Contribution of thermal fluctuations to the scattering and the gauge effect of longevity

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ABSTRACT
The distribution function of longevity of a sample under load due to thermal fluctuations is calculated. It reveals a size effect. Fair agreement is observed between theoretical results and available experimental data for a series containing about $10^2$ samples. This allows us to suppose that the usually observed scattering and the size effect of longevity are predominantly due to the thermally activated nature of the fracture process.

1. Introduction

Numerous experiments carried out by Zhurkov and co-workers have shown that fracture of solids under load is a thermally activated process and that the longevity (time to rupture) of a body under stress $\sigma$ is

$$\tau = \tau_0 \exp\left(\frac{U_0 - \gamma\sigma}{T}\right),$$

$T$ being the temperature in energetic units, $U_0$ a material constant, $\gamma$ a structure sensible parameter, $\tau_0$ the period of thermal vibrations [1]. Zhurkov's conception of thermally activated fracture provokes two theoretical problems.

A. Elucidation of the peculiarities of the thermally activated rearrangements of atoms in a body under stress and the calculation of the corresponding potential relief, i.e. of the stress-dependent activation energies controlling the elementary events of the energetically favourable development (creation and growth) of cracks.

B. Investigation of the process of surmounting the potential barriers, i.e. the building up of the fracture kinetics including the calculation of the time $\tau$ until the appearance of a main crack, $\tau$ being the longevity of the body. As the thermal fluctuations are random events, the crack development is a stochastic process and a complete description of $\tau$ requires the knowledge of its distribution function.

Up to now the first problem has not been answered for any material; for the second problem, only mean values of longevity have been calculated [2]. The aim of this paper is to present a brief account of the statistical kinetics of thermally activated fracture under isothermal creep conditions proposed by the present authors [3–5], and to solve the following open questions in the thermoactivational analysis of the fracture process:

(i) Are the experimentally observed scattering of longevities of nominally identical samples and the gauge effect due to the thermofluctuational nature of the fracture process, or are they due to variations of the defect structure and the testing conditions of the samples ("technological factors")?

(ii) Why has Zhurkov's empirical expression (1) for the longevity $\tau$, which is determined by the time of overcoming of numerous potential barriers, the appearance of the mean time of the thermally activated process for overcoming a single barrier?

In our approach the quantities that must be obtained in solving problem A are considered as given parameters of the theory. This is because on the one hand problem A has not been solved, and on the other hand we intend to elucidate general statistical features of the fracture process that do not depend on the details of its microscopic mechanism.
2. Kinetics of a single crack

Let us define the state \( i = 1, 2, \ldots \) of the sample containing a crack (or briefly the state of the crack) by a set \( q_i \{ q_1, q_2, \ldots \} \) of generalized coordinates \( q_i \) that vary in a discrete manner. Let us further suppose that as a result of the solution of problem A the path in configurational space \( \{ q_i \} \) corresponding to the energetically favourable thermally activated development of the crack in the loaded sample is known, along with the heights \( U_i \) of the potential barriers separating the states \( i-1 \) and \( i \) and the trail frequencies \( \theta_{oi}^{-1} \).

The movement of the configurational point along the potential surface occurs by means of thermal fluctuations and is a random process. Due to the inhomogeneities in the structure of the deformed sample the potential surface \( \{ U_i \} \) in general is non-monotonic. Overcoming barriers \( U_i \) may result in relaxational atomic rearrangements and in forming the next barriers \( U_{i+1} \). We suppose that these relaxation processes and the subsequent thermal equilibrium time occur much faster than the time to overcome the next barrier. In terms of probability theory, the described model may be considered as a Markov chain with continuous time and a discrete number of states.

We obtain a complete description of the development of the crack if we determine the probability \( F_{s', s}(t) \) that the time of the transition \( s' \rightarrow s \) does not exceed \( t \) if at the moment \( t=0 \) the crack was in the state \( s' \) \( [s(t=0)=s'] \). \( F_{s', s}(t) \) is the distribution function of random times \( t \) of reaching a fixed coordinate \( s \). The distribution function \( F_{s-1, s}(t) \) of the waiting times \( t \) for the change of the state of a homogeneous Markov system (in our case the probability of overcoming the barrier \( U_s \) during the time \( t \)) is known to be [6]

\[
F_{s-1, s}(t) = 1 - \exp\left(-t/\theta_s\right). \tag{2}
\]

According to rate theory [7] the mean time \( \theta_s \) of overcoming the barrier \( U_s \) is

\[
\theta_s = \theta_{0s} \exp\left(U_s/T\right). \tag{3}
\]

The desired function \( F_{s', s}(t) \) is determined in a recurrent way from expression (2) and the formula for the total probability [6] in the following way:

\[
F_{s', s}(t) = \int_0^t F_{s', s-1}(t') F_{s-1, s}(t-t') \, dt'. \tag{4}
\]

The dot denotes differentiation with respect to time. Equation (4) is similar to Smoluchowski's equation, and the sense of the similarity was earlier discussed [5]. The solution of (4) was obtained with the aid of a Laplace transform. In the case of equal \( \theta_i = \theta \), it was shown to be the \( \Gamma \)-distribution

\[
F_{s', s}(t) = \int_{0}^{\theta} x^{s-1} e^{-x} \left[ dx/\Gamma(n) \right], \quad n = s - s', \tag{5a}
\]

where \( \Gamma(n) \) denotes the gamma-function. In the case of different \( \theta_i \), the solution is the generalized Erlang distribution

\[
F_{s', s}(t) = 1 - \sum_{i=s'+1}^{\infty} \frac{\exp(-t/\theta_i)}{\prod_{j=s'+1}^{i} (1-\theta_{j}/\theta_i)} \tag{5b}
\]

The prime at \( \Pi' \) denotes omission of the term \( j = i \).

As mentioned above, at the present state of the theory the times \( \{ \theta_i \} \) are not known, thus the explicit expression (5b) is of little use in the following analysis. We search therefore for approximations that depend on fewer parameters. With this in mind we consider the