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DEFORMATION AND FRACTURE MECHANICS

Fracture Criterion and the Life of Materials during Brittle Fracture

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Abstract—A structural–statistical kinetic model is developed to describe the brittle fracture of materials at low stresses. Expressions are derived for the average life of a material at low stresses, and a kinetic meaning of the brittle fracture criterion is formulated.

Keywords: brittleness, fracture, life, stress

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1. INTRODUCTION

Most experimental and theoretical results of studying the life of materials [1, 2] belong to the tensile-stress range where Zhurkov's formula [3, 4], which was theoretically substantiated in [5, 6], holds true. These results allowed researchers to prove a thermal-fluctuation character of fracture and to find important characteristics of the process, such as the activation energy of an elementary act of bond rupture U, structure-sensitive coefficient γ, fluctuation volume V_a, and other limiting fracture characteristics of a material.

In the tensile-stress range where Zhurkov's formula holds true, the life of a material is short as compared to its operating time [1, 2]. It is obvious, however, that most materials must have the average operating time that is long enough for long-term operation. This means that all materials usually operate in the external-load range where the Zhurkov relation between average life τ and tensile stress σ is not valid [3, 4]. According to the experimental data obtained in a low stress σ range [2], the logarithm of the average life as a function of tensile stress σ does deviate from linear Zhurkov's dependence.

Since the average life of a material in a low-stress range is very long, it is practically impossible to experimentally study the dependence of the average life on tensile stress σ in this range. Therefore, it is very important to theoretically investigate the dependence of average life τ on stress σ in a low-stress range, which is the working range of most materials used in engineering and technology. It should be noted that brittle fracture, which is inherent in both metals and polymers under certain loading conditions, is the most dangerous type of fracture, since it usually occurs suddenly, without visible signs of preliminary plastic (in metals) and highly elastic (in polymers) deformation [5–7].

The theoretical works dealing with the fracture kinetics of materials are usually based on Zhurkov's kinetic fracture concept and are not focused on a low-stress range (see, e.g., [8, 9]). The purpose of this work is to develop a mathematical model to describe the brittle fracture of materials in a low-stress range [10–13].

2. FORMULATION OF THE MODEL

When simulating the fracture of materials, we have to take into account the following factors: (1) changes in the energy barriers when a system under external mechanical fields passes from a current state into a neighboring one (due to elementary fracture acts in fluctuation volume) in certain configuration space, which requires the calculation of stress fields in a material with allowance for cracks; (2) the distribution of cracks in the danger of induced fracture and a random character of this distribution; and (3) a stochastic character of the development of dangerous cracks in a material, which is caused by the thermal fluctuation mechanism of fracture of kinetic units (in particular, chemical bonds) in overstress regions, which are elementary fracture acts.

In the general case, the first and third factors include the structural relaxation processes (plastic deformation in metals and forced highly elastic deformation in polymers) that precede elementary fracture acts. In the case of brittle fracture, relaxation processes are "frozen" in time until material fracture; therefore, a local structure, on the scale of the nearest neighbors, is important here.

At low stresses, the main contribution to the life of a material with cracks is made at the stage of fracture

crack (FC) formation. The time of this stage depends on the imperfection of the initial (before loading) structure of a material and the kinetic processes that determine the structure development after the application of an external load [1, 11–13]. As a rule, FC is a crack with a small characteristic size and the most favorable (for fracture) orientation.

The life of a material at low stresses is determined by the time it takes to reach the FC state that corresponds to Griffith's fracture threshold and the time it takes to reach a critical state, after which a crack grows athermally and destroys the material. This total time can be estimated using a mathematical model for stochastic development of FC in a material. This model consists of an equation for function $P(\vec{l},t)$, which is the probability of the fact that FC at time t is in a state characterized by vector $\vec{l} = (l_1, l_2, \ldots l_n)$, where $l_1, l_2, \ldots, l_n$ is the set of parameters required for a unique determination of the state of FC.

