that) seems independent of K_D although the maximum number does increase with decreasing K_D.

(2) Similar to the rate of emission of dislocations, the rate of

plastic strain development (total dislocation displacement) increases with increasing σ, decreasing K_D and decreasing τ_F. Also similar to the time needed for emitting the maximum number of dislocations, the time needed to develop the saturation plastic strain depends more strongly on lattice friction than either the applied stress or the critical stress intensity factor for dislocation emission. Within the range of variables studied, the time needed for half saturation of plastic strain varies inversely with the fifth power of lattice friction, depends only about linearly with the applied stress and is almost independent of the critical stress intensity factor for dislocation emission.

(3) The size of the plastic zone (position of the last dislocation) varies with the square of the number of dislocations for any given σ and K_D independent of the lattice friction. Hence the rate of expansion of the plastic zone relates directly to the rate of emission of dislocations. The maximum size of the plastic zone increases with increasing applied stress and decreasing K_D.

(4) The dislocation density (number per unit distance along the x axis) is very high in the beginning. The dislocations are concentrated near the crack tip. With increasing number of dislocations emitted, the maximum density decreases and the dislocations are more uniformly distributed. The distribution approaches the static one obtained before (2) which agrees with the analytic results (3,4) for the continuous distribution of dislocations. Upon unloading, the dislocations one by one disappear into the crack. The number of dislocations left over depends on the lattice friction. The density of dislocations decreases first near the crack tip. Then it spreads to the middle while the plastic zone still expands. The position for peak density shifts to large x or farther away from the crack while the peak density decreases. For non-zero lattice friction, the final distribution will have a peak near the far end of the plastic zone rather than close to the crack tip. When the lattice friction is zero, all dislocations will eventually disappear into the crack.

(5) The dislocation-free zone expressed as the ratio between the position of the first dislocation and the spacing between the first and the second dislocation increases while the dislocations are emitted from the crack. It seems to increase linearly with the number of dislocations emitted when the lattice friction is zero. Compared at the same number of dislocations emitted, it is larger for larger critical stress intensity factor for dislocation emission or smaller applied stress but not much affected by lattice friction. However, compared at the maximum number of dislocation emitted, it is larger for larger critical stress intensity factor for dislocation emission or smaller lattice friction but not much affected by the applied stress. Upon unloading, the dislocation-free zone may decrease first but then it increases while the dislocations disappear into the crack (the zone is calculated after each disappearance). The zone reaches a largest value after the last disappearance. This value may be even larger than that before unloading.

(6) When the crack is allowed to propagate with a velocity proportional to a power function of the effective stress intensity factor, a steady state number of dislocations can be maintained in front of the crack. This number depends on the speed of the crack relative to that of the dislocation. Faster crack speeds can maintain only a smaller number of dislocations.

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