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HIERARCHY OF STRENGTH CRITERIA OF STRUCTURED BRITTLE MEDIA. SATELLITE INITIATION OF MICROCRACKS

V. M. Kornev

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The quasi-static growth of plane cracks in media with a regular structure is studied. The structures characterized by one linear dimension are considered. Consistent discrete-integral strength criteria for normal-rupture cracks for each structure are proposed. For three structures, the critical stress-intensity factor and the critical lengths of the normal-rupture cracks are estimated. For these critical parameters, a limiting passage is possible in the relations obtained where the stress-intensity factor and the crack lengths tend to zero (the classical relations do not admit this limiting passage). Modifications of the criteria proposed make it possible to describe the satellite initiation of a microcrack at the macrocrack tip if monocrystalline grains of the material are arranged in a special way in the vicinity of the macrocrack tip.

INTRODUCTION

In recent years, considerable attention has been given to strength and fracture analyses that take into account the real structure of the material from which a construction is made. Neuber [1] suggested that the failure in the presence of stress concentrations can be stated only after averaging the stresses over the material grain surface and comparing the averaged stresses with the strength characteristics of a structured solid. Novozhilov [2] introduced, in addition to the averaging, both necessary and sufficient criteria of brittle strength for crystalline solids. Following Novozhilov, Kornev et al. [3, 4] studied the sufficient criterion of brittle strength for real potentials of interatomic interaction for the case where there are vacancies near the crack tip. Kornev [5] proposed discrete-integral criteria for three types of cracks in which the averaging limits depend on the dimensions and location of defects in the vicinity of the crack tip. According to Novozhilov's terminology, the criteria proposed in [5] (in the absence of defects in the material) become necessary criteria. The characteristic linear dimensions of solids considered by Neuber [1], Novozhilov [2], and Kornev et al. [3–5] differ by several orders since grainy metals were studied in [1], whereas crystalline metals were considered in [2–5]. Mikhailov [6, 7] substantiated the averaging procedure in the Neuber–Novozhilov criteria. Studies [8–10] deal with strength of cracked porous bodies of regular structure, where the macroporosity of this structure is described by the characteristic linear dimension. Generally, there is no stress singularity at the apices of blunt cracks [1, 3, 8–10]. The refinement of Novozhilov's necessary and sufficient criteria of brittle strength for crystalline solids allows a qualitative description of the Rebinder effect [11–13].

To formulate strength criteria for both blunt and sharp cracks in continuous structured media, it is natural to use the Neuber–Novozhilov approach.

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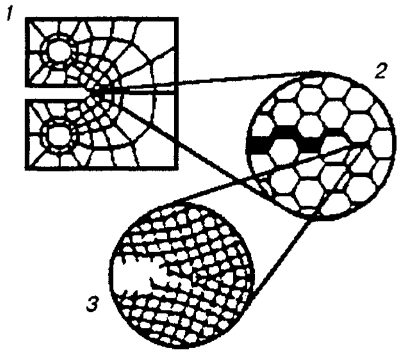

Fig. 1

1. STRESSES IN THE VICINITY OF CRACK TIPS

1.1. Mechanical Models for Normal-Rupture Cracks. We study the quasi-static growth of plane cracks in media with regular structures, each of them being characterized by one linear dimension. The linear dimensions for crystalline structures and massive building structures can range from 10^{-7} to 10^2 cm in order of magnitude. Two neighboring structures do not affect significantly each other when their dimensions differ by two orders. In view of the restrictions mentioned above, no more than five consistent criteria are possible in the considered range of linear dimensions. Let a cracked solid contain a hierarchy of regular structures (i^0 is the total number of the structures) such that their linear dimensions r_i ($i = 1, 2, \ldots, i^0$) are ordered as $r_i \gg r_{i+1}$ and each linear dimension r_i differs from the next one r_{i+1} by two orders or more. In [1–8], some discrete integral (necessary) strength criteria were proposed for the normal-rupture cracks for various structures. It should be noted that the classical approach, where only stress-intensity factors (SIF) $K_I^{(i)}$ in each structure are taken into account, is inapplicable here since for some structures the stress field can contain no singularity, i.e., $K_I^{(i^*)} \equiv 0$, $i^* = 1, 2, \ldots, i^0$. Moreover, certain difficulties arise in defining the concept of theoretical strength of the material of each structure. We note that this is the ideal strength for crystalline solids (see [14]).