Since the development of FC usually occurs due to a thermally activated transition from state $\vec{l} = (l_1, l_2, \ldots, l_n)$ to the neighboring state $\vec{l} + \vec{\lambda} = (l_1 + \lambda_1, l_2 + \lambda_2, \ldots, l_n + \lambda_n)$ or $\vec{l} - \vec{\lambda} = (l_1 - \lambda_1, l_2 - \lambda_2, \ldots, l_n - \lambda_n)$, an equation for function $P(\vec{l}, t)$ can be represented in the diffusion approximation [14]. Since the change in parameter $l_i (i = 1, 2, \ldots, n)$ occurs at various rates, the development of FC is determined by the parameter changing most slowly. Then, the equation for function $P(\vec{l}, t)$ is transformed to an equation for function $P(l, t)$, where l is the most slowly changing parameter of FC during its development.

The equation for function $P(l, t)$ was derived in [10, 11, 13] and has the following form for FC:

$$dP_m(l_i,t)/dt = w^+(l_{i-1},t)P_m(l_{i-1},t) - (w^+(l_i) + w^-(l_i))P_m(l_i,t) + w^-(l_{i+1},t)P_m(l_{i+1},t), \quad (1)$$
$$i = m+1, \ldots, k-1, \; t > 0,$$

$$dP_m(l_m,t)/dt = w^-(l_{m+1})P_m(l_{m+1},t) - w^+(l_m,t)P_m(l_m,t), \quad t > 0, \quad (2)$$

$$P_m(l_k,t) = 0, \quad t \geq 0, \quad (3)$$

$$P_m(l_i,0) = \delta_{mi}, \quad (4)$$

where $\delta_{mi} = \begin{cases} 1 & \text{at} \quad i = m \\ 0 & \text{at} \quad i \neq 0 \end{cases}$ is Kronecker's delta. Here, $P_m(l_i, t)$ is the probability of the fact that FC having parameter $l = l_m$ (characteristic size) at time $t = 0$ is in the state with $l = l_i$ at time t, and $w^+(l_i)$ and $w^-(l_i)$ are the probabilities of transition of FC from the state with $l = l_i$ to the states with $l = l_{i+1}$ and $l = l_{i-1}$ ($l_m < l_{m+1} < \ldots < l_k$), respectively.

Condition (3) means that the state of FC with $l = l_k$ is absorbing and corresponds to the beginning of athermal (barrier-free) FC growth, when the activation energy of transition to the next state $l_k + \lambda_n$ is zero.

Along with initial condition (4), Eqs. (1)–(3) represent a Cauchy problem for a set of linear first-order differential equations. From a formal standpoint, it is known how to solve this problem [15]. However, it can only numerically be solved and the number of equations in the system under study can be 10^3–10^5 or more. However, kinetic equations (1) and (2) make it possible to obtain exact expressions for the numerical characteristics of a random quantity, i.e., the life (its mathematical expectation, dispersion, etc.), if the frequencies of elementary fracture acts are time independent, i.e., during brittle fracture.

3. BASIC RESULTS

3.1. Life Distribution Function

Based on the solution of problem (1)–(4), we can find the life probability distribution density $\varphi_m(t)$ by the formula [1, 11, 13]

$$\varphi_m(t) = P_m(l_{k-1}, t - t_m^{(a)})w^+(l_{k-1}), \quad t \geq t_m^{(a)}, \quad (5)$$

$$\varphi_m(t) = 0, \quad t < t_m^{(a)}, \quad (6)$$

where $P_m(l_{k-1}, t - t_m^{(a)})w^+(l_{k-1})dt$ is the probability of the fact that FC with characteristic size $l = l_m$ at time $t \geq t_m^{(a)}$ is in the state with $l_i = l_{k-1}$, which passes to an absorbing state with $l_i = l_k$ at a probability $w^+(l_{k-1})dt$; $t_m^{(a)}$ is the time of athermal development of FC with characteristic initial size $l = l_m$ that is determined by the formula [1, 11, 13]

$$t_m^{(a)} = \frac{l_m - l_k}{v_k}, \quad (7)$$

where v_k is the velocity of sound in the material.

