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CALCULATION OF THE EVOLUTION OF PLASTIC YIELDING AT THE TIP OF A CRACK  
AND RELATED PHENOMENA

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The results of a computer calculation of the evolution of plastic yielding at the tip of a crack in a crystal are presented. The plastic yielding at the tip of the crack is due to thermally activated motion of dislocations in active slip planes of the crystal with the simultaneous action of an external tensile stress and thermal fluctuations. The plastic yielding and stress distributions at the tip of the crack at different instants of time are obtained. The effect of the plastic zone on the stress intensity factor (SIF) of the crack is calculated.

1. Introduction. In recent years microscopic models of the processes occurring in the neighborhood of a crack have become more and more widely used when investigating the mechanics of fracture. New ideas (the J-integral, the fine structure of the plastic zone, including the dislocation-free zone, etc.) have been proposed to describe them, while direct electron-microscope observations of the defect structure of the material in the region of the tip of the crack have, in turn, enabled the representation of the mechanics of fracture and the physical nature of the constants by which they operate to be refined.

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The common feature of the development of macroscopic cracks is the formation in front of them of the tip of a plastic zone of different form, the dimensions of which in plastic materials are often comparable with the length of the crack. However, there is still insufficient information on the actual structure of the plastic zone and the laws governing its evolution in different materials and under different loading conditions to be able to draw generalizing conclusions on how the fracture process develops under different conditions [1].

Experimental Results. In [2] it was possible to observe directly, using a transmission electron microscope, the modes of formation of a crack with a plastic zone in stainless steel with resolution of individual dislocations, under conditions III. An analysis of the contrast showed that the dislocations are cleaved screw dislocations. Their total number (greater than 300) corresponds to complete mutual displacement of the edges of the crack of about 90  $\mu\text{m}$ , which does not agree with theory [3]. This is obviously due to the complex geometry of the specimen - a thin foil of varying thickness, in which the crack grows from a thin edge, and in which (due to image forces) dislocations of the same kind are repelled more weakly than in the bulk material.

Another feature of the plastic zone was observed in [4], namely, in a part of the plastic zone, in the immediate vicinity of the tip of the crack, no dislocations are observed (there is a dislocation-free zone). This effect is due to the fact that in the immediate vicinity of the tip of the crack the acting stress is so high that it cannot be counterbalanced by the stress from the dislocations in the plastic zone. A detailed investigation of the dislocation-free zone at the tip of the crack in bulk metal crystals was carried out in [5].

Some Physical Models. Since a simple dislocation description of a crack with a plastic zone is available (proposed in [3] - the BCS model) which enables experimental data on the structure of the plastic zone to be interpreted quite easily, we will dwell in more detail on this model. In it the stress field of a plane crack of length  $2\ell$  under a stress  $\sigma$  is described by the distribution of cleavage dislocation in the section  $(-\ell, \ell)$ . The actual dislocations are distributed in the plastic zone  $(-a, -\ell)$ ,  $(\ell, a)$ . An external stress  $\sigma$  acts on the cleavage dislocations, and a stress  $\sigma - \sigma_0$  ( $\sigma_0$  is the lattice friction stress) acts on the dislocations in the plastic zone. The condition of equilibrium reduces to an integral equation for the distribution function  $\rho(x)$  of the dislocations

$$\frac{\mu b}{2\pi} \int_0^a \frac{\rho(x') dx'}{x-x'} = \sigma(x) - \sigma_0, \quad (1.1)$$

from the solution of which, in particular, the following relation is obtained:

$$\frac{l}{a} = \cos \frac{\pi}{2} \frac{\sigma}{\sigma_0} \quad (1.2)$$

( $\mu$  is the shear modulus and  $b$  is the Burgers vector), defining the dimensions of the plastic zone for a specified crack length  $\ell$ , and also an expression for the mutual displacement of the edges of the crack  $\varphi$ , which is equal to the overall Burgers vector of all  $n$  dislocations in the cluster in  $(+0, \ell)$ :

$$\varphi = b \int_0^l \rho(x') dx' = \frac{4\sigma_0 l}{\pi\mu} \ln \frac{a}{l}.$$

