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THE FRACTURE OF BRITTLE AND DUCTILE CRYSTALS. FORCE AND DEFORMATION CRITERIA†

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The growth and branching of sharp cracks in ideal single crystals are investigated. Neuber–Novozhilov force and deformation criteria are proposed for the branching of sharp cracks; these criteria describe the brittle, quasibrittle, quasiductile and ductile behaviour of materials on fracture. For internal cracks, simple relations are obtained that describe the branching of cracks when the Coulomb–Mohr single-crystal theoretical strength curves are known for a generalized stress state. The possibility of multiple branching of cracks is found, which is linked to the multiplicity of the eigenvalues on loss of stability of the system. It is established that, for ideal single crystals, the principle of local symmetry is satisfied in the vicinity of the crack tip if the axis of symmetry of the crystal coincides with the axis of the crack. When there are asymmetrical disturbances of the atomic lattice in the vicinity of the crack tip, or when the axis of symmetry of the single crystal does not coincide with the crack axis, the principle of local symmetry is not satisfied.

1. INTRODUCTION

The problem of the stable growth of sharp cracks (or their branching) for certain types of loading of a body with a rectilinear sharp crack is of undoubted interest. In the vicinity of the tip of a normal-cleavage sharp crack, a complex stress–strain state (SSS) arises. Under certain conditions, blunting of sharp cracks may occur due to the large shear stresses and strains. There is still no definite answer to the question as to whether a sharp cleavage crack is stable in an ideal Bravais crystal lattice on account of the presence of shear stresses or shear strains in the vicinity of the crack tip, and how this stability is related to the ideal tensile and shear strength of the single crystal or the limiting deformability of the crystal lattice under shear.

Kelly, Tyson and Cottrell [1–3] presented a condition of stability for a cleavage crack in the form

$$\tau_{I\max}/\sigma_{I\max} < \tau_m/\sigma_m \tag{1.1}$$

where τ_I and σ_I are the shear and tensile stresses arising in the vicinity of the tip of the normal-cleavage crack, and τ_m and σ_m are the theoretical (ideal) shear and tensile strengths of the single crystal [4]. Qualitative considerations reduced to the following [1]: an interatomic bond at the tip of a sharp crack should be extended almost to its critical state, but then, in the vicinity of the crack tip, these tensile stresses will be transformed (possibly only partially) into high shear stresses, and, since the theoretical tensile strength τ_m is greater than the theoretical shear strength σ_m, condition (1.1) arises, superimposed on the blunting of the crack. This condition is a typical force criterion.

Rice and Thomson [2, 3, 5] proposed a different condition of stability for a cleavage crack in the form of an approximate relation if the real geometry of the atomic lattice is ignored

$$Gb/\gamma \gtrsim 10 \tag{1.2}$$

where G is the shear modulus, b is the Burgers vector of dislocation and γ is the surface energy of the material. Criterion (1.2) was obtained from the classic concepts of solid-state physics [5]: a crack that is sharp at the atomic level is blunted due to dislocation emission from the crack tip. Unlike force criterion (1.1), criterion (1.2) is the deformation criterion. We emphasize that the blunting of cracks according to these criteria can occur, generally speaking, at different points with respect to the crack tip.

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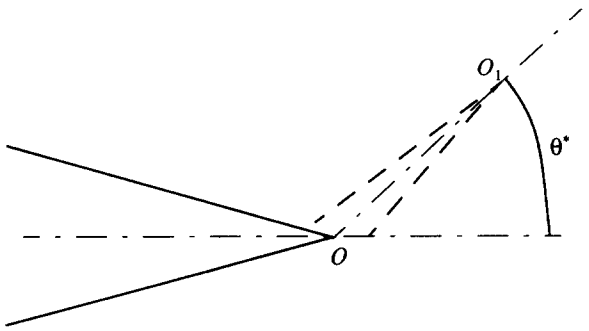

Fig. 1

2. THE STRESS–STRAIN STATE IN THE VICINITY OF THE CRACK TIP

In an isotropic material, we will consider an internal crack that is sharp at the atomic level. An internal rectilinear crack is modelled by a two-sided cut of length $2l$. For a normal-cleavage crack, let the stresses be specified at infinity, σ_∞. We will examine the stability of the growth of sharp cracks, understanding this problem to be their branching.

The continuous curve in Fig. 1 represents the right-hand tip of such a crack in the first quadrant, and the dashed line shows the expected new position of the crack during branching, where $\pm\theta^*$ represents the angle of branching for a crystal symmetrical about the crack, and points O and O_1 correspond to the old and new positions of the crack tips for an elementary act of crack propagation. Below, this constraint, requiring the presence of a certain symmetry of the crystal in relation to the crack/cut, will be removed.