Formulas (5) and (6) can be applied when only FC is present in a material in the initial state. A material usually contains a set of cracks, which are described by their initial size distribution. In this case, the life probability distribution density $\varphi(t)$ can be represented in the form [1, 11]

$$\varphi(t) = \exp\left[-\sum_{m=1}^{n} \bar{N}_m W_m(t - t_m^{(a)})\right] \sum_{m=1}^{n} \bar{N}_m \varphi_m(t). \quad (8)$$

Here,

$$W_m(t - t_m^{(a)}) = w^+(l_{k-1}) \int_0^{t - t_m^{(a)}} P_m(l_{k-1}, x)dx, \quad (9)$$

$\bar{N}_m = C_m V$ is the average number of cracks in the material with characteristic initial size l_m, and C_m is their concentration in material volume V (number of cracks per unit volume).

The sum in Eq. (8) is taken over the entire set $\{l_m\}$, $m = 1, 2, ..., n$ ($l_1 < l_2 < ... < l_n$) of initial cracks, which are normal to external tensile stress σ. If the initial crack size distribution has a crack with a large initial size (initial length), which differs radically from other cracks, the expression for distribution function $\varphi(t)$ is simplified and can be written as [1, 11]

$$\varphi(t) = \sum_{m=1}^{n} p_m \varphi_m(t), \quad (10)$$

where

$$p_m = (1 - \exp(-\bar{N}_m)) \exp\left[-\sum_{i=m+1}^{n} \bar{N}_i \right] \quad (11)$$

is the probability of the fact that a crack of size $l = l_m$ is the crack with the maximum characteristic initial size.

3.2. Average Life

The average life of a material τ is

$$\tau = \int_0^\infty \varphi(t) t dt. \quad (12)$$

Substituting Eq. (10) into Eq. (12), we obtain (this case is considered below)

$$\tau = \sum_{m=1}^{n} p_m \tau_m, \quad (13)$$

where partial lives τ_m are

$$\tau_m = \langle t_m \rangle + t_m^{(a)}, \quad \langle t_m \rangle = w^+(l_{k-1}) \int_0^\infty P(l_{k-1}, t) t dt. \quad (14)$$

According to [1, 10, 11], we have

$$\tau_m = \sum_{i=m}^{k-1} \frac{1}{w^+(l_i)} \left[1 + \sum_{j=i+1}^{k-1} \prod_{n=i+1}^{j} \frac{w^-(l_n)}{w^+(l_n)} \right] + t_m^{(a)}. \quad (15)$$

To calculate τ_m by Eq. (15), we have to find transition frequencies $w^+(l_i)$ and $w^-(l_i)$. According to the fluctuation theory, the authors of [1, 10, 11] obtained

$$w^-(l_{i+1}) = w^+(l_i) \exp\left[\frac{\lambda}{k_B T} \frac{d\Delta\Phi(l_i)}{dl_i} \right], \quad (16)$$

$$w^+(l_i) = \nu \exp\left[-\Delta\Phi^+(l_i)/k_B T \right], \quad (17)$$

$$\Delta\Phi^+(l_i, \sigma) = U - V_a \sigma^*(l_i, \sigma). \quad (18)$$

Here, $\Delta\Phi^+(l_i, \sigma)$ is the change in the thermodynamic potential of the sample during the thermal-fluctuation-induced transition of a crack from the state with l_i to a metastable state between l_i and l_{i+1}; $\sigma^*(l_i, \sigma)$ is the tensile stress in the transition region, i.e., at the crack front; λ is the characteristic change in parameter l_i during the transition of FC into neighboring states $l = l_{i+1}$ and $l = l_{i-1}$; $\Delta\Phi(l_i, \sigma)$ is the increment of the thermodynamic potential of the material containing FC with initial size $l = l_m$ during its evolution to size l_i; k_B is the Boltzmann constant; T is the absolute temperature; and ν is the oscillation frequency of the kinetic units in fluctuation volume V_a that determine the transition of FC from a given state into the neighboring one.