In each structure, only plane rectilinear cracks are considered, whose planes coincide and whose rectilinear fronts are parallel, i.e., a plane problem of the theory of elasticity is studied. We propose a family of discrete-integral criteria of brittle strength for normal-rupture cracks

$$\frac{1}{k_i r_i} \int\limits_0^{n_i r_i} \sigma_y^{(i)}(x_i, 0)\, dx_i \leqslant \sigma_m^{(i)} \qquad (i = 1, 2, \ldots, i^0, \text{ where } \quad i^0 \leqslant 5), \tag{1.1}$$

which are consistent for each structure. Here $\sigma_y^{(i)}$ are the normal stresses at the crack continuations (they can contain singularities or not), $O_i x_i y_i$ are the Cartesian coordinate systems oriented relative to the right parts of the cracks of different scale [the origins for the cracks of different scales can differ; in this case, the limits of integration in (1.1) are changed accordingly], r_i is the characteristic linear dimension of a particular structure, n_i and k_i are integers ($n_i \geqslant k_i$), k_i is the number of active bonds acting at the crack tip of the ith structure, $n_i r_i$ are the intervals of averaging, and $\sigma_m^{(i)}$ are the theoretical strengths of the material of a particular structure (for crystalline solids, this is the ideal strength of perfect crystals [14]).

The limits of stress averaging in the discrete-integral criteria (1.1) depend on the presence, dimension, and location of microdefects in the ith structure in the vicinity of the crack tip ($n_i \geqslant k_i$). The magnitudes of these averaged stresses [1, 2] must not exceed the theoretical breaking strength of an ideal material of the ith structure. The quantities k_i/n_i characterize damage of the ith material at the crack continuation. In the specific implementation [15, 16] of the nonlocal strength criterion [6, 7], the damage of the material is ignored (see [15, relations (5)] and [16, relations (12)]).

The stress fields $\sigma_y^{(i)}$ at the crack continuations can be calculated after the corresponding linear problems of the theory of elasticity for specified loads (i^0 is the total number of these problems) are solved. The proposed approach accounting for the hierarchy of structures is illustrated in Fig. 1 (the emblem of the 5th International Conference on Fundamentals of Fracture), in which 1 is the macrolevel (standard specimen), 2 is the mesolevel (regular graininess of material), and 3 is the microlevel (particular atomic structure in the vicinity of the crack tip). In the simplest cases, exhaustive information on the stress fields $\sigma_y^{(i)}$ at the crack continuation can be obtained for an arbitrary i so that $\sigma_y^{(i)} = F(\sigma_\infty^{(1)})$, where F is a certain function and $\sigma_\infty^{(1)}$ are the stresses acting in the normal direction to the crack plane and specified at infinity or on a certain contour of the body for the first structure. The solution for stresses at the continuation of sharp cracks $y = 0$ can be expressed in terms of SIFs $K_I^{(i)}$ to give

$$\sigma_y^{(i)}(x_i, 0) \simeq \sigma_\infty^{(i)} + \frac{K_I^{(i)}}{(2\pi x_i)^{1/2}} \qquad (i = 1, 2, \ldots, i^0). \tag{1.2}$$

In (1.2), only the leading terms that characterize the stressed state near the crack tip are written, the second term having an integrable singularity. Relation (1.2) corresponds to the origin located at the crack tip. A smooth component of the solution in (1.2) makes it possible to describe the initiation of cracks at any step.

We now consider an approximate method of constructing $\sigma_y^{(i)}$ for porous media with cracks (notches), where i^{00} is the number of porous structures ($i^{00} \leqslant i^0$). Let there be a porous medium for $i = 1$, i.e., for the first structure. At the first step, we construct a solution for the macrostructure $i = 1$ for an internal or edge crack by using the known stresses $\sigma_\infty^{(1)}$ acting in the normal direction to the crack plane. As a result, we obtain the stress field near the tip of a blunt crack. The form of the solution for the stresses $\sigma_y^{(1)}$ at the continuation of the blunt crack with the curvature radius ρ_1 is more complicated than (1.2). These stresses $\sigma_y^{(1)}$ can be represented in the form (1.2) only in the limiting case as $\rho_1 \to 0$. The stresses $\sigma_\infty^{(1)}$ being specified, the stresses $\sigma_\infty^{(i)}$ for $1 < i \leqslant i^{00}$ are determined from the relations

$$\int\limits_0^{n_i r_i} \sigma_y^{(i)}(x_i, 0)\, dx_i = \sigma_\infty^{(i+1)} \qquad (i = 1, 2, \ldots, i^{00} - 1). \tag{1.3}$$