When $\theta^* = 0$, the crack propagates in a stable manner, remaining rectilinear, when $\pm\theta^* \neq 0$ it will branch, changing its direction, and here, when $\theta^* = \pm\pi/2$, blunting of the crack occurs as it opens. In brittle fracture of the material [1–3, 5], the cleavage crack propagates rectilinearly, i.e. $\theta^* = 0$. In the case of ductile fracture of the material [1–3, 5], two dislocations are emitted from the crack tip, since $\theta^* = \pm\pi/2$. Below it will be shown that both quasibrittle ($\theta^* \cong \pm 0$) and quasiductile ($\theta^* \cong \pm\pi/2$) behaviour of the material is possible when $\pm 0^* \neq 0$, $\theta^* < \pi/2$. We emphasize that no constraints, apart from symmetry, are imposed in advance on the behaviour of the system (unlike existing approaches [1, 2]). Therefore, generally speaking, regimes are possible where multiple branching occurs when, for example, $\theta^*_{21} \neq \theta^*_{22} \neq \theta^*_{23}$ (the subscripts correspond to the number of the material and the type of loading). The multiple branching is related both to the complexity of the SSS in the vicinity of the crack tip and to the strength characteristics of the isotropic material with a complex stress state.

In describing the branching of cracks, it is necessary to have information on the stress field in the polar coordinate system $Or\theta$ for the force criterion, while for the deformation criterion, when describing the blunting of cracks, it is necessary to know the displacement of the sides of the crack in the rectangular system of coordinates Oxy in the vicinity of the crack tip. The SSS and the displacements of the crack sides in the vicinity of the right-hand tip of the normal-cleavage crack can be written in the form [6, pp. 15–17]

$$\sigma_\theta(r, \theta) = \frac{K_I}{\sqrt{2\pi r}}\cos^3\frac{\theta}{2} + O(r^0)$$
$$\tau_{r\theta}(r, \theta) = \frac{K_I}{\sqrt{2\pi r}}\sin\frac{\theta}{2}\cos^2\frac{\theta}{2} + O(r^0), \quad K_I = \sigma_\infty\sqrt{\pi l} \tag{2.1}$$

$$2v(x, 0) = \frac{\kappa + 1}{G}K_I\sqrt{\frac{|x|}{2\pi}} + O(x), \quad x \leq 0 \tag{2.2}$$

where $\sigma_\theta(r, \theta)$ and $\tau_{r\theta}(r, \theta)$ are the normal and shear stresses, K_I is the stress intensity factor (SIF), $2v(x, 0)$ is the opening of the crack surfaces, G is the shear modulus, and $\kappa = 3 - 4\nu$ for plane strain and $\kappa = (3 - \nu)/(1 + \nu)$ for a plane stress state, where ν is Poisson's ratio. According to known recommendations [7], for crystals it is more convenient to study plane strain. The stress field [see relation

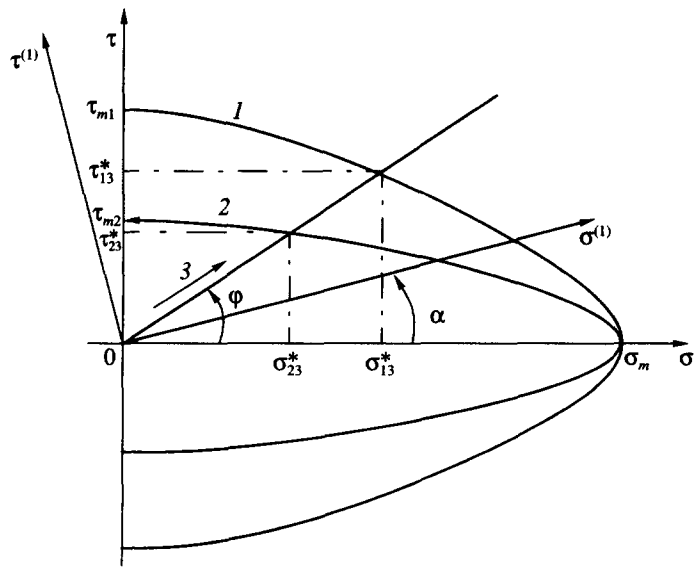

Fig. 2

(2.1) and Fig. 1] was determined inside the single crystal [cf. relation (1.1)], while the opening of the crack surfaces [see relation (2.2) and Fig. 1] was determined outside the single crystal [cf. relation (1.2)].

We will investigate the brittle–ductile transition during the fracture of single crystals for fairly long cracks, more precisely, for cracks of length $2l > 20r_e$, where r_e is the atomic lattice constant. Under such constraints, relations (2.1) and (2.2) can be simplified: terms $O(r^0)$ are omitted in relation (2.1), and terms $O(x)$ are omitted in relation (2.2). Below, the Neuber–Novozhilov approach will be used for materials with a structure, and the atomic lattice constant r_e is selected as the characteristic linear size of the isotropic single crystal. The interval of averaging when this approach is used for an ideal single crystal is equal to r_e or $2r_e$ and coincides with the length of the segment OO_1 in Fig. 1.

3. FORCE AND DEFORMATION CRITERIA

When there is a gradual increase in the stresses σ_∞, we have proportional loading with a complex stress state in the vicinity of the crack tip. Branching of the crack is possible [8–10] or the emission of dislocations [11]. The selection by the system of a particular branching path is related to the strength characteristics of the material.