The BCS model was generalized to the case of plastic zones consisting of several clusters of dislocations in slip planes inclined to the plane of the crack at an angle  $\alpha$ . The distribution of the dislocations in the clusters, the stress at the tip, the opening of the tip of the crack  $\delta$ , and the value of the J-integral were obtained in [6] as a function of the angle of inclination  $\alpha$  and the applied stress. A similar model was calculated in [7], where, in particular, an approximate expression was obtained for the distance  $\Delta u$  between the edges of the crack at the point  $x - \ell$  as a function of the length of the crack  $\ell$

$$\Delta u - \delta \approx (l-x) [\ln(l-x)]^\gamma, \quad \gamma \geq 1,$$

and it was also found that the main tensile stress is an order of magnitude greater than the main shear stress along the extension of the plane of the crack in the region of its tip.

The occurrence of dislocations of opposite sign directly at the tip in a model close to [3], was found in [8]. It was assumed in [8] that these "negative" dislocations (due to the effect of image forces) accumulate at the crack and blunt it.

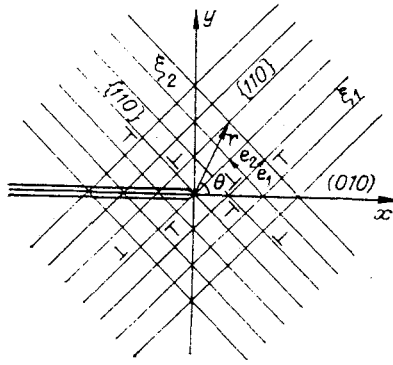


Fig. 1

The behavior of the dislocations in the plastic zone was considered in [9]. Here the conditions for the generation of dislocation loop-dipoles in the region of the crack and the equilibrium configurations of the dislocations are calculated in the discrete approximation.

Screening of the elastic field of the crack by dislocations situated in the plastic zone in different configurations were considered in [10, 11]. In the simplest case of  $2N - 1$  similar screw dislocations, parallel to the tip of the crack of transverse shear (mode III), and situated equidistantly on the surface of a cylinder of radius  $r^*$ , whose axis coincides with the tip of the crack, the reduction in the stress intensity factor is

$$K_D = -\frac{\mu b}{\sqrt{2\pi r^*}} \frac{4N}{\pi}. \quad (1.3)$$

For a dislocation density  $\rho = 10^{10} \text{ cm}^{-2}$  and  $N \approx 19^4$ , we have  $K_D = -50 \text{ MPa}\cdot\text{m}^{1/2}$ , which is comparable with the fracture viscosity of steel at medium temperatures. Consequently, the increase in  $K_c$  in plastic yielding is due not only to blunting of the crack, but also to screening of elastic field by the dislocations.

Hence, new physical models of the rearrangement of the dislocation structure at the tip of the crack in a highly deformed material has enabled the representations on the initiation and growth of cracks to be extended considerably. This paper is devoted to a further development of these ideas.

2. The Dislocation Model of Plastic Yielding at the Tip of a Fixed Plane Crack in a bcc Crystal. A Method of Calculating the Evolution of Plastic Yielding. A crack is situated in the (010) cleavage plane of an infinite crystal having a body-centered cubic lattice (Fig. 1). A uniform stress  $\sigma_{yy}(t) = \sigma_a'(t)$ , which increases monotonically to a value  $\sigma_a$  sufficient for plastic yielding of the crystal but insufficient to increase the crack, is applied to the  $y = \pm\infty$  crystal planes.

Plastic yielding of the crystal is deformation of pure shear along the {110} easy slip planes. The {110} planes, intersecting the xy plane, form two families of slip lines  $\xi_j$  ( $j = 1, 2$ ). The positive directions on the lines are specified by the unit vectors  $e_j$ , making angles  $\beta_j = (\pi/2)j - \pi/4$  with the x axis. The St. Venant plasticity criterion holds for the crystal with a correction for local strengthening of the material. Sources of rectilinear dislocations, perpendicular to the xy plane, are distributed uniformly over xy in the crystal, generating edge dislocations with Burgers vectors  $\pm be_j$ .