3.3. Calculation and Asymptotics of the Average Life

The experimental data collected and presented in [2] demonstrate that the kinetic units that are responsible for an increase in the FC size are usually atoms or molecules, the breaking of bonds between which at the FC tip leads to crack development. The authors of [1, 11, 13] showed that

$$\Delta\Phi(l_i, \sigma) = -\frac{\pi\sigma^2\lambda_\pi}{2E}(l_i^2 - l_m^2) + 2\alpha_s\lambda_\pi(l_i - l_m), \quad (19)$$

for an edge linear FC of length l_i in a thin plate of thickness λ_π under uniaxial stress σ,

$$\Delta\Phi(l_i, \sigma) = -\frac{\pi\sigma^2\lambda_\pi}{4E}(l_i^2 - l_m^2) + 2\alpha_s\lambda_\pi(l_i - l_m), \quad (20)$$

for an initial through linear FC of length l_i in a thin plate of thickness λ_π under uniaxial stress σ, and

$$\Delta\Phi(l_i) = -\frac{8\sigma^2(1-\mu^2)}{3E}(l_i^3 - l_m^3) + 2\pi(l_i^2 - l_m^2)\alpha_s, \quad (21)$$

for a disk FC of radius l_i. Here, α_s is the free specific surface energy, E is Young's modulus, and μ is Poisson's ratio.

An analysis of Eq. (5) [1, 11, 13] demonstrates that the expression under the sum sign in Eq. (15) has a maximum at $l_i = l^*$, where l^* is the root of the equation $d\Delta\Phi(l)/dl = 0$ at stress σ, at low tensile stresses σ, i.e., the stresses in the range $0 < \sigma < \sigma_G$, where σ_G is Griffith's fracture threshold determined by the condition $d\Delta\Phi(l)/dl = 0$. Therefore, we can estimate sum (15), which enters into Eq. (13) and determines τ_m, by the Laplace method provided $l_m \ll l^*$; as a result, we have [1, 11, 13]

$$\tau_m \approx \frac{kT}{\lambda^2 w^+(l^*)\Delta\Phi'(l_m)} \times \sqrt{\frac{2\pi k_B T}{|\Delta\Phi''(l^*)|}} \exp\left(\frac{\Delta\Phi(l^*)}{k_B T} \right) + t_m^{(a)}. \quad (22)$$

Griffith's fracture threshold for a material with FC of initial size l_m is determined from Eq. (21),

$$\sigma_G = \sqrt{\pi\alpha_s E / (2(1-\mu^2) l_m)}. \quad (23)$$

When σ decreases, the condition $l_m \ll l^*$, where $l^* = \pi\alpha_s E/(2(1 - \mu^2)\sigma^2)$, is met for FC with an increasing initial size until the situation where none of the samples with FC that meet this condition is pres-

ent among the set of identical samples of a given material. In this case, we have $\ln(\lambda\Delta\Phi'(l_m)/(k_BT)) \ll \Delta\Phi(l^*)/k_BT$; therefore, all terms in Eq. (13) cease to depend on the FC size distribution for a given material. Since $\sum_{m=1}^{n} p_m = 1$ and $\langle t_m \rangle \gg t_m^{(a)}$ and the other quantities entering into Eq. (22) are independent of the FC size distribution in a given material, we arrive at the following average life asymptotics during brittle fracture:

$$\tau \approx \frac{1}{\lambda w^+(l^*)}\sqrt{\frac{2\pi k_BT}{|\Delta\Phi''(l^*)|}}\exp\left(\frac{\Delta\Phi(l^*)}{k_BT}\right). \quad (24)$$

