

## KINETIC ASPECT OF THE LIFE OF TENSILE SPECIMENS: A COMPARISON OF TWO APPROACHES

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UDC 536.42:539.424

*This paper considers two approaches to estimating the life of specimens: kinetic strength theory and homogeneous nucleation theory. Using aluminum as an example, it is shown that homogeneous nucleation theory overestimates the real life of tensile metal specimens by two order of magnitude and gives values close to the theoretical strength of metals. The use of experimental data on the lifetime of a superheated and stretched liquid (hexane) allows one to couple both approaches taking into account the time scale of occurrence of metastability.*

**Key words:** *strength theory, nucleation theory, stretched liquid.*

The overall tension of a condensed medium corresponds to a negative external pressure  $p < 0$  and stresses  $\sigma_{ii} = -p > 0$ . A stretched solid or liquid is in a metastable phase state [1], which is characterized by a finite time  $\tau$  to failure (loss of continuity). For solid crystalline and glass-like specimens, the average value and standard deviation of  $\tau$  as functions of the stress  $\sigma$  and the temperature  $T$  are usually determined in uniaxial tension tests [2]. This, however, is not a fundamental hindrance to a similar consideration of liquid specimens with isotropic stresses.

The kinetic aspect of life implies that the thermal fluctuation mechanism participates in the initial stage of failure. In this case, two models for the development of the process are possible. The first model, which will be called heterogeneous, assumes the presence of fixed microscopic defects (bubbles or cracks) in the specimen and their subsequent fluctuation growth to the critical size at a given stress. The second model — the homogeneous nucleation (HN) model — assumes that all segments of the specimen are equivalent and that the nucleation and growth of all defects involve fluctuation mechanisms.

In this model, the stationary nucleation rate  $J$  for a unit volume has the following form [3]:

$$J = N_1 B \exp(-W_*/(kT)). \quad (1)$$

Here  $N_1$  is the number of molecules per unit volume,  $B$  is the kinetic factor ( $B \approx 10^{11} \text{ sec}^{-1}$  for low-viscosity liquids),  $W_*$  is the work of formation of a nucleus of the critical size, and  $k$  is Boltzmann's constant. For a stretched liquid ( $p < 0$ ), the critical radius of a spherical nucleus  $r_*$  (ignoring vapor pressure) depends on the surface tension  $\alpha = \alpha(T)$  and the stress  $\sigma = -p$ :

$$r_* = -2\alpha/p = 2\alpha/\sigma. \quad (2)$$

The work  $W_*$  can be expressed in terms of the product of the volume of the critical nucleus  $v_*$  by the stress or it can be written in a form that does not explicitly contain the nucleus size [3]:

$$W_* = \frac{1}{2} v_* \sigma = \frac{16\pi}{3} \frac{\alpha^3}{\sigma^2}. \quad (3)$$

The goal of the present study is to compare these two approaches using two groups of experimental data: on the life of solids  $\tau_1$  [2] and on the average lifetime  $\tau_2$  of superheated and stretched liquids [3, 4]. In the HN model, the average time before the occurrence of the first nucleus in a volume  $V$  is given by

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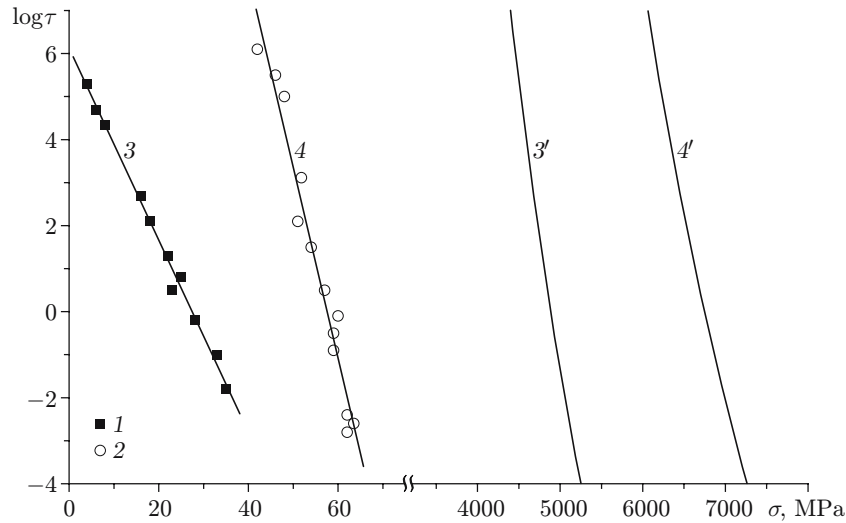


