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A MODEL OF THE VISCOUS–BRITTLE TRANSITION UPON FRACTURE OF METALS AND ALLOYS

L. B. Zuev

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A model of the viscous–brittle transition upon fracture of metals and alloys that is based on the competition of the processes of microcrack development and dislocation generation is proposed. Micropores which occur in the region of stress concentration in the coagulation of vacancies are regarded as defects of one or another type. The kinetics of development of a micropore and the micropore-assisted generation of microcracks or prismatic dislocation loops are estimated quantitatively. The temperature dependence of the embrittlement of metals and alloys and also the influence of the loading rate and doping on the embrittlement temperature are considered.

At present, the problem of viscous–brittle transition upon low-temperature fracture of metals and alloys (cold brittleness) is still far from solution despite years of fairly thorough investigations [1–3]. The engineering methods of suppression of this dangerous phenomenon, which permit the threshold of cold brittleness to be shifted to low temperatures unattainable in the nature, are rather clear [4], but this is not the case with the physics of embrittlement. A distinguishing feature of this process is a cardinal change of the character of fracture with a comparatively insignificant change of the experimental or operating temperatures. In essence, at present the Yoffe–Davidenkov model remains the most comprehensive [2, 5]. According to this model, embrittlement at low temperatures is caused by the difference between the temperature runs of the strength and plasticity limits. In addition, at a qualitative level, this model sufficiently correctly explains the specifics of the phenomenon, but it is of little use for a quantitative description and the more so predictions of the properties of materials. However, precisely this model underlies various theories of brittle fracture, which are additionally supported by the use of the linear mechanics of fracture [6], an allowance for the scale factor [7], an analysis of the behavior of the sets of microdefects of various types [8], etc. Common for all approaches is the idea that viscous fracture and brittle fracture are fundamentally different from the moment of generation. In fact, this is connected with the kernel of the Yoffe–Davidenkov model in which either brittle fracturing or plastic flow, the nature of each process being independent and not specified, first occurs, depending on the temperature.

In the present paper, we develop a model of the viscous–brittle transition proposed in [9]. According to this model, the initial stage of the process is the same for both types of materials behavior, and the distinction arises at the later stages and is determined by a number of factors such as the temperature and the regime of loading application. The basic points of the developed model are as follows.

Let there be a concentrator of stresses in a loaded body, or a crack in our context. As is known [1, 2, 10], real objects usually contain cracks, which can develop in a brittle or viscous manner, depending on a combination of many factors. In the first case, the growth of such a (main) crack is connected with the coalescence of microcracks occurring on its extension [11–13] and, in the second case, the crack growth is associated with the generation and development of dislocation flows [14] or the rougher macroscopic bands of sliding [15] from its mouth. It is obvious that the mouth of a crack is a source of vacancies, so that the zone directly ahead of this mouth turns out to be oversaturated by these defects. At some distance from the

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concentrator the vacancies can coagulate, thus forming flat vacancy disks bounded by planes with a minimum value of the surface-energy density γ. As the critical size r_c is reached, these disks collapse with formation of prismatic dislocation loops of vacancy type [16]. This was frequently observed [17] in metals hardened by the electron-microscopic method. There is direct evidence [18] in support of the formation of prismatic loops in front of the stress concentrator (the double) the elastic field of which is similar to the crack field [19]. The critical size of a vacancy disk r_c is estimated from the equality [16]

$$2\pi r_c^2\gamma = 2\pi r_c G b^2.$$

Here the left-hand side is the surface energy of the flat vacancy agglomerate, the right-hand side is the energy of the prismatic vacancy loop with the Burgers vector b, and G is the modulus of shear. For various materials, the critical value of the radius of the vacancy disk $r_c = Gb^2/\gamma$ is $10b$–$40b$ (see Table 1) [20]. The basic idea of the proposed model consists in the following: the character of fracture is determined by whether the flat vacancy disk will grow to the critical size and will become a dislocation loop before the moment when it begins to develop as a crack under the action of the elastic field of the stress concentrator (the main crack) [11]. Viscous fracture will occur in the first case and brittle fracture in the second (hereinafter, the point is microcracks with a size considerably smaller than the length of a Griffith crack [1]: $r_c \ll r_G \simeq E\gamma/\sigma^2$).

