MODELING OF EVOLUTION OF METAL UNDER CREEP

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Damage evolution in metals is considered by studding a boundary problem for a system of quasilinear parabolic equations. By standard linear stability analysis the presence of the stress threshold, below which the damage formation does not progress is shown. The estimations of the threshold stress value and conditions of damage dissipative structure development are obtained. For each loading level above the threshold the model suggests a corresponding limit void formation density value that is in good agreement with literature data. The distribution of microdamage formed due to evolution under stresses depends only indirectly on the initial conditions of the problem. Largely it is provided by the dissipative system peculiarities, that differs substantially this approach from the conventional damage theories.

INTRODUCTION

Usually high temperature fracture of structures is brittle and proceeds along the grain boundaries. The voids and cracks appear after particular incubation period. Comparison of the fracture mechanisms and deformation maps (Ashby (1)) under service conditions shows a good agreement between intergranular creep fracture mechanism and boundary diffusional flow. However, the available quantitative theories of damage evolution under creep usually do not reflect the mentioned peculiarities of the process. They can not be used for description of the qualitative transformation that consists in accumulation of microdamages in a grain boundary local place and spontaneous void nucleation after the incubation period.

The object of the present paper is the construction of a model that describes the first step of the damage evolution that causes the void nucleation in the originally continuous and nearly homogeneous material.

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FORMULATION OF A PROBLEM

We assume the following:

1. Grain boundary is an open thermodynamic system that is a mixture of two "reagents": vacancies and microvoids. We consider the microvoids as the clusters of vacancies (bivacancies, threevacancies, etc.) that have ability to diffuse.
2. The system is isothermal.
3. The system is in the state of mechanical equilibrium (loading values are low enough, so there are no viscous flows in material).
4. Vacancy and microvoid fraction gradients are small (concentrations do not change at the distance of the ' free run ' of vacancies).

We use the terms of 'reagents' because the main metallophysic mechanisms of damage growth resemble a chemical reaction (Nicolis and Prigogine (2)). Assumptions 2 and 3 reduce our problem to the isothermal one for an elastic material. Assumption 4 is equivalent to the principle of thermodynamic system local equilibrium (2). For a system, containing reagents it means that their contact, which causes reaction processes, happens very seldom.

We create the evolution equations for the reagents fractions basing on the principle of balance. The convective processes are absent (assumption 3), i.e. the concentration growth due to exchange can result only from a diffusion. Suggesting the diffusion coefficients for the components are independent of the concentration and diffusional flows are inconjugated because of the mixture dilution (assumption 4), we have:

$$\frac{\partial c}{\partial t} = D_c \operatorname{div}(\operatorname{grad} c) + f_c(c, z, \ldots); \quad \frac{\partial z}{\partial t} = D_z \operatorname{div}(\operatorname{grad} z) + f_z(c, z, \ldots). \tag{1}$$

The functions f_c, f_z were constructed by Skrypnyk and Nykyforchyn (3) in analogy to (2) taking into account the following damage formation micromechanisms:

1. Microvoid growth due to vacancies' absorption (mechanism Raj and Ashby, (4)) $\{\pm Rcz\}$;
2. Initiation of vacancies under the stress influence and already existing ones $\{A\sigma + Bc\}$;
3. Microvoid coalescence under the influence of stress field $\{K\sigma^{\alpha}(z - z_o)^2\}$;
4. Microvoid elimination as a result of microplastic deformation $\{-F\sigma\}$.