Fig. 1. Life versus stress for aluminum: the points refer to experimental data at  $T = 300$  (1) and  $18^\circ\text{C}$  (2); curves 3 and 4 refer to calculations using the heterogeneous nucleation model at  $300$  and  $18^\circ\text{C}$ , respectively; curves 3' and 4' refer to calculations using the homogeneous nucleation theory at  $300$  and  $18^\circ\text{C}$ , respectively.

$$\tau_2 = (VJ)^{-1} = (VN_1B)^{-1} \exp(W_*/(kT)). \quad (4)$$

The heterogeneous model uses the relation [2]

$$\tau_1 = A \exp(-\gamma\sigma/(kT)) \quad (5)$$

or

$$\tau_1 = \tau_0 \exp((U_0 - \gamma\sigma)/(kT)). \quad (6)$$

Here the parameter  $\gamma$  has the dimension of volume,  $\tau_0$  is close in order of magnitude to the period of thermal oscillations of molecules (atoms) in a solid, and  $U_0$  is close to the heat of sublimation (destruction) per one molecule. The parameters  $A$ ,  $\tau_0$ ,  $U_0$ , and  $\gamma$  depend on the temperature but do not depend on the stress  $\sigma$ . If  $\gamma$  is expressed in terms of the volume  $v_0$  per one molecule:  $\gamma = nv_0$ , life data processing usually yields  $n = 10\text{--}100$  [2]. This approach and formulas (5) and (6) are named after Zhurkov in recognition of his contribution to research into the life of solid materials [5–7], although they have prehistory [2].

In contrast to the homogeneous nucleation model (4), model (5) is formulated phenomenologically, the parameter  $\gamma$  has no physical meaning and is found by life data processing. The logarithm of the average time to specimen failure decreases linearly with increase in the product  $\gamma\sigma$ , where  $\gamma$  is the characteristic volume that participates in the thermal-fluctuation failure of the specimen in the presence of defect nuclei.

Obviously, the structures of formulas (4), (5), and (6) with respect to stress  $\sigma$  are different. Their common feature is the form of the derivatives

$$\frac{\partial \ln \tau_1}{\partial \sigma} = -\frac{\gamma}{kT}; \quad (7)$$

$$\frac{\partial \ln \tau_2}{\partial \sigma} = -\frac{v_*}{kT}, \quad (8)$$

i.e., the slopes of the life isotherms in the coordinates  $\ln \tau$  and  $\sigma$  in both cases are determined by the characteristic volume  $\gamma$  or  $v_*$ . A considerable difference between relations (7) and (8) is that relation (8) is obtained taking into account the dependence of the volume of the critical bubble on  $\sigma$ . According to formula (2), we have  $v_* \sim \sigma^{-3}$ .

To compare the two approaches to determining the life of solids, we use experimental data for aluminum at two temperatures [2, 6]. Figure 1 shows the common logarithm of life as a function of the uniaxial tensile stress  $\sigma$ . In calculations using formula (6),  $\gamma = 4.11 \cdot 10^{-27} \text{ m}^3$  ( $18^\circ\text{C}$ ),  $\gamma = 4.06 \cdot 10^{-27} \text{ m}^3$  ( $300^\circ\text{C}$ ) are determined from the slope of curves 4 and 3 (Fig. 1). In calculations using formula (4),  $V = 10^{-9} \text{ m}^3$ , which is close to the specimen