Allowing for Eq. (19), from Eq. (24) we obtain the following asymptotic expression for the average life for a surface FC [1, 11]:

$$\tau \sim \exp(2\alpha_s^2 E\lambda_\pi/\pi\sigma^2 k_BT). \quad (25)$$

We now consider the case of a circular disklike FC in more detail [13]. As follows from Eqs. (10) and (11), the cracks having the maximum size l_0 (in our case, l_0 is the radius of a disklike crack) mainly contribute to τ. According to [13], l_0 can be estimated if the limiting (theoretical) $\sigma_{th} = U/V_a$ and breaking $\sigma_b(V)$ strengths of a material of volume V are known. Assuming $\sigma^* = \sigma_{th}$ and $\sigma = \sigma_b$ in the formula $\sigma^*(l_i, \sigma) = \frac{2\sigma}{\pi}\sqrt{\frac{l_i}{2\lambda}} + \sigma = \sigma^*$, which deter mines the stress at the FC front [1], we obtain $l_0 = \lambda((\sigma_{th} - \sigma_b)/(\sigma_b\chi))^2$, where $\chi = \sqrt{2}/\pi$ is the form factor of FC. In this case, Griffith's fracture threshold for a material of given volume is equal to Griffith's fracture threshold for an internal disklike FC of radius l_0, i.e., $\sigma_G = \sqrt{\pi\alpha_s E/(2(1-\mu^2)l_0)}$. Allowing for the l_0 expression, we obtain

$$\sigma_G = \frac{\sigma_b\chi}{\sigma_{th} - \sigma_b}\sqrt{\pi\alpha_s E/(2\lambda(1-\mu^2))}. \quad (26)$$

Thus, the low-stress range depends on both the theoretical and breaking strengths of a material and is determined by the following condition in our case:

$$0 < \sigma < \frac{\sigma_b\chi}{\sigma_{th} - \sigma_b}\sqrt{\pi\alpha_s E/(2\lambda(1-\mu^2))}. \quad (27)$$

The substitution of $\Delta\Phi(l^*)$ and $|\Delta\Phi''(l^*)|$ into Eq. (24) with allowance for Eq. (21) leads to the following average life asymptotics in the case of a circular disklike FC [12, 13]:

$$\tau \approx \frac{k_BT}{\lambda^3\nu}\frac{1}{4\pi\alpha_s}\left(\frac{\sigma_b\chi}{\sigma_{th} - \sigma_b}\right)^2 \times \sqrt{\frac{k_BT}{2\alpha_s}}\exp\left(\frac{\pi^3\alpha_s^3E^2}{6(1-\mu^2)^2\sigma^4 k_BT}\right). \quad (28)$$

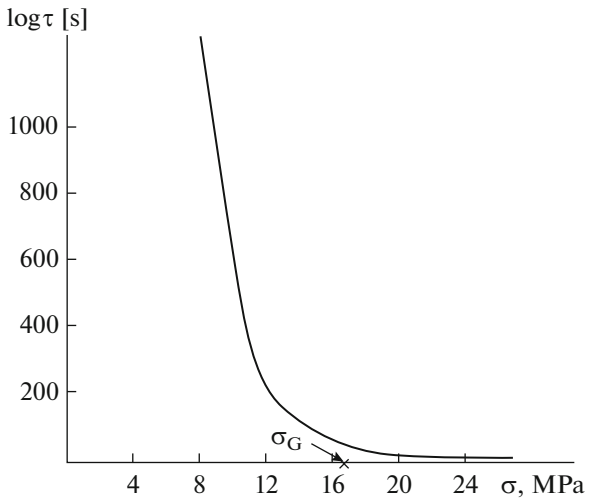

Fig. 1. Average life of organic glass at low stresses and T = 293 K, σ_G = 16.7 MPa, U = 134 kJ/mol, $V_a = 1.4 \times 10^{-28}$ m^3, $\lambda = 23 \times 10^{-10}$ m, $\lambda_\pi = 8 \times 10^{-10}$ m, $\alpha_s = 39 \times 10^{-3}$ J/m^2, $\mu = 0.33$, $E = 3.93 \times 10^9$ N/m^2, $l_0 = 1.7 \times 10^{-7}$ m, and $\nu = 10^{13}$ s^{-1} [17].