The averaged stresses $\sigma_\infty^{(2)}$ are used in criterion (1.1) for $i = 1$ and in the formulation of the boundary conditions of the elastic problem for the blunt crack in the next porous structure $i = 2$. For $i = 2$, the stressed state $\sigma_y^{(2)}(x_2, 0)$ is constructed [see a similar relation (1.2) for $i = 2$]. Problems for edge cracks are usually obtained for $i > 1$, then the stresses are averaged according to relation (1.3) for $i = 2$, etc. [see criteria (1.1) and relations (1.2) and (1.3)]. After appropriate transformations, we obtain the estimate of the critical SIF $K_I^{*(i)}$ for a sharp normal-rupture crack

$$K_I^{*(i)}/\sigma_\infty^{(i)} \leqslant [(\sigma_m^{(i)}/\sigma_\infty^{*(i)})(k_i/n_i) - 1](\pi n_i r_i/2)^{1/2} \qquad (i = 1, 2, \ldots, i^0), \tag{1.4}$$

where $\sigma_\infty^{*(i)}$ is the critical value of $\sigma_\infty^{(i)}$. A modification of estimate (1.4) for a blunt crack is given below.

We construct necessary criteria of brittle strength for a medium that has three structural levels $i^0 = 3$ (Fig. 2). The microscope principle is used, which allows one to study the behavior of the material in the vicinity of the crack tip in more detail. A porous solid body ($i^{00} = 1$) with an internal macrocrack that has a microcrack at its tip is studied. Let an unbounded porous medium contain regularly located cylindrical cavities whose centers form a regular lattice with a square cell [8–10]. The internal macrocrack of length $2l_{n_1k_1}^{(1)}$ appears due to the breakage of certain bonds in the porous body of regular structure (Fig. 2a). We assume that the body is loaded at infinity by the stresses $\sigma_\infty^{(1)}$. The distance between the centers of the cylindrical cavities is denoted by r_1 and the radius of the cylindrical cavities by ρ_1. Let the porous material have macrodamages in front of the macrocrack tip which are described by the parameters $n_1 = 2$ and $k_1 = 1$, i.e., there is one force bond at this tip (Fig. 2a). Let the material of the force lintels of the porous body consist of monocrystalline grains whose location is shown in Fig. 2b (r_2 is the characteristic linear scale of the