As a result of the concentration of the stress at the tip of the crack and the relaxation of the stresses by plastic yielding [12], high densities of effective dislocations are reached in this region (excess dislocations of one sign among dislocations with parallel Burgers vectors) and, consequently, an internal elastic field arises [which does not disappear when the external load  $\sigma_a'(t)$  is removed], which has a considerable effect on the evolution of plastic yielding.

The plastic zones formed in the crystal are immediately adjacent to the tips of the crack and have linear dimensions in the xy plane that are so much smaller than  $\ell$  that we are justified in describing the plastic yielding of the crystal at an individual crack tip as plastic yielding at the tip of a semiinfinite crack.

The rate of plastic yielding in the crystal is determined by the slip of the dislocations along  $\xi_j$  ( $j = 1, 2$ ) with thermally activated surmounting of the energy barriers [13], and over an area with normal  $n_j$  ( $n_1 = e_2, n_2 = -e_1$ ) at the crack tip has the form

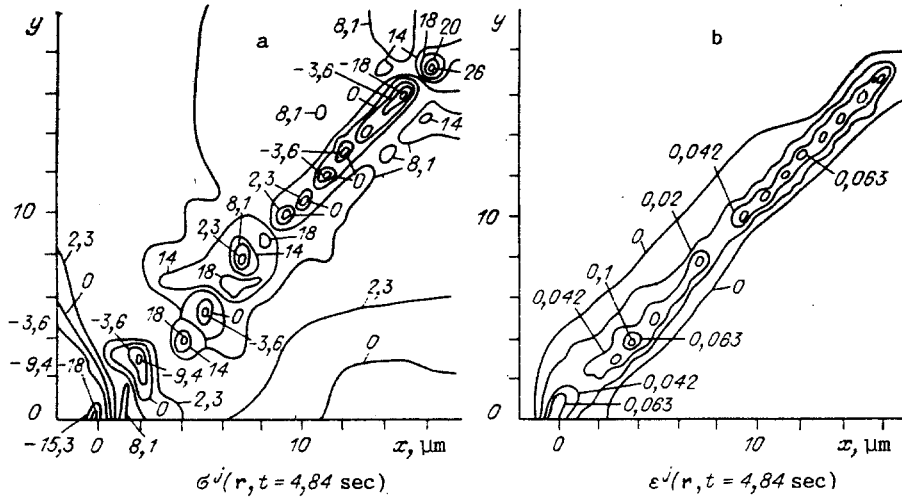


Fig. 2

$$\frac{d\epsilon^j(r, t)}{dt} = \epsilon_0 \exp \left\{ -\frac{U_0 \langle 1 - [\sigma_e^j(r, t)/\tau_0]^{1/2} \rangle}{KT} \right\} \text{sign } \sigma_e^j(r, t), \quad (2.1)$$

where  $\mathbf{r} = xe_x + ye_y$ ,  $(x, y)$  are the coordinates of the point of the plane in a Cartesian rectangular system of coordinates  $xy$ ,  $e_x$  and  $e_y$  are unit vectors specifying the positive direction of the axes of the  $xy$  system of coordinates,  $\epsilon_0$ ,  $\tau_0$ ,  $U_0$ ,  $K$ ,  $T$  are constants ( $U_0$  is the activation energy,  $K$  is Boltzmann's constant, and  $T$  is the temperature), and

$$\sigma_e^j(r, t) = \begin{cases} |\sigma^j(r, t) - \sigma_s(r, t)| \text{sign } \sigma^j(r, t), & \text{if } |\sigma^j(r, t)| > |\sigma_s(r, t)|, \\ 0, & \text{if } |\sigma^j(r, t)| \leq |\sigma_s(r, t)| \end{cases} \quad (2.2)$$

is the effective shear stress on the area with normal  $n_j$ . In (2.2)  $\sigma^j(r, t)$  is the shear stress determined by the components of the stress tensor

$$\sigma(r, t) = \sigma^c(r, t) + \sigma^f(r, t), \quad (2.3)$$

characterizing the elastic field in the region of the crack tip, while

$$\sigma_s(r, t) = \sigma_0 + \sigma_f(r, t) \quad (2.4)$$

is the stress impeding plastic shear due to friction of the lattice  $\sigma_0$  and local strengthening of the material  $\sigma_f$ . In (2.3)

