On the Nucleation of Microcracks in Metals under External Loading

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In earlier works [1,2] was suggested a theory of formation of nuclei of vacancy clusters in a single crystal metal subject to the uniaxial strain. After assuming an analogy with the process of formation of a new phase in a liquid-vapour system, the nucleation rate equation was derived. On the basis of energy considerations the change of the activation energy of the vacancy motion, due to the crystal elongation, was also found in the form

$$\Delta U = aR_0^{-m}\left\{1-(1+\varepsilon)^{-m}-\frac{m}{n}\left[1-(1+\varepsilon)^{-n}\right]\right\} \quad , \qquad (1)$$

where a, m, n, are material constants, ε is the linear strain of the crystal, and R_0 is the lattice constant.

The aim of the paper is to investigate the microcrack nucleation rate in a polycrystalline metal subject to the uniaxial strain. As it is known, the vacancy clusters are formed much easier on the grain boundaries than within the grains. Thus, one of the ways which can bring us closer to the early stage of fracture mechanism consists in investigating the process of heterogeneous nucleation of the microcrack. The considerations are based on assuming an analogy with the process of vapour condensation on a substrate. On the other hand, the treatment of heterogeneous nucleation requires an atomistic approach since in our case very high supersaturations are expected. Consequently, for the analysis of the problem the description of vapour deposits on a substrate, carried out on the basis of

statistical mechanics and proposed by Walton[3], was chosen.

Let us consider a sample of a polycrystal subject to the uniaxial strain. The assumptions may be listed as follows: (i) Dislocation density is negligibly small everywhere except on the grain boundaries. (ii) Grain boundaries are free from preferential adsorption sites. (iii) Only single advacancies (adsorbed vacancies) are mobile on the grain boundaries. (iv) Only single advacancies may desorb directly from the boundaries. (v) Aggregate nucleation and growth occur only by the addition of single vacancies due to the surface diffusion. (vi) A quasi-steady state is established.

Let us now consider an internal region of the crystal containing a grain boundary. The problem has been analysed via the petit canonical ensemble and reduced to that of calculating the partition function of a two-dimensional adsorbed gas composed of different aggregates.

The partition function has the form

$$Z = \sum_i \exp\left(-\frac{E_i}{kT}\right)$$

where E_i is the energy of state i, k is Boltzmann's constant, T is the absolute temperature, and the sum is taken over all possible configurations of the N advacancies on the grain boundary.

Let N_o be the density of discrete adsorption sites per unit area of the boundary ($\approx 10^{15} cm^{-2}$), N_n - the equilibrium surface density of clusters of n advacancies, and ϵ_n - the potential energy of an aggregate of size n. Assuming that $N_o \gg \sum_{i=1}^{n} N_i$, N_1 aggregates can be distributed over N_o positions in

$$\binom{N_o}{N_1} = \frac{N_o(N_o-1)\ldots(N_o-N_1+1)}{N_1!} \approx \frac{1}{N_1!} N_o^{N_1} \text{ ways,}$$

and its contribution to the partition function is

$$T_1 = (1/N_1!)N_o^{N_1}\exp(N_1\epsilon_1/kT) \quad . \tag{2}$$

The total contribution to Z of all the aggregates is the product of all the terms (2), and the partition function is the sum of all these products over all possible distributions

$$Z = \sum_{k=1}^{n} \prod_{i=1}^{k} \frac{1}{N_1!} \left[N_o\exp\left(\frac{\epsilon_1}{kT}\right)\right]^{N_1} \tag{3}$$

The most probable distribution of aggregates N_n corresponds to the minimum of free energy F. This, owing to the relation $F = -kT\ln Z$, leads to the maximum of $\ln Z$ with the condition

$$\sum_{i=1}^{n} iN_i = N \tag{4}$$

Thus, the problem is reduced to the solution of a set of two equations: (4) and

$$\frac{\partial}{\partial N_j}\left[\ln Z + \ln\lambda\left(\sum_{i=1}^{n} iN_i-N\right)\right] = 0 \tag{5}$$

where $\ln\lambda$ is the Lagrangian multiplier.