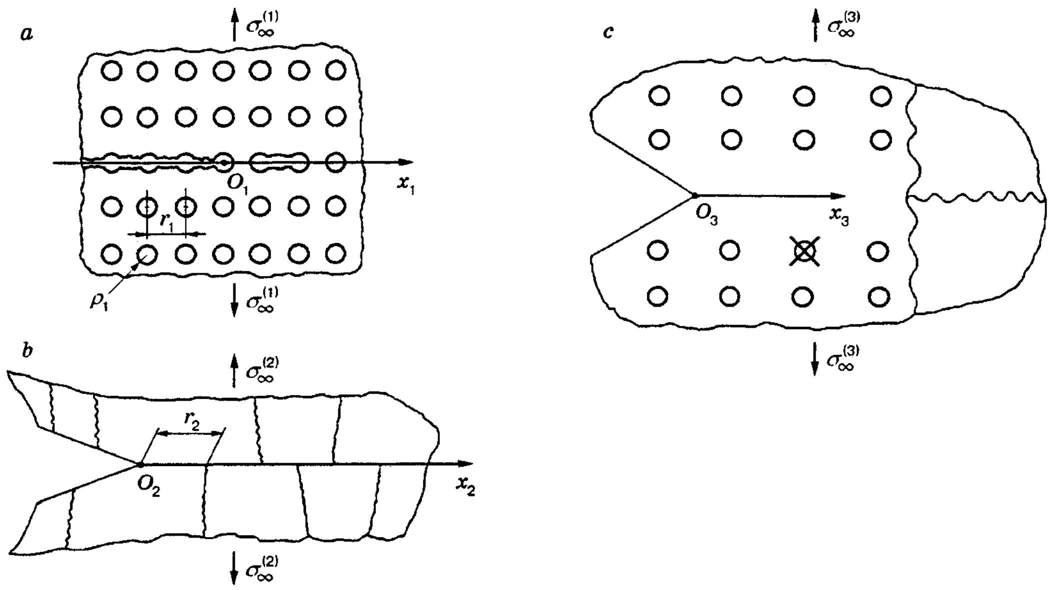

Fig. 2

grain). Let the first force lintel have a surface crack; then in another scale, we have an edge crack of length $l^{(2)}_{n_2k_2}$ for a grainy material of regular structure (microdamages of the grainy structure are described by the parameters $n_2 = 2$ and $k_2 = 1$). The procedure of determining $\sigma^{(2)}_\infty$ is outlined above. Let the crack tip end in a monocrystalline grain of the material as shown in Fig. 2c. We consider the simplest crystal lattice which is oriented "properly" relative to the crack plane; r_3 is the crystal lattice distance and the cross denotes a vacancy ($n_3 = 2$ and $k_3 = 1$). In this case, we obtain again an edge crack of length $l^{(3)}_{n_3k_3} = l^{(2)}_{n_2k_2}$ for a specified loading $\sigma^{(2)}_\infty$. Obviously, $r_1 \gg r_2 \gg r_3$.

We now give three consistent criteria: for a porous body with an internal crack (Fig. 2a), a grainy material with an edge crack (Fig. 2b), and a monocrystalline material with an edge crack (Fig. 2c).

Below, we consider relations for the critical parameters of internal sharp, edge sharp, and internal blunt cracks, which are used to construct all the consistent necessary criteria.

1.2. Internal Sharp Crack. We consider an internal crack of length $2l^{(i)}_{n_ik_i}$. We recall that the SIF of this crack is $K^{(i)}_I = \sigma^{(i)}_\infty\sqrt{\pi l^{(i)}_{n_ik_i}}$. Substituting the critical SIF for this crack into relation (1.4), we obtain the critical length $2l^{*(i)}_{n_ik_i}$ of the sharp internal normal-rupture crack

$$2l^{*(i)}_{n_ik_i}/r_i = (\sigma^{(i)}_m/\sigma^{*(i)}_\infty - n_i/k_i)^2 k_i^2/n_i. \tag{1.5}$$

1.3. Edge Sharp Crack. We consider a half-plane with an edge crack of length $l^{(i)}_{n_ik_i}$ subjected to the tensile stresses $\sigma^{(i)}_\infty$ applied perpendicularly to the crack. The SIF of this crack is $K^{(i)}_I = 1.1215\sigma^{(i)}_\infty\sqrt{\pi l^{(i)}_{n_ik_i}}$ (see [17]). Substituting the critical SIF for this crack into relation (1.4), we obtain the critical length $l^{*(i)}_{n_ik_i}$ of the sharp edge normal-rupture crack

$$2.52\, l^{*(i)}_{n_ik_i}/r_i = (\sigma^{(i)}_m/\sigma^{*(i)}_\infty - n_i/k_i)^2 k_i^2/n_i. \tag{1.6}$$

1.4. Internal Blunt Crack. We consider an internal blunt crack of length $2l^{(i)}_{n_ik_i}$ or, more precisely, a crack with the curvature radius ρ_i at the tip. The stress-strained state at the tip of a narrow notch is well known [17]. Note that there is no stress singularity at the crack tip for a finite ρ_i. After some manipulations [5], we obtain the critical SIF of the notch $K^{*(i)}_I$, which is expressed in terms of the SIF $K^{*0(i)}_I$ for a sharp crack of the same length:

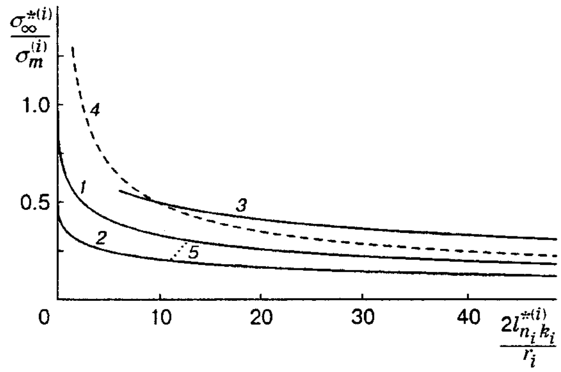

Fig. 3

$$K_I^{*(i)} = K_I^{*0(i)}(\rho_i/(2n_ir_i)+1)^{1/2}. \tag{1.7}$$

It is obvious that the limiting passage from the blunt to the sharp crack is possible as $\rho_i \to 0$. Using equality (1.7) and the SIF of the sharp crack $K_I^{0(i)} = \sigma_\infty^{(i)}\sqrt{\pi l^{(i)}_{n_ik_i}}$, we obtain the critical length of the blunt crack

$$2l^{*(i)}_{n_ik_i}/r_i = (\sigma_m^{(i)}/\sigma_\infty^{*(i)} - n_i/k_i)^2(\rho_i/(2n_ir_i)+1)k_i^2/n_i. \tag{1.8}$$

Expressions (1.7) and (1.8) for the critical parameters involve the nondimensional quantity ρ_i/r_i that characterizes the notch curvature.