Figure 2 shows the Coulomb–Mohr single crystal theoretical strength curves [12] for two different materials and shows the loading path. The following notation is used: σ and τ are the normal and shear stresses on the examined area in a complex stress state when the axis of symmetry of the crystal coincides with the cut; curves 1 and 2 are curves of the theoretical strength of single crystals symmetrical about the crack, such that $\sigma_m = \sigma_{m1} = \sigma_{m2}$ are the theoretical (ideal) tensile strengths of the single crystals [4], and $\tau_{m1} \neq \tau_{m2}$ are the theoretical (ideal) shear strengths of the single crystals [4] (if the theoretical tensile strengths of the materials are the same, the theoretical shear strengths of the materials differ considerably); the arrow 3 shows the proportional path of loading; $\sigma^{(1)}$ and $\tau^{(1)}$ are the normal and shear stresses on the examined area in a complex stress state when none of the axes of symmetry of the crystal coincides with the cut; α is the angle between the axis of symmetry of the crystal and the cut. The path of loading 3 is characterized by the following relation: $\sigma^*_{13}/\tau^*_{13} = \sigma^*_{23}/\tau^*_{23} = C_3 = \text{const}$ (the notation σ^* and τ^* is used for stresses of critical states, with subscripts corresponding to the number of the material and the type of loading); besides the constant C_3, the loading path can be specified by the angle φ. This constant C_3 or the angle φ defines the type of loading, and the type of loading does not depend on the strength characteristics of the materials.

The force criterion. Let a single crystal containing a crack be symmetrical about the crack and have no defects, for example, vacancies. We will examine the force discrete-integral brittle strength criterion [8–10] of the Neuber–Novozhilov type for crack growth in selected directions ± 0, defined by the angles of branching (see Fig. 1)

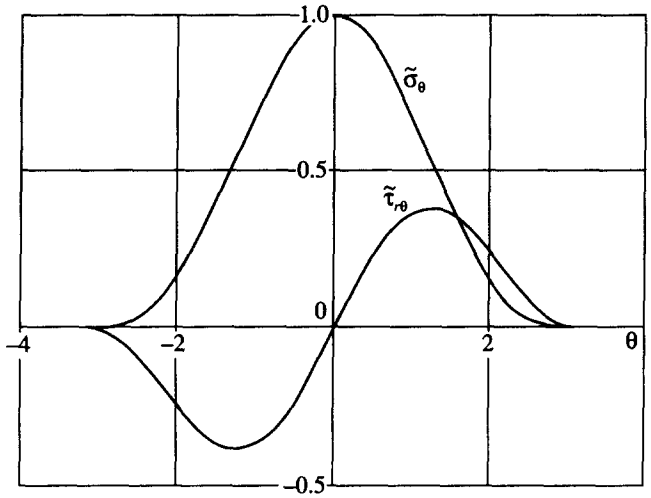

Fig. 3

$$\langle\sigma_\theta(\theta)\rangle \le \sigma^*, \quad \langle\tau_{r\theta}(\theta)\rangle \le \tau^*$$

$$\langle\sigma_\theta(0)\rangle = \frac{1}{nr_e}\int_0^{nr_e}\sigma_\theta(r,\theta)dr, \quad \langle\tau_{r\theta}(\theta)\rangle = \frac{1}{nr_e}\int_0^{nr_e}\tau_{r\theta}(r,\theta)dr; \quad n = 1,2 \tag{3.1}$$

where $\langle\sigma_\theta(\theta)\rangle$ and $\langle\tau_{r\theta}(\theta)\rangle$ are the averaged normal and shear stresses in the selected directions $\pm\theta$ in an ideal single crystal. When $\langle\sigma_\theta(\theta)\rangle < \sigma^*$ and $\langle\tau_{r\theta}(\theta)\rangle < \tau^*$, the crack does not propagate (there is no branching). When the averaged stresses $\langle\sigma_\theta(\theta)\rangle$ and $\langle\tau_{r\theta}(\theta)\rangle$ are identical with the stresses of the critical state σ^* and τ^*, criterion (3.1) is satisfied: in the selected directions $\pm\theta^*$, (a) a rectilinear crack propagates by the averaging interval if $\theta^* = 0$ (there is no branching), and (b) branching of an internal crack of length $2l$ occurs if $\theta^* \neq 0$, and the crack tip is displaced from point O quasistatically to point O_1 and a point symmetrical to it (see Fig. 1). When crack propagation occurs at $\theta^* = 0$, criterion (3.1) is applied repeatedly to a rectilinear crack of length $2(l + nr_e)$ to assess the possibility of the branching of a new crack. When branching occurs at $\theta^* \neq 0$, it is necessary to refine the SSS for a crack with a complex break (see, for example, the reference book [6] and the paper [13], and also the bibliography in them), and then to repeat the procedure in order to assess the possibility of crack branching with breaks. However, when $\theta^* \neq 0$, for a crack with a complex break, the SSS is complicated considerably, since, besides the first mode, a second mode of deformation appears.