Figure 1 shows the average life calculated by Eqs. (13) and (15) in the range $0 < \sigma < \sigma_G$ according to the method developed in [17, 18].

If the conditions of loading by constant stress σ are such that $\sigma > \sigma_G$, from Eq. (15) we have

$$\tau = \sum_{m=1}^{n} p_m\left(\sum_{i=m}^{k-1}\frac{1}{w^+(l_i)} + t_m^{(a)}\right). \quad (29)$$

The following well-known Zhurkov formula follows from Eq. (29) according to [1, 11] and Eqs. (17) and (18) [3–5]:

$$\tau = \tau_0\exp[(U - \gamma\sigma)/k_BT], \quad (30)$$

where $\tau_0 = 2k_BTl_0/(\nu V_a\lambda\beta\sigma)$, $\beta = 1 + \chi\sqrt{l_0/\lambda}$ is the notch-sensitivity index, and $\gamma = V_a\beta$.

Asymptotic formulas (25) and (28) for the average life demonstrate that it remains long but finite at any low uniaxial tensile stress σ. Thus, the vertical asymptote of the average life is the line $\sigma = 0$ rather than $\sigma = \sigma_G$, as follows from [6, 19].

One could think that, at such a long average life, a forecast will also be favorable for the time ensured at a given functionally probability. However, the estimated dispersion of the average lives degrades this forecast. Indeed, the proposed structural–statistical kinetic approach to simulating the brittle fracture kinetics makes it possible to estimate the dispersion $D\tau$ of the life using the well-known formula

$$D\tau = \int_0^\infty t^2\varphi(t)dt - \tau^2. \quad (31)$$

The calculations performed in [17, 18] gave $D\tau \sim \tau^2$. This means that the root-mean-square deviation of the life is $\sigma_\tau \sim \tau$; that is, the scatter of the lives increases with the average life. This finding degrades the possibilities of the life forecast for a material in a brittle state from the average life. The situation can be improved by decreasing the dispersion of the lives by designing materials with a multielement structure [1], e.g., by creating composite materials.

In conclusion, we note that, to calculate the thermal-fluctuation break frequencies and the bond restoration frequencies in an overstress range, the mathematical model developed for the brittle fracture of materials uses the mathematical theory of cracks based on the elasticity theory, which gives infinite stresses at the crack front. This stress singularity is removed in the model as follows: these stresses are assumed to be equal to the stresses reached at a certain distance (on the order of the intermolecular distance) λ from the point of singularity. The singularity can also be removed by introducing cohesion forces between crack edges in terms of the Khristianovich–Barenblatt model of cracks [20]. The adequacy of this model was considered and supported by calculations in [21].

4. CONCLUSIONS

Using a structural–kinetic probabilistic model of the brittle fracture of materials, we showed the following: (1) The average life of a material increases infinitely when tensile stress σ decreases infinitely. (2) Griffith's fracture criterion determines the lower boundary of the tensile stress range in which thermally activated irreversible crack growth takes place during brittle fracture until athermal crack growth. (3) The upper boundary of low-stress range $0 < \sigma < \sigma_G$ depends on both the theoretical and breaking strengths of a material; as the breaking strength, this boundary is a random quantity, which depends on an initial crack size distribution. (4) In the range $0 < \sigma < \sigma_G$, the dispersion of the lives should be taken into account to predict the functionality time of a material.

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