1.5. Fracture Curves. Limiting Passage to Defect-Free Materials. We consider curves that describe the fracture according to the Neuber–Novozhilov criteria proposed [see the initial criterion (1.1) and implementations of this criterion in (1.5) and (1.6) for the corresponding types of cracks] and the classical criterion where the lengths of internal cracks $2l^{*(i)}_{n_ik_i}/r_i$ are specified.

We give relations that determine dimensionless critical loads for the blunt (structures have microdefects: $n_i > k_i$) and the sharp (microdefects are absent: $n_i = k_i$) internal cracks:

$$\frac{\sigma_\infty^{*(i)}}{\sigma_m^{(i)}} = \left[\frac{n_i}{k_i} + \frac{\sqrt{n_i}}{k_i}\sqrt{\frac{2l^{*(i)}_{n_ik_i}}{r_i}}\left(1+\frac{\rho_i}{2n_ir_i}\right)^{-1/2}\right]^{-1}, \quad \frac{\sigma_\infty^{*(i)}}{\sigma_m^{(i)}} = \left(1+\sqrt{\frac{2l^{*(i)}_{n_ik_i}}{n_ir_i}}\right)^{-1}. \tag{1.9}$$

In the first relation, the limiting passage from the blunt to the sharp crack is possible as $\rho_i \to 0$. For an arbitrary i, relations (1.9) can be regarded as equations that describe a unified fracture curve; moreover, the theoretical strengths $\sigma_m^{(i)}$ and the characteristic linear dimensions r_i of regular structures serve as units of measurements for stresses and linear dimensions, respectively. To estimate the strength of materials with and without defects that have sufficiently long blunt cracks, one can use the approximate equalities

$$\sigma_\infty^{*(i)}/\sigma_m^{(i)} \simeq (k_i/\sqrt{n_i})\sqrt{(r_i/(2l^{*(i)}_{n_ik_i}))(1+\rho_i/(2n_ir_i))} \tag{1.10}$$

relating the critical parameters.

An increase in the critical length of the crack by two orders leads to a decrease in the critical load by one order with allowance for defects of the material and bluntness of the crack.

Two types of defects are possible, namely, macrodefects and microdefects at each structural level. The macrodefects are described by the crack dimension (for example, we have a set of parameters r_i and $2l^{*(i)}_{n_ik_i}$ for an internal crack). The microdefects correspond to damages of the material in the vicinity of the crack tip and are described by the parameters n_i and k_i. Figure 3 shows five fracture curves: curves 1 and 2 describe, respectively, the fracture of defect-free materials ($n_i = k_i = 1$) and materials with defects ($n_i = 2$ and $k_i = 1$) that contain a sharp crack; curve 3 describes the fracture of defect-free materials ($n_i = k_i = 1$) with a narrow notch [$\rho_i/(2r_i) = 3$ and $2l^{*(i)}_{n_ik_i}/r_i \geqslant 10\rho_i/(2r_i)$]; curve 4 is the classical fracture curve, which has a singularity at zero [see the second relation of (1.9) where the unity is omitted inside the brackets]; and dotted curve 5 is a conventional curve that describes the passage from the defect material to the defect-free material for the growing crack. It is obvious that, according to the criteria proposed, materials with or without microdefects cannot sustain stresses that exceed the theoretical strengths of the corresponding structures.

Thus, the effect of the smooth components of the solutions $\sigma_\infty^{(i)}$ in (1.2), the material microdefects in front of the crack tip k_i/n_i, and the crack bluntness ρ_i/r_i on the critical loads $\sigma_\infty^{*(i)}$ [see relations (1.5), (1.8), and (1.9)] is qualitatively estimated. We emphasize that, according to Novozhilov's terminology, curve 1 in Fig. 3 corresponds to the necessary strength criterion. It is noteworthy that, for the critical parameters in relations (1.4)–(1.6), (1.8), and (1.9), we can pass to the limit as $K_I^{*(i)} \to 0$ and $l_{n_i k_i}^{*(i)} \to 0$ [in the classical relations like in (1.10), this passage is impossible].