We will assess the type of stress state in the vicinity of the crack tip as a function of the angle θ ($-\pi < \theta < \pi$). Figure 3 shows the distribution of the stresses σ_θ and $\tau_{r\theta}$ in accordance with the simplified formulae (2.1) when terms $O(r^0)$ are omitted. All quantities relate to $K_I/\sqrt{2\pi r_0}$, where $r_0 = \text{const}$, i.e. $\tilde{\sigma}_\theta = \sigma_\theta/[K_I/\sqrt{2\pi r_0}]$ and $\tilde{\tau}_{r\theta} = \tau_{r\theta}/[K_I/\sqrt{2\pi r_0}]$. For a certain angle θ, the following relation is satisfied

$$\tau_{r\theta}(r,\theta)/\sigma_\theta(r,\theta) = \langle\tau_{r\theta}(\theta)\rangle/\langle\sigma_\theta(\theta)\rangle = \operatorname{tg}(\theta/2) \tag{3.2}$$

Thus, as the crack $\theta = 0$ propagates, pure elongation $\sigma_0 \neq 0$, $\tau_{r\theta} = 0$ is realized; in the immediate vicinity of the sides of the crack, when $\theta \to \pm\pi$, in the vacinity of the crack tip a preferentially shear form of the SSS is realized; at arbitrary angles $-\pi < \theta < \pi$, a generalized stress state $\sigma_\theta \neq 0$, $\tau_{r\theta} \neq 0$ occurs.

Suppose a certain crystalline material is specified, the SSS of which, after averaging, is described quite well by the equations of isotropic elasticity theory [see (2.1) and (2.2)]. When the axis of symmetry of the crystal coincides with the cut, the limiting curve of the strength of a single crystal of the Coulomb–Mohr type in the plane σ–τ is described by the function $\rho(\varphi) = \rho(-\varphi) = f(\varphi) = f(-\varphi)$ (see Fig. 2 and [12]), which may be related to the principle of local symmetry [14]. Then the theoretical tensile and shear strengths of the single crystal are respectively equal to $\sigma_m = f(0)$ and $\tau_m = f(\pi/2)$, and the stresses of the critical states are defined as follows:

$$\sigma^* = f(\varphi)\cos\varphi, \quad \tau^* = f(\varphi)\sin\varphi; \quad \tau^*/\sigma^* = \operatorname{tg}\varphi \tag{3.3}$$

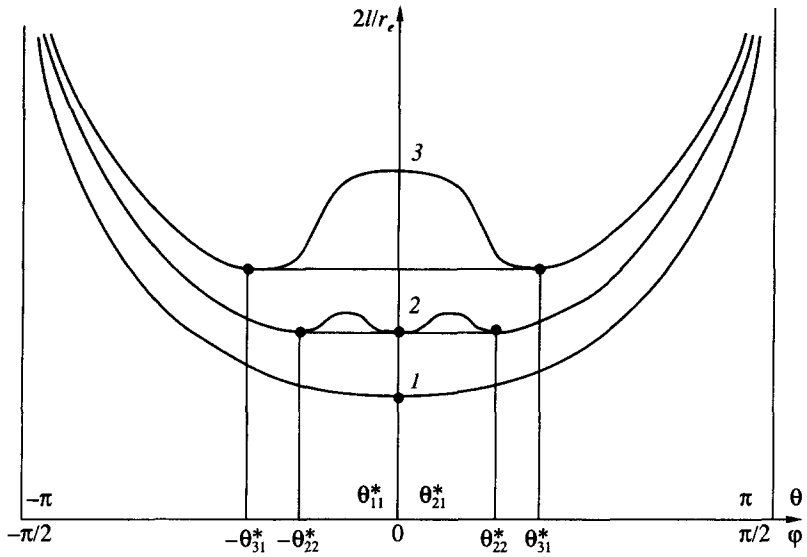

Fig. 4

Comparing relations (3.2) and (3.3), we obtain $\varphi = \theta/2$: when $\varphi = \theta/2 = 0$ we have elongation, and when $\varphi = \theta/2 = \pi/2$ we have shear. Thus, it is very easy to switch from the type of loading in the vicinity of the crack tip to the type of loading in the σ–τ plane.

The necessary transformations are carried out in relations (3.1) to (3.3) when, in equalities (2.1), terms $O(r^0)$ are omitted. Note that the use of the first or second relations from (2.1) and (3.3) under proportional loading leads to identical results [8–10]. The equations describing the branching of internal cracks have the form

$$\frac{2l(\theta)}{r_e} = \frac{nf^2(\theta/2)}{\sigma_\infty \cos^4(\theta/2)}, \quad 0 \le \theta \le \pi; \quad \frac{2l(\varphi)}{r_e} = \frac{nf^2(\varphi)}{\sigma_\infty \cos^4 \varphi}, \quad 0 \le \varphi \le \frac{\pi}{2} \tag{3.4}$$