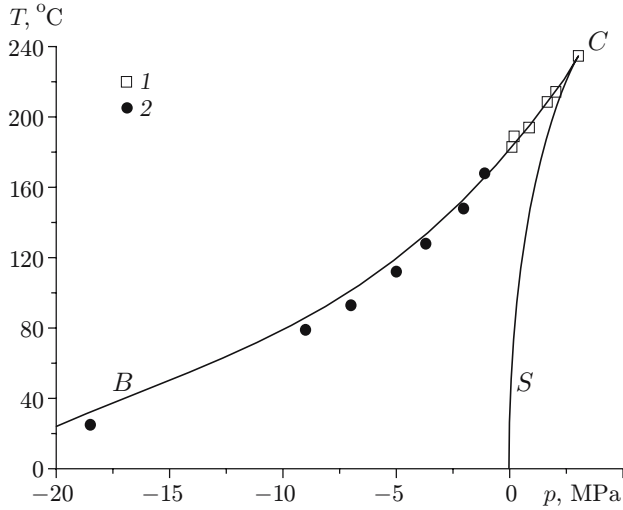


Fig. 2

Fig. 2. Boundary of limiting stresses for stretching of  $n$ -hexane: points 1 and 2 are experimental data of [10] and [11], respectively; the curve  $BC$  refers to calculations using homogeneous nucleation theory for  $J = 10^{12} \text{ m}^{-3} \cdot \text{sec}^{-1}$ ; curve  $SC$  is the liquid-vapor equilibrium curve;  $C$  is the thermodynamic critical point of  $n$ -hexane.

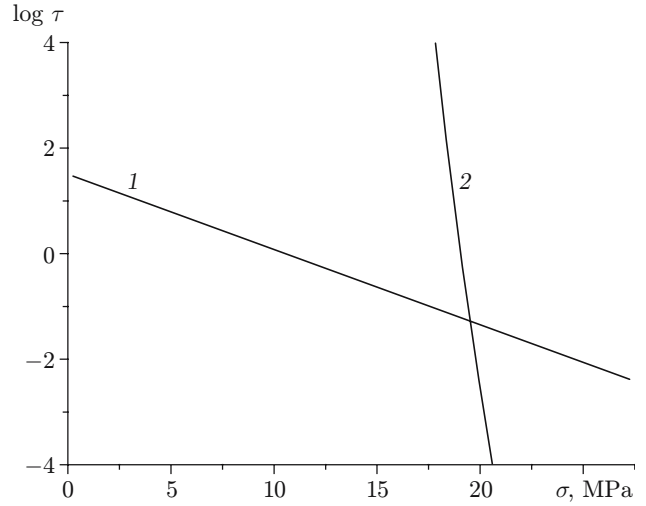


Fig. 3

Fig. 3. Life of  $n$ -hexane versus tensile stress at  $25^\circ\text{C}$ : curve 1 refers to calculations using formula (6); curve 2 refers to calculations using homogeneous nucleation theory.

volume in the experiments of Zhurkov and his colleagues, and  $N_1 B = 10^{39} \text{ m}^{-3}/\text{sec}$ . For the surface tension  $\alpha$ , we use the values  $\alpha = 1.164 \text{ J/m}^2$  at  $18^\circ\text{C}$  and  $\alpha = 1.105 \text{ J/m}^2$  at  $300^\circ\text{C}$  [8]. Estimating the volume of the critical nucleus  $v_*$  for  $\tau_2 = 10 \text{ sec}$  and the stress of the experiment with aluminum, we find that for the indicated temperatures,  $v = 2.7 \cdot 10^{-22} \text{ m}^3$  and  $v = 3.7 \cdot 10^{-21} \text{ m}^3$ , respectively. As one might expect, the volume  $\gamma$  is smaller than the volume of a nucleus capable of growth at the specified  $\sigma$ . According to the HN theory, the life interval shown in Fig. 1 is reached using relation (4) for stresses  $\sigma$  that are two orders of magnitude higher than those in the experiments (curves 3' and 4'). The values  $\sigma \sim 10^9 \text{ Pa}$  are close to the theoretical strength of aluminum. This suggests the heterogeneous mechanism in the initial stage of failure in the experiments.