2. CRITICAL CRACK PARAMETERS ESTIMATED BY MULTISCALE CRITERIA

We consider a body with a hierarchy of structures for which the characteristic linear dimensions and theoretical strengths are given by

$$r_i/r_{i+1} = A_i, \qquad \sigma_m^{(i+1)}/\sigma_m^{(i)} = B_i \qquad (i = 1, 2, \ldots, i^0 - 1), \tag{2.1}$$

where $A_i = \text{const} \gg 1$ and $B_i = \text{const} \gg 1$ are constants, which, in general, differ by orders [see (1.10)]. As a rule, we have

$$\min r_i = r_{i^0}, \qquad \min \sigma_m^{(i)} = \sigma_m^{(1)} \qquad (i = 1, 2, \ldots, i^0).$$

We consider an internal sharp crack of length $2l_{n_i k_i}^{(i)}$ and assume that the defectness parameters of the material k_i/n_i are known. The minimum critical load $\min \sigma_\infty^{*(i)}$ that is observed for a certain structure $i = i^*$ can readily be determined from the approximate relations (1.10) for given A_i and B_i. If necessary, this load can be refined [see (1.9)]. Depending on geometrical and force parameters and parameters that characterize the material defects, the minimum critical load $\min \sigma_\infty^{*(i)}$ corresponds to one or another structure. Other conditions being equal, the crack resistance of a structured material increases as the linear dimension of the particular structure r_i is increased, since the relative dimension of the crack $2l_{n_i k_i}^{(i)}/r_i$ decreases for its length fixed. The same result was obtained by the methods of similarity theory in [18] (the available experimental data were also analyzed therein). Serious difficulties arise in manufacturing defect-free materials $k_i/n_i = 1$ or materials with a prescribed relative level of defects $k_i/n_i = \text{const} < 1$ when the dimension r_i increases.

Let the load parameter for a certain particular structure $i = i^*$ reach a critical value under continuously added loading. Then unstable growth of the crack for this structure occurs. Moreover, uncontrollable macrofracture begins if $i^* = 1$, and quasi-static growth of the crack occurs if $i^* > 1$. In the case of uncontrollable fracture, the body is split into fragments. When the crack extends in the structure $i^* > 1$, either cessation of fracture of the structure $i^* > 1$ or intensification of fracture of the structures $i < i^*$ is possible. The fracture can stop when, for example, the crack tip meets a grain of an ideal monocrystal [the passage from the material with microdefects to the defect-free material (curve 5 in Fig. 3)]. The fracture is intensified when, for the quasi-static extension of the i^*th structure crack, criterion (1.1) holds for the ith structure such that $1 \leqslant i < i^*$. It should be noted that, for $i^* = 1$, the passage to uncontrollable macrofracture is observed. The most unfavorable case (catastrophic failure) occurs when the critical loads are exceeded simultaneously for two or more structures among which there is the macrostructure $i^* = 1$.

Bearing the foregoing in mind, we consider the behavior of sufficiently long cracks. The necessary information on the critical parameters of internal cracks (see Sec. 1) is supplemented by the approximate equality for the edge sharp cracks [cf. (1.10)]

$$\sigma_\infty^{*(i)}/\sigma_m^{(i)} \simeq (k_i/\sqrt{n_i})\sqrt{r_i/(2.52 l_{n_i k_i}^{*(i)})}. \tag{2.2}$$

We assume that there is only one bond at the crack tip in each structure, and the relative linear dimensions and material defects for each structure have the form

$$r_1/r_2 = A_1 = O(10^4), \quad r_2/r_3 = A_2 = O(10^2), \quad n_1 = n_2 = n_3 = 2, \quad k_1 = k_2 = k_3 = 1, \tag{2.3}$$

where $2r_i$ are the intervals of averaging ($i = 1$, 2, and 3) and r_3 is the lattice distance. It is also assumed that theoretical strengths for each structure differ by orders [$\sigma_m^{(3)}$ is the ideal strength of a monocrystalline body]:

$$\sigma_m^{(2)}/\sigma_m^{(1)} = B_1 = O(10^2), \qquad \sigma_m^{(3)}/\sigma_m^{(2)} = B_2 = O(10), \tag{2.4}$$

which corresponds to the case where the strength of the structural material in the macrostructure differs from the ideal strength of a crystalline body by three orders. Taking relations (1.10) and (2.2) and equalities (2.3) and (2.4) into account, we infer that, for sufficiently long cracks, the minimum critical load is reached in one of the structures $i = 1$, 2, and 3 depending on the geometrical and force parameters and parameters characterizing the material defectness.