We will present qualitative reasoning explaining the functional relations (3.4) for fairly smooth functions $f(\varphi)$ (there are no discontinuities of the first kind). Remember that, when $\varphi = 0$, pure elongation occurs and $f(0) = \sigma_m > 0$, while, when $\varphi = \pi/2$, pure shear occurs and $f(\pi/2) = \tau_m > 0$ (see Fig. 2). It is obvious that $l(0) > 0$ and $l(\varphi) \to \infty$ when $\varphi \to \pi/2$, and here $l'(\varphi) > 0$ when $\varphi \to \pi/2$. We will make use of results given in [4]. The relative estimates of the theoretical tensile strength σ_m and shear strength τ_m in limiting cases are alike [4]: (1) for crystals prone to cleavage, $\sigma_m \gtrsim \tau_m$; (2) for crystals with low resistance to the emission of dislocations, $\sigma_m \gg \tau_m$. We will estimate the number of extrema of the function $l(\varphi)$ in the interval $(-\pi/2, \pi/2)$. For the first case, when $l(\varphi) \approx$ const we have a minimum at the point $\varphi^* = 0$, i.e. the crack propagates rectilinearly. For the second case $\sigma_m \gg \tau_m$, an angle $\pm\varphi^*$ will appear at which $l'(\pm\varphi^*) = 0$, and three relations are possible: (2.1) $l(0) < l(\pm\varphi^*)$ (the crack propagates rectilinearly); (2.2) $l(0) = l(\pm\varphi^*)$ (triple branching of the crack); (2.3) $l(0) > l(\pm\varphi^*)$ (double branching of the crack).

The functional dependences (3.4) of the critical lengths of cracks $2l/r_e$ on the branching angle θ or the type of stress state φ are presented in Fig. 4. Three curves are given, characterizing the branching of cracks in different materials at a prescribed loading level σ_∞: curve *1* describes the behaviour of the first material, for which $\theta^*_{11} = 0$; curve *2* describes the behaviour of the second material, for which $\theta^*_{21} = 0$, $\pm\theta^*_{22} \neq 0$; and curve *3* describes the behaviour of the third material, for which $\pm\theta^*_{31} \neq 0$. The differences in the behaviour of the materials are related to the strength characteristics $f_i(\varphi)$ of the first ($i = 1$), second ($i = 2$) and third ($i = 3$) materials. At a prescribed level of loading σ_∞ for the first, second and third materials, the critical lengths of cracks $l^*_1(\theta^*_{11})$ (no branching of the crack), $l^*_2(\theta^*_{21}) = l^*_2(+\theta^*_{22}) = l^*_2(-\theta^*_{22})$ (triple branching) and $l^*_3(+\theta^*_{31}) = l^*_3(-\theta^*_{31})$ (double branching) are obtained respectively, and here, according to the force criterion, the critical lengths of the cracks for these materials are defined as $l^*_i = \min l_i(\theta)$ with $i = 1, 2, 3$; to these critical lengths l^*_i there correspond the branching angles θ^*_{11}, θ^*_{21}, θ^*_{22} and θ^*_{31}. The principle of local symmetry is satisfied [14]. Note that the appearance of a more complex behaviour of the materials, for example multiple cracking, is also possible. If the

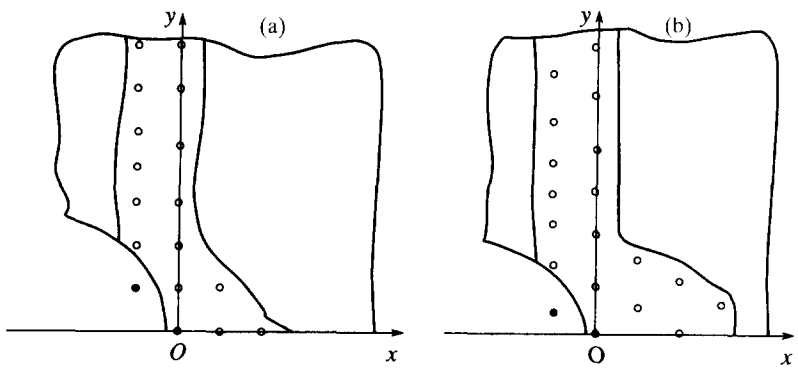

Fig. 5

first material behaves like a brittle material, since $\theta_{11}^* = 0$, the third material ($\pm\theta_{31}^* \neq 0$ and $\theta_{31}^* < \pi/20$) behaves like a quasibrittle material at $\theta_{31}^* \approx 0$, and like a quasiductile material at $\theta_{31}^* \approx \pi/2$. It is difficult to classify the second material, when $\theta_{11}^* = 0$ and $\theta_{22}^* \approx \pi/2$. The transition from critical lengths of internal cracks l_i^* to SIFs $K_{Ii}^* = \sigma_\infty\sqrt{\pi l_i^*}$ ($i = 1, 2, 3$) is obvious.

Experimental results [15] are consistent with the principle of local symmetry [14] and the above reasoning; for example, a micrograph of the tip of a branching crack during the multiple cracking of ceramics has been given ([15], Fig. 7). We recall that criterion (3.1) is related to loss of stability of the crystal lattice. For the first material there is no branching of the crack (a simple eigenvalue), while for the second material triple branching occurs [15] (a triple eigenvalue). Only for the first type of material does a rectilinear crack propagate stably, since it does not change its direction during quasistatic growth.