$$\sigma^c(r, t) = K^c(t) (2\pi r)^{-1/2} \Theta(\theta) \quad (2.5)$$

is the stress field external to the crystal [which disappears together with  $\sigma_a^1(t)$ ], which is determined by the Westergaard formulas [14] corresponding to the type of loading for the linear asymptotically elastic field at the tip of the crack, while

$$\sigma^l(r, t) = \sum_{k=1}^2 \int_{D_k} \sigma^k(r, r') \Delta \rho_k(r', t) dr' \quad (2.6)$$

is the stress field produced at the tip of the crack by dislocations of the plastic zone. To calculate  $\sigma_f$  in (2.4) we will use the relation

$$\sigma_f(r, t) = \sigma_1 \left[ \sum_{j=1}^2 |\epsilon^j(r, t)| \right]^m \quad (2.7)$$

( $\sigma_1$  and  $m$  are constants) which is a generalization of the empirical relationship  $\sigma_f = \sigma_1 \epsilon^m$  [13]. In (2.5)  $K^c(t) = \sigma_a^1(t) \sqrt{\pi l}$  is the Irvine stress intensity factor and  $(r, \theta)$  are polar coordinates (see Fig. 1). In (2.6)  $\sigma^k(r, r')$  is the stress tensor of the edge dislocation of the crystal, which intersects the  $xy$  plane at the point  $r'$ , which has a Burgers vector  $b e_k$  and is related to the discontinuity of the displacements on the part  $\xi_k(r')$  lying at the point  $r'$  while

$$\Delta \rho_k(r', t) = -\frac{1}{b} \frac{d}{d\xi_k} \epsilon^k(r', t) \quad (2.8)$$

is the density at the point  $r'$  of effective dislocations with Burgers vector  $b e_k$  [15]. Both  $\sigma^k(r, r')$  and  $\sigma^c(r, t)$  were calculated using the linear theory and correspond to the Inglis-Griffiths-Irvine model of a brittle crack.

Equations (1.1)-(1.8) form a system from which, with the initial condition

$$\varepsilon^j(\mathbf{r}, t=0) = 0, \quad \sigma'_a(t=0) = 0$$

and the boundary condition

$$\sigma_{xy}, \sigma_{yy}(x \leq 0, y = 0, t) = 0,$$

$\varepsilon^j(\mathbf{r}, t)$  and  $\sigma(\mathbf{r}, t)$  are found.

The integration in (2.6), the differentiation in (2.8), and the integration of the differential equation (1.1) are carried out numerically. The integrals in (2.6) were evaluated using the rectangle rule, and to calculate the derivatives in (2.8) we used their simplest representation by central finite differences; the differential equation (1.1) was integrated using the explicit Euler difference scheme

$$\varepsilon^j(\mathbf{r}, t_i) = \Delta t_{i-1} \dot{\varepsilon}_0 \exp \left\{ -\frac{U_0 \langle 1 - [\sigma'_e(\mathbf{r}, t_{i-1})/\tau_0]^{1/2} \rangle}{KT} \right\} \text{sign } \sigma'_e(\mathbf{r}, t_{i-1}) + \varepsilon^j(\mathbf{r}, t_{i-1})$$

( $t_i = t_{i-1} + \Delta t_{i-1}$ ) with an integration step  $\Delta t$  which varied depending on the computational situation. Since the problem is symmetrical about the x axis the calculations were only carried out for the upper half-plane.