We dwell in greater detail on the choice of the quantity $\sigma_m^{(1)}$ that characterizes the theoretical strength of the bond in a porous body. When it is necessary to perform particular calculations and compare experimental results with theoretical concepts [9, 10], one should choose the upper limit of the strength of the specimen-witness [9, 10] obtained in a full-scale experiment as the theoretical strength of this bond. We emphasize that experiments on smooth specimens gave greater scatter than those on specimens-witnesses. In fact, microdamages of the pore surfaces were modeled on the specimens-witnesses; as a result, the macrostructures failed earlier than the structures with ideal-surface pores did.

Remark. In criterion (1.1) it is assumed that, for a material with damages, the fracture begins at the crack tip rather than at the microdamage tips. A more detailed estimate of the failure pattern due to interaction between sharp cracks and various holes (blunt cracks) can be found in [19, 20].

3. INITIATION OF MICROVOIDS IN FRONT OF THE CRACK TIP FOR LOW-ANGLE BOUNDARIES

The multiscale criteria for brittle strength proposed above are free of restrictions of the classical approach and make it possible to describe the initiation of satellite microcracks: "... crack growth in ductile materials can occur by both continuous tearing and by void formation ahead of the advancing crack tip" [21, p. 409]; "there is growing evidence that, in multiphase polycrystalline materials, the stress concentration caused by second-phase particles or by grain boundaries causes microvoids to form, which eventually coalesce into macrovoids" [21, p. 411].

To describe the initiation of microvoids in front of a crack in a material with defects, we modify criterion (1.1). Further, we consider the formation of microvoids in a continuous solid at the continuation of the normal-rupture macrocrack (see [21, Figs. 13 and 15]). Let the right tip of the internal macrocrack of length $2l$ stop at a defect-free monocrystal (its x-length is $n_{i^0} r_{i^0}$, where r_{i^0} is the lattice distance, the subscript $i^0 = 2$ is assigned to the crystalline structure; for example, we have $r_2 = r_e = 2.9$ Å for α- and β-iron and $r_2 = r_e = 3.6$ Å for γ-iron). Moreover, let the low-angle boundary of the other two monocrystals be located at the right continuation of the crack [the subscript $i = 1$ is assigned to the structure with the low-angle boundary, and the low angle characterizes the disorientation of these monocrystals (see Fig. 2b and c)]. We assume that, for a specified load $\sigma_\infty^{(1)}$, the crack length $2l$ is critical neither for $i = 1$ nor for $i^0 = 2$ [see criteria (1.1)].

We model a regular low-angle boundary of two monocrystals by clusters composed of vacancies. It is assumed that the two monocrystals come into contact along a certain straight line, on which the vacancies are located regularly. The number of vacancies is $n_1 - k_1$, where $k_1 = O(1)$ is the number of working interatomic bonds between the upper and lower monocrystals that form the low-angle boundary (for example, $k_1 = 1$, 2, and 3) and $n_1 r_1$ is the recurrence interval of the regular structure, $n_1 \gg 1$ (for example, $n_1 = 10$ and 20). For definiteness, we assume that the structure $i = 1$ originates in the cluster from $n_1 - k_1$ vacancies followed by k_1 atoms that ensure interatomic interaction of crystalline structures of the two monocrystals.

A sharp crack is modelled by a two-sided notch; the condition for formation of the first microvoid on the right continuation of the crack for a certain particular structure $i = i^*$ (for low-angle boundaries, we have $i^* = i^0 - 1 = 1$) has the form

$$\max \frac{1}{kr} \int\limits_{n^{(1)}r}^{n^{(2)}r} \sigma_y(x,0)\,dx = \sigma_m^{(1)}. \tag{3.1}$$

Here $\sigma_y = \sigma_y^{(i^*)}(x_{i^*},0)$ are the normal stresses at the crack continuation [they can have a singularity only at the crack tip for the i^0th structure and do not have one for the (i^0-1)th structure], $O_{i^*}x_{i^*}y_{i^*}$ is the Cartesian coordinate system oriented relative to the right part of the crack, $r = r_{i^*}$ is the characteristic linear dimension of the i^*th structure, in (3.1) and below the symbol i^* is omitted, $n^{(2)}r$ and $n^{(1)}r$ are the upper and lower limits of integration, $n^{(1)} > 0$, k is the number of active bonds acting in the averaging interval $(n^{(1)}r,\ n^{(2)}r)$ such that $n^{(2)} - n^{(1)} \gg k$, and $\sigma_m^{(1)}$ is the theoretical strength of the material.