The duration t_σ of the existence of a body with defects at stress σ can be calculated by Zhurkov's formula [21]:

$$t_\sigma = t_0 \exp\left[(U_0 - \eta\sigma)/kT\right], \tag{1}$$

where U_0 is the activation energy of fracture (the potential barrier), $\eta\sigma$ is the decrease in the barrier at the expense of work of external forces, t_0 is a constant, k is the Boltzmann constant, and T is the temperature. Obviously, the activation volume is $\eta = \eta(r)$; the form of this function will be discussed below. On the other hand, the disk-shaped agglomerate of vacancies grows diffusively according to the law [22]

$$r \sim (D_v t)^{1/2} \tag{2}$$

or more exactly [23] $r \sim (D_v t)^{3/4}$ (D_v is the diffusivity of the vacancies). If the time for which the flat disk grows to the critical size r_c turns out to be shorter than that determined by (1), viscous fracture occurs, because dislocations are born in the area of the crack tip (the stress concentrator). In the opposite case, the disk in the macrocrack field is potentially capable of beginning to propagate [11] and to generate fracture without plastic deformation (brittleness). For analysis of the model, an explicit form of the above-mentioned function $\eta(r)$ is required. Bearing in mind that the decrease in the potential fracture barrier is $\eta\sigma = \alpha V_0\sigma$ [21] ($V_0 \simeq a^3$ is the atomic volume and α is a coefficient which includes the stress concentration at the crack tip and also the decrease in the effective cross section as the crack grows), we write [21]

$$\alpha = \alpha_0(1 + r/a)(1 + r/L).$$

Here a is a lattice parameter, L is the characteristic transverse size of the loaded body, and α_0 is a constant which describes the change of the coupling forces in the vicinity of the crack tip [21]. For a microcrack, we have $a \ll r \ll L$, and, hence, $\alpha = \alpha_0 r/a$. With allowance for the aforesaid, relation (1) takes the form

$$t_\sigma = \varphi(r) = t_0 \exp[(U_0 - \alpha_0 a^2 r\sigma)/kT]. \tag{3}$$

For temperatures $T_1 < T_2$, this dependence is shown in Fig. 1 (curves 1′ and 2′) in the coordinates $\ln t$–r. In the same coordinates, the curves $r(t)$ of the dependences (2) are shown for the same temperatures (curves 1 and 2). The boundary value $r = r_c$ divides the field of the diagram into two parts, and the character of fracture can be defined based on the positions of the points S_1 and S_2 of intersections of curves 1 and 1′ and 2 and 2′ for corresponding temperatures. Obviously, the point S_1 with the abscissa $r < r_c$ corresponds to the case of microcrack propagation and brittle fracture. In contrast, the point S_2 at $r > r_c$ indicates viscous fracture after the birth of sliding dislocations from prismatic loops. It is seen from Fig. 1 that at the higher temperature T_2, the intersection occurs in the right part of the scheme, which corresponds to dislocation production, and this occurs in the left part at the lower temperature T_1. In the latter case, the disk-shape

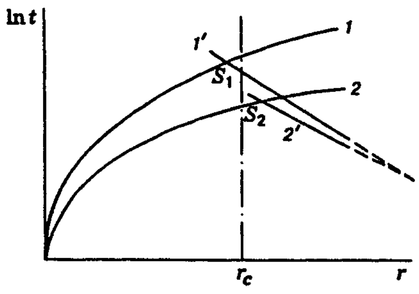

Fig. 1

TABLE 1

Crystal	$G \cdot 10^{-5}$, MPa	γ, J/m^2	r_c/b
MgO	3.08	2.33	13
LiF	1.08	0.78	20
NaCl	0.345	0.345	20
Si	1.75	1.27	26
W	3.89	3.32	26
α-Fe	2.22	1.71	26
Cu	1.31	0.82	41
Zn	1.09	0.85	30
Cd	0.81	0.73	29

agglomerate of vacancies works as a microcrack. Thus, at a qualitative level, the model considered correctly describes a change of the mechanism of fracture at lower temperatures (cold brittleness), and the temperature (threshold) of cold brittleness Θ lies within the range $T_1 < \Theta < T_2$.