We will now consider the interpretation of the stability condition (1.1). We will refine the left-hand side of this relation: we use relations (2.1), ignoring terms $O(r^0)$ in them. It is obvious that the stresses σ_θ and $\tau_{r\theta}$ reach an extremum at $\theta_\sigma = 0$ and $\theta_\tau = \pm 2 \arcsin(1/\sqrt{3})$ respectively, i.e. at different points $\theta_\sigma \neq \theta_\tau$ (see Fig. 3). In obtaining criterion (1.1), qualitative reasoning was given [1] in substantiating the transition from the stress field in the vicinity of the crack tip to the theoretical tensile and shear strength of the material.

Thus, more general approaches have been proposed in investigating the problem of the branching of cracks when the limiting curve $\rho(-\varphi) = \rho(-\varphi) = f(\varphi) = f(-\varphi)$ of the strength of the material of the Coulomb–Mohr type is known [see (3.1) and (3.4)].

Deformation criterion. We will now consider the deformation criterion for ductile materials. Let a single crystal containing an internal crack be symmetrical about the crack and not have any defects, for example, vacancies. Under load, two dislocations can be emitted from the crack tip [5]. We will take into account the actual geometry of the atomic lattice in the vicinity of the crack tip [16] for the plane case. We will use the simplest Frenkel–Kontorova model of dislocation [11]. This model is characterized by two geometrical parameters which will be used below: the distance between the two layers of atoms r^* (this distance may not be the same as the atomic lattice constant r_e), and the critical displacement h_m. Let $\pm\beta$ be the angle between the normal to the plane of the crack and the planes along which the dislocations emerge ($-\pi/2 < \beta < \pi/2$). A real crack, which is modelled by a two-sided cut, is formed in the following way: two atoms are removed along the crack line, it is assumed that atoms lying on the sides of the crack do not interact with each other. The supercritical states of systems after the emergence of two dislocations are given in Fig. 5 for the subcritical arrangement of atoms at points of the tetragonal lattice (a) and at points of the close-packed layer of atoms (b). In relation (2.2), the crack tip is chosen as the reference point, and the displacement of the sides of the crack is estimated at distance $x = -r^* \cos\beta$ from its tip [11] (terms $O(x)$ in relation (2.2) are omitted). It is proposed to use a deformation criterion describing the symmetrical emission of two dislocations from the tip of an internal crack

$$2v(-r^*\cos\beta, 0) = \frac{\kappa+1}{G} K_I \sqrt{\frac{r^*\cos\beta}{2\pi}} \leq \frac{2h_m}{\cos\beta}, \quad K_I = \sigma_\infty\sqrt{\pi l} \tag{3.5}$$

where h_m is the critical displacement in the atomic lattice with specific packing of the atoms such that, during deformation of the system, with geometrical and physical non-linearity, the theoretical shear strength τ_m is exceeded (see [11]). For critical displacement in a close-packed layer of atoms, estimates [8–10] $h_m \cong (0.3, \ldots, 0.4)r_e$ were obtained, and the specific values of h_m depend on the interatomic interaction potentials.

When $v(-r^* \cos\beta, 0) < h_m/\cos\beta$, no dislocations are emitted. Let the constraint $\langle\sigma_\theta(\theta)\rangle < \sigma^*$, $\langle\tau_{r\theta}(\theta)\rangle < \tau^*$ be satisfied for criterion (3.1). Then, if deformation criterion (3.5) is satisfied, when $v(-r^* \cos\beta, 0) = h_m/\cos\beta$, extremely effective blunting of the crack occurs on account of the emission of two dislocations (a double eigenvalue). For a blunt crack, Khristianovich's hypothesis on the finiteness of stresses at the crack tip [6] is satisfied. Materials in which the crack is blunted by the emission of dislocations are either ductile when $\beta = 0$ or quasiductile when $\beta \approx 0$. For the types of materials examined, from deformation criterion (3.5) for critical SIFs K_{Ii}^{**} and critical crack lengths l_i^{**}, the following simple relations hold

$$K_{Ii}^{**} = \frac{2h_m}{\cos\beta}\frac{G}{\kappa+1}\sqrt{\frac{2\pi}{r^*\cos\beta}}, \quad l_i^{**} = \frac{K_{Ii}^{**}\sigma_\infty}{\pi}; \quad i = 1, 2, 3 \tag{3.6}$$

It is difficult to classify a material in the case of multiple cracking, when the force criterion (3.1) and the deformation criterion (3.5) are satisfied simultaneously. Given $\langle\sigma_\theta(\theta)\rangle = \sigma^*$, $\langle\tau_{r\theta}(\theta)\rangle = \tau^*$, and $v(-r^* \cos\beta, 0) = h_m/\cos\beta$, it is open to question whether a material of this kind exists among practical materials in the form of ideal single crystals; however, if there are considerable perturbations of the atomic lattice ahead of the crack tip similar behaviour of the material is not ruled out (see below). The blunting of cracks at the atomic level was described in detail in [17, 18]. However, in [17] there are no simple expressions for the critical parameters K_{Ii}^{**} and l_i^{**} [see relations (3.6)]. After the emission of dislocations, the material is damaged. Now, in a material with damage, it is simplest to examine a blunt crack [18, 19], or, more precisely, a notch with a radius of curvature at the tip. These radii of curvature for the systems shown in Fig. 5 are approximately $R \approx 1.5\, r_e$ (a) and $R \approx 1.5\sqrt{0.75}\, r_e$ (b).