Below we consider the system (1) in one-dimensional case. Taking into account the explicit expressions for f_c, f_z (3), equations (1) can be written as:

$$\frac{\partial c}{\partial t} = D_c \Delta c + A\sigma + Bc - Rcz; \quad \frac{\partial z}{\partial t} = D_z \Delta z + K\sigma^{\alpha}(z - z_o)^2 + Rcz - F\sigma; \tag{2}$$

$$0 \le x \le l.$$

The boundary conditions for this problem are considered to be the following:

$$c(0,t) = c(l,t) = c_o; \quad z(0,t) = z(l,t) = z_o. \tag{3}$$

The initial conditions include the concentration fluctuations:

$$c(x,0) = c_o + \delta c(x); \quad z(x,0) = z_o + \delta z(x). \tag{4}$$

THE BOUNDARY PROBLEM ANALYSIS

Investigation of the system is performed by the linear stability analysis method (2). The trivial solution c_o, z_o to system (2) is obtained from the condition $f_c = f_z = 0$:

$$c_o = \frac{F-A}{B}\sigma, \qquad z_o = \frac{FB}{R(F-A)}. \tag{5}$$

We want to find a solution to the boundary problem (2)-(4):

$$c(x,t) = c_o + \delta c(x,t); \quad z(x,t) = z_o + \delta z(x,t). \tag{6}$$

The linearized system of equations is expressed in terms of the operators:

$$\frac{d}{dt}\begin{pmatrix}\delta c\\ \delta z\end{pmatrix} = \mathbf{L}\begin{pmatrix}\delta c\\ \delta z\end{pmatrix}, \quad \mathbf{L} = \begin{vmatrix} D_c\nabla^2 + B - Rz_o & -Rc_o \\ Rz_o & D_z\nabla^2 + Rc_o \end{vmatrix} \tag{7}$$

Next, we present the solution (6) as:

$$\begin{pmatrix}c\\ z\end{pmatrix} = \begin{pmatrix}c_o\\ z_o\end{pmatrix} + \sum_m a_m e^{\lambda_m t}\begin{pmatrix}u_m\\ v_m\end{pmatrix}; \quad \begin{pmatrix}u_m\\ v_m\end{pmatrix} = \begin{pmatrix}b_1\\ b_2\end{pmatrix}\sin\left(\frac{m\pi x}{l}\right), \quad m \in N \tag{8}$$

Thus, the stationary solution (5) is asymptotically stable if all eigenvalues have a negative real part. We assume $l=\pi$ for simplicity. Upon substitution of (8) into operator equation (7) we obtain an 'eigenvalue' equation:

$$\lambda_m^2 + B\left[(d_1+d_2)m^2 + f - r\sigma - 1\right]\lambda_m + B^2\left[(d_1m^2 + f - 1)(d_2m^2 - r\sigma) + fr\sigma\right] = 0 \quad ,(9)$$

where $f = F/(F-A)$; $r = R(F-A)/B^2$; $d_1 = D_c/B$; $d_2 = D_z/B$. (10)

Basing on the analysis of the quadrature equation (9) we examine the conditions of the onset of instability and periodicity of the problem solution (Fig.1). The following symbols were used to denote the obtained dependencies:

$$\sigma_{1,2} = \left(\sqrt{f} \pm \sqrt{1-(d_1-d_2)m^2}\right)^2 / r; \; \sigma^* = \left((d_1+d_2)m^2 + f - 1\right)/r;$$

$$\tilde{\sigma} = d_2m^2\left(1 + f/(d_1m^2 - 1)\right)/r; \; m^* = \sqrt{1/d_1}; \quad m^{**} = \sqrt{1/(d_1 - d_2)}; \tag{11}$$

$$\sigma^{\min} = D_z\left(1+\sqrt{f}\right)^2/(D_c r) \quad \text{at} \quad m_0 = \sqrt{(1+\sqrt{f})/d_1}. \tag{12}$$

The quantity $\sigma^{\min}$ is a conservative estimation of the material damage threshold: if the inequality $\sigma<\sigma^{\min}$ is satisfied any fluctuation decay to zero in time. Since $Dz \ll Dc$, that suggests $\sigma^{\min}<\sigma_1(m=0)$, we can draw a conclusion that there is no periodical pulsation. At $\sigma>\sigma^{\min}$ the fluctuations growth results in formation of dissipative sine structures with $m_1<m<m_2$ (see Fig.1). By rising the stress the range $(m_1;m_2)$ increases and maximum mode m_2 grows too.