A trivial analysis shows that the model considered correctly predicts the role of the surface-energy density. Since the critical size of the planar agglomerate decreases as the quantity γ grows, the dividing line in Fig. 1 is displaced to the left, and the intersection of the corresponding curves in the $r < r_c$ area becomes possible only at a lower temperature, which is equivalent to a decrease in the temperature of the viscous–brittle transition. The effect of the loading rate is correctly predicted as well.

In accordance with data of [21], in the case of rate increase, the lifetime becomes shorter, i.e., the straight lines in Fig. 1 are steeper, and they will intersect the curves at smaller values of r, which is equivalent to higher probability of brittle fracture. This is supported by experiments.

Thus, it is possible to regard that all the factors that displace the point S to small values of r embrittle the material, and when this point is displaced to the right, the tendency toward the viscous character of fracture is manifested. In this connection, of interest is the problem of the action of doping elements on the position of the cold-brittlement threshold [4]. This effect can be connected with the change in the density of the surface energy, on the one hand, and with a significant effect of admixtures on the diffusivity of vacancies [24]. Thus, a detailed account of the role of admixtures in the embrittlement of alloys becomes possible.

We shall estimate some characteristic temporal scales of the processes monitoring the choice between the viscous and the brittle character of fracture. For a diffusive formation of a flat vacancy disk with critical radius r_c, the time τ is required. This time can be estimated from the following simple arguing: the volume of such a disk should be equal to the total volume of vacancies contained in the volume $\sim R^3$, which managed "to be discharged" for this time with the formation of a vacancy agglomerate [23], i.e., $\xi R^3 = ar_c^2$, where ξ is the concentration of the vacancies. As $R^2 \simeq D_v\tau$, we have

$$\tau \simeq D_v^{-1}(ar_c^2/\xi)^{2/3}. \tag{4}$$

Bearing in mind a pronounced oversaturation of the lattice by vacancies near a source, which is the mouth of a crack, we set $\xi \simeq 10^{-4}$ and roughly estimate the diffusivity of vacancies, assuming that the energy of their migration is ~0.6 eV [24]. Then $D_v \simeq 3 \cdot 10^{-18}$ m^2/sec, and it follows from (4) that $\tau \simeq 30$ sec. On the other hand, it is easy to calculate the time before fracture by means of (3) using the values of the constants, given in [21], which differ little for the majority of metals. Assuming that $t_0 = 10^{-13}$ c, $a = 3 \cdot 10^{-10}$ m, $\alpha_0 = 20$, $\sigma = 150$ MPa, $T = 300$ K, $U_0 \simeq 2$ eV, and $r = r_c = 3 \cdot 10^{-9}$ m, we obtain $t_\sigma \simeq 10$ sec, which is close to the above estimate τ and indicates the realistic possibility of the choice between two cross points in Fig. 1. It is necessary to consider the large value of the diffusivity of the vacancies, which is of significance for our calculation. Vladimirov and Khannanov [24] explained the small energies of migration by diffusion of bivacancies. In addition, the vacancies diffuse in the stress-gradient field, which increases their mobility and accelerates the formation of a flat agglomerate.

The presented model seems to be promising, because it allows one to take into account quantitatively the effect of most of the factors on which the character of fracture depends as the temperature varies. At the same time, it is necessary to bear in mind the preliminary character of the estimates that we made. It is clear that, for a defect whose scale is slightly larger than the atomic scale, the concepts of cracks and dislocation loops, which work well in the other scale, should be used with care. One can assume that the micronucleus of a fracture-shift considered here is an analog of the previously proposed defects [25] like the "dilaton," the "strongly excited state" [26], and the "frustron" [27], which can be considered to be the predecessors of the usual lattice defects.

The present model can be further developed in two directions: experimental check of the proposed relations and refining of the atomic structure of a fracture-shift nucleus. It is not improbable that a defect that can become a crack (the topological dimensionality 2) or a dislocation line (the dimensionality 1) occupies the intermediate position between them and has the fractal dimensionality $1 < D_f < 2$ [28].

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