The proposed deformation criterion (3.5) and its consequences (3.6) enable us to describe the loss of stability of the atomic lattice in the vicinity of the crack tip when dislocations are emitted, and the parameter of critical displacement in the atomic lattice h_m introduced is similar physically to the energy parameter characterising the loss of stability of the atomic lattice [20]. This criterion is probably simpler than the criterion from [20]; this is partly due to the fact that, in criterion (3.5), a simpler Frenkel–Kontorova dislocation model [11] is used, rather than the Peierls model [20].

Comparing the critical crack lengths l_i^* and l_i^{**} or the critical SIFs K_{Ii}^* and K_{Ii}^{**} respectively according to the force criterion (3.1) and the deformation criterion (3.5), we will establish which of these criteria is realized during branching of the crack ($i = 1, 2, 3$):

(1) if $K_{Ii}^* < K_{Ii}^{**}$ and $l_i^* < l_i^{**}$, then branching of cracks occurs according to the force criterion without the emission of dislocations;

(2) if $K_{Ii}^* > K_{Ii}^{**}$ and $l_i^* > l_i^{**}$, then the emission of dislocations occurs according to the deformation criterion;

(3) if $K_{Ii}^* = K_{Ii}^{**}$ and $l_i^* = l_i^{**}$, then both branching of the crack according to the force criterion and emission of dislocations according to the deformation criterion occur.

4. BREAKDOWN OF THE PRINCIPLE OF LOCAL SYMMETRY

The principle of local symmetry proposed in [14], which has been widely used above, may break down if, instead of studying ideal Bravais lattices for single crystals, one considers more or less real crystals [16]. We will assume that:

(1) besides the crack, the single crystal has defects of the vacancy, dislocation or impurity atom type, arranged arbitrarily with respect to the crack tip;

(2) the axes of symmetry of the crack and ideal single crystal do not coincide.

The *influence of perturbations*. Suppose edge dislocations are arranged at an arbitrary angle to the crack line in the vicinity of its tip. We will determine more precisely the arrangement of vacancies and impurity atoms. We will assume that a single crystal has atomic lattice defects in the form of a single vacancy or a single impurity atom and clusters of two vacancies or two impurity atoms in the immediate vicinity of the crack tip, and here the vacancies or impurity atoms, which cause the atomic lattice to lose its symmetry, are not positioned on the crack surfaces. For impurity atoms it is assumed that the values of the crystal lattice constants of the base material r_e and the impurity $r_e^{(1)}$ are practically identical, i.e. $r_e \approx r_e^{(1)}$, and any significant difference is related to the interatomic interaction constants [1]. The force and deformation criteria will be written in a slightly different form

$$\langle\sigma_\theta(\theta)\rangle \le \sigma^{**}, \quad \langle\tau_{r\theta}(\theta)\rangle \le \tau^{**}, \quad \sigma^{**} = f^*(\varphi)\cos\varphi, \quad \tau^{**} = f^*(\varphi)\sin\varphi \tag{4.1}$$

$$v(-r^* \cos\beta, 0) \le h_m^*/\cos\beta \tag{4.2}$$

where σ^{**} and τ^{**} are the stresses of the critical states of the material with defects, and h_m^* is the critical displacement in the atomic lattice with defects, for which loss of stability occurs. Due to the presence of defects, there is a change in the limiting curve $\rho^*(\varphi) = f^*(\varphi)$ of the strength of the material of the Coulomb–Mohr type in the σ–τ plane, and here, in the general case, $\rho^*(\varphi) \neq \rho^*(-\varphi)$, this function $\rho^*(\varphi)$ possibly having discontinuities of the first kind. Thus, in the modified force criterion (4.1) and deformation criterion (4.2), the characteristics of the material change compared with the initial criteria (3.1) and (3.5) [see, for example, (3.6)].

It is comparatively easy to obtain estimates of the reduction in the strength of the initial material when the perturbations are related only to vacancies, and the limiting curve for the initial ideal single crystal $f(\varphi)$ is known. The procedure for averaging is carried out taking into account the bonds that are really active [18], and we then have the estimates

$$\sigma^{**} \simeq (k/n)\sigma^*, \quad \tau^{**} \simeq (k/n)\tau^* \tag{4.3}$$

where k is the number of interatomic bonds acting in the averaging interval nr_e, and here, in the case in question, $k \ge 1$ and $k \le n \le 4$. The number of interatomic bonds k which appears depends on the angle θ, and the parameter k/n characterises the damage to the material (for an ideal single crystal $k/n = 1$). For material with impurity atoms it is necessary to plot a curve $\rho^*(\varphi) = f^*(\varphi)$ of the strength of material of the Coulomb–Mohr type; the loss of stability of atomic chains with impurity atoms was investigated in [19].