3. Method of Calculating the Evolution of the Stress Intensity Factor of a Crack in the Crystal. We have the following relation for the stress intensity factor of a crack:

$$K(t) = K^c(t) + K^p(t),$$

where  $K^c(t)$  is the term of the stress intensity factor of the crack ignoring the effect of plastic yielding on it, while  $K^p(t)$  is determined exclusively by this effect:

$$K^p(t) = \sum_{k=1}^2 \int_{D_k} \widehat{K}^p(z', \beta_k) \Delta \rho_k(z', t) dz'.$$

The contribution to  $K^p(t)$  by an individual dislocation situated at the point  $z' = x' + iy'$  in the complex plane, is calculated from the formula [16]

$$\widehat{K}^p(z', \beta_k) = -\text{Re} \sqrt{\frac{2}{\pi}} \int_{-\infty}^0 [P_y^k(\xi, z') - iP_x^k(\xi, z')] \frac{d\xi}{\sqrt{-\xi}},$$

from which, carrying out the integration, we obtain

$$\widehat{K}^p(z', \beta_k) = \text{Re} \frac{A}{\sqrt{2\pi}} [J_1 \sin \beta_k - iJ_2 \cos \beta_k].$$

Here

$$A = \frac{\mu b}{2\pi(1-\nu)}; \quad J_1 = -\pi \left[ \frac{1}{\sqrt{z'}} + \frac{3}{2\sqrt{z'}} - \frac{z'}{2(z')^{3/2}} \right]; \quad J_2 = -\pi \left[ \frac{1}{\sqrt{z'}} + \frac{1}{2\sqrt{z'}} + \frac{z'}{2(z')^{3/2}} \right];$$

$\mu$  is the shear modulus and  $\nu$  is Poisson's ratio.

4. Results of Computer Calculations and Conclusions. Calculations were carried out for a crystal of  $\alpha$ -Fe with the following values of the constants:  $l = 1$  mm,  $r_0 = 0.1$   $\mu\text{m}$ ,  $\Delta x = 1$   $\mu\text{m}$ ,  $\sigma_a = 6$  MPa,  $\varepsilon_0 = 10^{11}$   $\text{sec}^{-1}$ ,  $U_0 = 0.9$  eV,  $\tau_0 = 330$  MPa [17],  $T = 300$  K,  $\sigma_0 = 18$  MPa,  $b = 2.47 \cdot 10^{-4}$   $\mu\text{m}$ ,  $\sigma_1 = 2$  GPa,  $\mu = 60$  GPa [18], and  $\nu = 0.3$ . The crystal was loaded at a rate  $\sigma'_a = 20$  MPa $\cdot\text{sec}^{-1}$  from 0 to  $\sigma_a$ . After reaching the upper loading limit the external tensile stress remained constant.

The calculations showed that two stages can be distinguished in the evolution of  $\varepsilon^j(\mathbf{r}, t)$ . In the first stage (from  $t = 0$  to  $t \approx 2.5$  sec) the plastic zone gradually grows, its shape changes in a similar way to itself, and the distribution  $\varepsilon^j(\mathbf{r}, t)$  in the plastic zone is largely a repetition of the distribution  $\sigma'_c(\mathbf{r}, t)$ , and in the second stage (when  $t > 2.5$  sec) a considerable change occurs in the form of the plastic zone and the redistribution of  $\varepsilon^j(\mathbf{r}, t)$  in it due to the effect of the dislocation structure of the crystal. Note that there are considerable quantitative discrepancies in the distribution of  $\sigma^j(\mathbf{r}, t)$  and  $\sigma'_c(\mathbf{r}, t)$ , which become greater as the plastic yielding process develops (Fig. 2a, b).

Calculations showed that there is a lag between  $K(t)$  and  $K^c(t)$ , its development is extremely nonharmonic, and there is a tendency for it to decrease (and consequently there is an increase in the margin of stability of a fixed crack) during plastic yielding at the tip of the crack (Fig. 3).

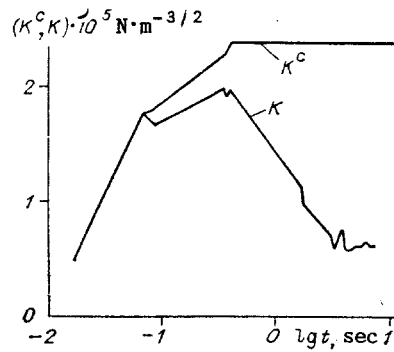


Fig. 3

Hence, our calculations have given the following main results:

- 1) the evolution of the elastic field of the crystal due to a change in its dislocation structure at the tip of a crack has a considerable effect on the development of plastic yielding in this region;
- 2) plastic yielding at the tip of a crack in a crystal usually increases the stability of the crack.

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