Replacing the sum (3) by the largest component T (the method of the maximum term), assuming that $N_1 \gg 1$ and applying Stirling's formula $\ln N_1! = N_1\ln N_1-N_1$, we obtain

$$\ln T = \ln\prod_{i=1}^{n}\frac{1}{N_1!}\left[N_o\exp\left(\frac{\epsilon_1}{kT}\right)\right]^{N_1} = \sum_{i=1}^{n}\left[-N_1\ln N_1+N_1+N_1\left(\ln N_o+\frac{\epsilon_1}{kT}\right)\right] \tag{6}$$

Formal differentiating of Eq.(5), Eq.(6) being taken into account, leads to

$$\frac{\partial}{\partial N_j}\left[\ln T+\ln\lambda\left(\sum_{i=1}^{n} iN_i-N\right)\right] = +\ln N_o+\frac{\epsilon_1}{kT} + j\ln\lambda- \ln N_j = 0 \tag{7}$$

Hence, $N_j = N_0 \exp(\epsilon_j/kT) \lambda^j$ and putting $j=1$ we can find λ and the density of critical clusters N_{n*}

$$N_{n*} = N_0 (N_1/N_0)^{n*} \exp(E_{n*}/kT) , \qquad (8)$$

where $n*$ is the number of advacancies in a critical cluster, and $E_{n*} = \epsilon_{n*} - n* \epsilon_1$ is the net gain in energy when the cluster is formed from $n*$ advacancies (binding energy).

The nucleation rate J is the rate of promotion of critical clusters, containing $n*$ vacancies, to the smallest stable clusters (nuclei) by advacancy capture

$$J = N_{n*} w_{n*} , \qquad (9)$$

where w_{n*} is the capture rate of single advacancies by a cluster of size $n*$.

The mean lifetime of an advacancy before desorption is $\tau_a = \nu^{-1} \exp(E_a/kT)$ where $\nu \approx 10^{13}$ is the atomic vibrational frequency, and E_a is the adsorption energy of a single vacancy. If we denote by P_p the incidence rate of vacancies, the equilibrium advacancy population N_1 can be expressed as

$$N_1 = P_p \tau_a = P_p \nu^{-1} \exp(E_a/kT) \qquad (10)$$

The incidence rate may be written approximately as $P_p = vc$, where v is the average velocity of a vacancy which can be determined as $v = \nu R_0 \exp\left[-(U_m - \Delta U)/kT\right]$ with U_m denoting the activation energy of motion of vacancies and ΔU given by (1); c is the current volume vacancy concentration in the strained crystal ($\varepsilon > 0$). On the other hand, the initial concentration of vacancies ($\varepsilon = 0$) is given by the known formula $c_0 = \mathcal{N} \exp(-U_f/kT)$, where $\mathcal{N}$ is the total number of atomic sites per unit volume and U_f is the activation energy of formation of a vacancy. If we assume that, due to the

strain, this energy will be lowered by ΔU, then $c = \mathcal{N} \exp\left[-(U_f - \Delta U)/kT\right] = c_0 \exp(\Delta U/kT)$. Thus, the incidence rate is

$$P_p = \nu R_0 c_0 \exp\left[-(U_m - 2\Delta U)/kT\right] . \qquad (11)$$

The capture rate w_{n*} can be reckoned from kinetic considerations. When advacancies diffuse over the grain boundary with a mean velocity $v_d = d\nu \exp(-E_d/kT)$, where d is the distance between adsorption sites and E_d is the activation energy for surface diffusion, and b_n is the capture width of the critical aggregate, then

$$w_{n*} = b_{n*} d \nu N_1 \exp(-E_d/kT) . \qquad (12)$$

Substituting (8) and (12) into (9) and taking into account (10) and (11) as well as putting $N_0 \approx 1/d^2$, we finally obtain the microcrack nucleation rate in the loaded crystal

$$J = (R_0 c_0)^{n*+1} d^{2n*-1} b_{n*} \nu \exp\left\{\left[(n*+1)(E_a - U_m + 2\Delta U) + E_{n*} - E_d\right]/kT\right\} \qquad (13)$$

where ΔU, as a function of strain ε, is given by (1).

The proposed mechanism of microcrack nucleation explains to some degree the beginning of the process of fracture and the nature of formation of small cracks. Once the growing nucleus of a microcrack has reached the size of the order of a Griffith crack, its further growth can follow the existing continuum hypotheses.

References

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