In the continual model, the stressed state in the vicinity of the crack tip has an integrable singularity [see (1.2)] and the SIF of the internal crack is related to its half-length and the load specified at infinity σ_∞ by $K_I = \sigma_\infty\sqrt{\pi l}$. Substitution of the above-mentioned relations into the integrand in (3.1) and necessary manipulations yield the formula

$$\frac{\sigma_\infty^*}{\sigma_m^{(1)}} = \left[\max\left(\frac{n^{(2)}-n^{(1)}}{k} + \frac{\sqrt{n^{(2)}}-\sqrt{n^{(1)}}}{k}\sqrt{\frac{2l^*}{r}}\right)\right]^{-1},$$

which describes the initiation of the first microvoid and relates the critical load σ_∞^* and the macrocrack length $2l^*$ [cf. (1.9)]. The critical load σ_∞^* satisfies the following restrictions [criterion (3.1) is fulfilled first rather than criteria (1.1)]:

$$\sigma_\infty^*/\sigma_m^{(1)} < \sigma_\infty^{*(1)}/\sigma_m^{(1)}, \qquad \sigma_\infty^*/\sigma_m^{(1)} < \sigma_\infty^{*(2)}/\sigma_m^{(2)}.$$

Here $\sigma_\infty^{*(2)}$ and $\sigma_\infty^{*(1)}$ are the critical loads of the monocrystal and polycrystal with a low-angle boundary, respectively, where the critical length of the internal crack is $2l^* = 2l^{*(1)} = 2l^{*(2)}$ [see (1.9)]. In the last inequalities, the critical parameters are compared again. If the critical parameter $\sigma_\infty^*/\sigma_m^{(1)}$ becomes equal to at least one of the critical parameters $\sigma_\infty^{*(1)}/\sigma_m^{(1)}$ and $\sigma_\infty^{*(2)}/\sigma_m^{(2)}$, catastrophic failure occurs.

In the case of low-angle boundaries, the left side of relation (3.1) reaches its maximum when

$$n^{(1)} = n_2, \qquad n^{(2)} = n_2 + 2n_1 - k_1, \qquad k = k_1,$$

and hence, the length of the new void formed is $L = (2n_1 - k_1)r_1$. One can easily verify that all restrictions are fulfilled, for example, for $k_1 = 1$, $n_1 = 21$, and $n = 4$, i.e., for sufficiently weak low-angle boundaries.

The discrete-integral criteria (1.1) and (3.1) are hybrid criteria since they are based on both discrete and continual approaches: the stress-strain state near the crack tip is determined with the use of the continual model of mechanics of continuous media, whereas the loss of stability of an atomic lattice with defects for a specified load is determined using the discrete approach in accordance with models of the physics of solids.

In a defect-free material, criteria (1.1) are satisfied first, then criterion (3.1) is fulfilled. In the presence of significant defects at the crack continuation, criterion (3.1) can be fulfilled first, then the stress-strained state alters because of the formation of microvoids. Thus, only after the effect of the structure in the vicinity of the crack tip on fracture is taken into account does it become possible to explain why, under certain conditions, the failure occurs not at the crack tip, but at a certain distance from it (the problem, in principle, cannot be solved within the framework of the continual model of the theory of elasticity since, in view of the singularity at the crack tip predicted by the continual model, whichever criterion is used, the failure must begin precisely at this tip) [22, p. 56].

After the formation of the first microvoid, the following events are possible: 1) appearance of a second microvoid; 2) propagation of the main crack (uncontrollable failure); 3) expansion of the first microvoid-crack (see [23, Fig. 77]). In the first case, an analog of criterion (3.1) is used and in the second and third cases, analogs of criteria (1.1) are used. To describe the quasi-brittle process of initiation of microvoids, their growth, and propagation of the main crack, criteria (3.1) and (1.1) become somewhat complicated since in the integrands it is necessary to use normal stresses at the crack continuation with allowance for the microvoids-cracks already formed [19, 20]. The development of the microvoids, in general, cannot be described by quasi-brittle (necessary) criteria of the type (1.1) and (3.1) since "the plastic deformation involved in void coalescence is often on such a fine scale as to escape macroscopic level, but is locally of a high degree of deformation, comparable to hundreds or thousands of percent in a tensile test" [23]. A complete description of the microvoids will be possible after multiscale sufficient criteria of strength are constructed.

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