Let us compare the two approaches to determining the life  $\tau_1$  and  $\tau_2$  using experimental data for stretched liquids. Instead of  $U_0$  in (6) we use the heat of vaporization at the corresponding temperature. The factor  $\tau_0$ , which contains the contribution of collective motions in the liquid, is evaluated from experimental data. Experiments with spontaneous boiling of liquids have been performed with various substances over a wide range of pressures [3]. Calculations using HN theory [formulas (1) and (4)] provide a good approximation of experimental data for low values of  $\tau_2$ . In [9], negative pressures were produced by reflection of pressure pulses from a free liquid surface. This made it possible to observe the cavitation boundary at negative pressures of the order of  $p_{\text{cr}}$  or higher ( $p_{\text{cr}}$  is the critical pressure of the substance). Figure 2 shows the saturation curve  $SC$  and the curve  $BC$  of the cavitation boundary calculated using HN theory [formulas (1) and (3)] for a nucleation rate  $J = 10^{12} \text{ m}^{-3} \cdot \text{sec}^{-1}$  for  $n$ -hexane. In experiments at  $p > 0$  [10], the volume of superheated droplets was  $V \approx 10^{-11} \text{ m}^3$  and their average lifetime was  $\tau_2 = (VJ)^{-1} \approx 0.1 \text{ sec}$ . In Fig. 2, points 1 correspond to the experimental data of [10] at positive pressures, and points 2 to the experimental data of [11] at negative pressures. Both types of points are in agreement with calculations using HN theory.

To compare the two approaches to determining the life of stretched hexane at a certain point near the curve  $BC$ , we proceed as follows. At this point, let  $\tau_1 = \tau_2 = \tau_*$ . Using formulas (4) and (6), we continue the curves of  $\tau_2(\sigma)$  and  $\tau_1(\sigma)$  beyond their common point ( $\tau_1 = \tau_2 = \tau_*$ ) and compare the slopes of these curves (see curves 1 and 2 in Fig. 3). Near the curve  $BC$ , we take the point ( $T = 25^\circ\text{C}$ ,  $p = -19.5 \text{ MPa}$ ). By the HN theorem [formula (4)], we have all necessary data for such construction. To use formula (6) for  $\tau_1 = \tau_*$ , it is necessary to

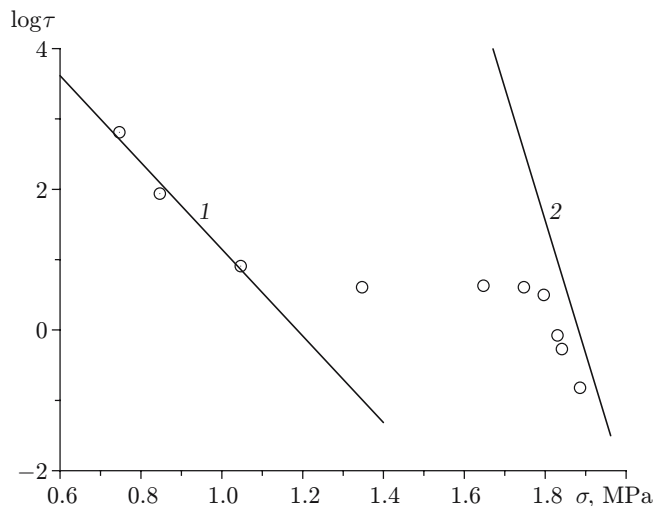


Fig. 4. Life versus stress  $\sigma = p_S - p$  for ethane at 269 K: curve 1 refers to a linear interpolation of experimental data in the region of heterogeneous boiling and curve 2 refers to calculations using homogeneous nucleation theory.

estimate the parameters  $\tau_0$  and  $\gamma$ . Assuming a weak temperature dependence of  $\tau_0$  for hexane, we obtain  $\tau_0$  from formula (6) for  $\sigma = 0$  and an average life time  $\tau_2 = \tau_*$  identical for the entire curve  $BC$  in Fig. 2 ( $\tau_* = 0.1$  sec). In Fig. 2, the value  $\sigma = 0$  corresponds to a temperature of 180°C, a heat of vaporization  $U_0 = 2.78 \cdot 10^{-20}$  J, and  $\tau_0 = 10^{-4}$  sec. Using the value of  $\tau_0$  at the chosen point of the equality of  $\tau_1$  and  $\tau_2$ , we calculate the parameter  $\gamma$  at this point:

$$\gamma = \frac{kT}{\sigma} \left( \ln \frac{\tau_0}{\tau_*} + \frac{U_0}{kT} \right). \quad (9)$$