The principle of local symmetry [14] in the system with the defect considered:

(1) is satisfied if the function $f(\theta)^*$ is even;

(2) is violated when the function $f(\varphi)^*$ is not even.

If considerable damage exists ahead of the crack tip, where the damage parameter k/n is considerably less than unity [see Eq. (4.3)], and if there is no other damage, then a case where criteria (4.1) and (4.2) hold simultaneously can probably be realized; such material is difficult to classify. Crack propagation in brittle and quasibrittle materials when there are defects has been discussed in [21].

Mismatch of the axes of an ideal single crystal and a crack. We will assume that the axis of symmetry of an ideal single crystal is rotated by a certain angle $\alpha \neq 0$ with respect to the cut (agreement must undoubtedly be reached regarding the sign of the shear stresses τ). In the new axes $\sigma^{(1)} - \tau^{(1)}$ (see Fig. 2), let the limiting curve of the strength of the single crystal of the Coulomb–Mohr type be described by the function $\rho(\varphi - \alpha) = f(\varphi - \alpha)$.

The force criterion (4.1) formally retains its form if the stresses of the critical states σ^{**}, τ^{**} are defined in the appropriate way, namely

$$\begin{aligned} &\langle \sigma_\theta(\theta) \rangle \le \sigma^{**}, \quad \langle \tau_{r\theta}(\theta) \rangle \le \tau^{**}, \quad \sigma^{**} = f(\varphi - \alpha)\cos(\varphi - \alpha) \\ &\tau^{**} = f(\varphi - \alpha)\sin(\varphi - \alpha) \end{aligned} \tag{4.4}$$

The functional dependence of the critical crack lengths $2l(\varphi)/r_e$ differs from (3.4) by the presence of the angle $\alpha \neq 0$.

The deformation criterion acquires the form

$$v(-r^* \cos\beta^{\pm}, 0) \le h_m^*/\cos\beta^{\pm} \tag{4.5}$$

since the angles between the normal to the crack plane and the planes in which the dislocations are emitted above and below the crack plane do not coincide in absolute magnitude, i.e. $\beta^+ \neq |\beta^-|$.

It is obvious that the local principle of symmetry [14] breaks down both for the force criterion (4.4) and for the deformation criterion (4.5), since $f(\varphi - \alpha) \neq f(-\varphi + \alpha)$ and $\beta^+ \neq |\beta^-|$.

5. DISCUSSION

The growth and branching of sharp cracks both in ideal single crystals and in crystals with perturbations have been investigated. Force and deformation criteria have been plotted for these crystals. With successive additional loading of a body with a crack, a stress–strain state is produced such that either the force or the deformation criterion is satisfied (simultaneous satisfaction of these criteria is also

possible). In the vicinity of the crack tip, the atomic lattice of the material loses its stability. Competition between the brittle and quasibrittle behaviour of materials and the quasiductile and ductile behaviour occurs, which, generally speaking, is defined by the ratio σ_m/τ_m [1]. The latter ratio in practical structural materials can be changed by using metal physics processes. The principle of local symmetry [14] is satisfied for symmetrical systems and is violated for systems without symmetry. The compactness of the proposed exposition of the problem of branching (see [17, 20, 21]) is due to reinterpretation and formalization of the results from the neighbouring area of knowledge – solid-state physics (metal physics). In the exposition proposed, use is made of: 1) not only the concept of the theoretical tensile and shear strength [4] but also the entire Coulomb–Mohr single crystal theoretical strength curve for the generalized stress state (see [8–10]); when defects of the single crystal are present in the vicinity of the crack tip, this curve can have discontinuities of the first kind; 2) another definition of the nucleus of dislocation (see [11]) where the critical displacement of the atoms in the Frenkel–Kontorova model corresponds to the theoretical shear strength of the crystal lattice.

The atomic lattice can have multiple eigenstates. With multiple eigenstates the critical loads of the different states are the same, and multiple cracking of the material occurs. For certain crystal lattices, crowding of the critical loads of the eigenstates exists in the vicinity of the smallest critical load. When perturbations take effect, under multiple critical loads and with their crowding [22–25], large spreads are observed in full-scale experiments and certain difficulties arise in describing the supercritical behaviour of systems in a numerical experiment [25, 26].

The atomistics of fracture was discussed in [25, 26]. We emphasize that the first of these reviews [25] is devoted to a numerical experiment in micromechanics in the presence of defects. Occasionally, in numerical calculations [25] the principle of local symmetry [14] is violated in symmetrical systems due to roundings off in the calculations. The judicious application of the finite element method to the supercritical deformation of atomic lattices in the presence of perturbations has been demonstrated [27].

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