We use the heat of vaporization  $U_0(T)$  is taken at a temperature of 25°C. Curve 1 in Fig. 3 is plotted by formula (6) for  $\gamma = 1.35 \cdot 10^{-27}$  m<sup>3</sup> and  $\tau_0 = 10^{-4}$  sec. It is evident that HN theory yields a steeper curve of life  $\tau$  versus tensile stress  $\sigma = -p$  than that obtained for the Zhurkov formula. (At the point of intersection of the curves,  $\partial \log \tau_1 / \partial \sigma = -0.14$  MPa<sup>-1</sup>,  $\partial \log \tau_2 / \partial \sigma = -2.7$  MPa<sup>-1</sup>,  $\gamma = 1.35 \cdot 10^{-27}$  m<sup>3</sup>, and  $v_* = 2.6 \cdot 10^{-26}$ .)

Experimental data on the life of stretched liquids provide a better understanding of the relation between the two models in the strength theory of condensed media. This is due to the fact that in experiments with liquids, one can observe both homogeneous boiling (cavitation) at small times of occurrence of metastability and heterogeneous boiling of liquids under rather slow stretching or heating [3]. The curves of lifetime (life) on isotherms or isobars have steep segments and flat tails.

Figure 4 shows this curves for ethane [12] at a temperature of 269 K. (The liquid superheated in a bubble chamber had a volume of about 65 mm<sup>3</sup>.) Curve 2 is plotted in accordance with homogeneous nucleation theory without using adjusting parameters. Here  $\sigma = p_S - p$ , where  $p_S$  is the saturated-vapor pressure and  $p$  is the ambient pressure. The right group of experimental points is located close to this curve. As the life increases, the experimental points form a flat transition segment and then the straight line 1, which can be approximated by the Zhurkov formula (5). For the straight line 1 at  $T = 269$  K, we have  $\log A = 7.31$ ,  $\gamma = 5.3 \cdot 10^{-26}$  m<sup>3</sup>, and  $r_\gamma = 2.33 \cdot 10^{-9}$  m. These values of the characteristic volume  $\gamma$  for the thermal-fluctuation loss of continuity of the specimen and the corresponding bubble radius  $r_\gamma$  are much smaller than the values  $v_* = 4 \cdot 10^{-24}$  m<sup>3</sup> and  $r_* = 10^{-8}$  m for boiling at  $\sigma = 1$  MPa by the homogeneous nucleation mechanism.

One reason for the occurrence of the tails is the initiating action of natural background radiation [3], but this is not the only reason. The deviation from HN theory is especially apparent for water [13]. Background radiation does not provide this effect. One has to assume that water purified by conventional methods also contains microscopic gas bubbles, which grow up to the critical radius at a degree of metastability far below the boundary indicated by HN theory. The transition from the HN region to the heterogeneous cavitation mechanism can be shown using Fig. 3. At the specified temperature and a fixed value  $\tau > \tau_*$ , if one moves to the left from the point

of intersection of curves 1 and 2 ( $\log \tau_* = -1$  and  $\sigma = 19.5$  MPa), then for the stretching of the specimen, straight line 1 will be intersected at a lower stress  $\sigma_1$  than the stress  $\sigma_2$  for curve 2. This implies that cavitation occurs at the nucleus (defect). In view of the aforesaid, the Zhurkov formula (6) can be used to describe the flat tails on the life curve of stretched/superheated liquids, which requires an additional analysis of experimental data [3].

This work was supported by the Russian Foundation for Basic Research (Grant No. 04-02-16251-a) and the program of basic research of the Presidium of the Russian Academy of Sciences “Thermal Physics and Mechanics of High-Energy Action.”

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