Presence of the strong autocatalytic mechanism (such as mechanism 3, when damage increases due to microvoid coalescence, is described by function $K\sigma^{\alpha}(z-z_0)^2$(3)) causes formation of the 'pin structures' (Samarskij et al, (5)). On the localized zones the autocatalytic mechanism prevails over the dissipative ones and after finite time period a problem solution tends to infinity. So, irrespective of the initial values of c and z, the latter in a certain period of time achieves the unity, thus we may speak about nucleation of a macrovoid (local fracture) in this place. These nucleations are expected to appear at the maximums of the dissipative structure. Thus, by increasing the stress the possible maximum void density grows.This result is in good agreement with the experimental data (Lombard (6)).

RESULTS OF NUMERICAL INVESTIGATION

The void formation of X8CrNiNb1613 steel was simulated at temperatures 600°C, for which the experimental graphs 'stress - mean average void formation density' are known (6). Additional data (1) on the diffusion along the grain boundaries were used. As a result we obtained the following model parameters (3):

$$A= 2.78\cdot10^{-14},\ B=4.00\cdot10^{-3},\ K= 2.28\cdot10^{-11},\ R= 4.75\cdot10^{-1},\ F= 5.30\cdot10^{-14},$$
$$D_c=5.56\cdot10^{-17},\ D_z= 2.78\cdot10^{-19},\ \alpha=1.5. \qquad (13)$$

Modeling was performed by a finite difference method. The Runge-Kutta fifth order integral with automatic step selection was used for time integration. Fig.2 presents the numerical solution of the boundary problem. Depending on the initial conditions (4) (Fig.2,a) the sine-shaped structures with different modes m (Fig.3) were realized, then progressing into the 'pin structures'. The location of the damage maximums for initial distribution (2) (Fig.2,b) and the sites of the formed macrovoids do not always coincide. This principally differs the proposed model from the conventional damage theories.

To model the initial inhomogeneity of the material, a constant A was replaced by a l-periodical function $A(x)$ (Fig.4,a). This can be explained as a inhomogeneous distribution of vacancies' sources along the grain boundary. As a result the formed structure sinusoidality breaks (Fig.4,b). This causes the macrovoids appearance to be prolonged in time, that was observed during experiments (6). However, the problem of an influence of the $A(x)$-function structure and its amplitude value on the solution needs more profound analytical and numerical investigations.

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USED SYMBOLS

A,B,F,K,R,α = material constants at fixed temperature

c,z = concentrations of vacancies and microvoids

c_o,z_o = stationary trivial solution for system (2)

Dz,Dc = diffusion factors for vacancies and microvoids (m^2/s)

f_c,f_z = functions of sources, which model internal irreversible processes

l = modeling range of grain boundary (m)

$\{ u_m, v_m \}$ = eigenvector of linearized operator **L**

λ_m = eigenvalue of linearized operator **L**

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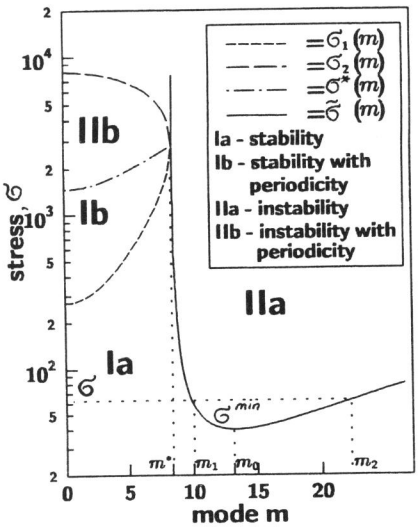

Fig.1. Schematic presentation of instability and periodicity of system (2) solution.

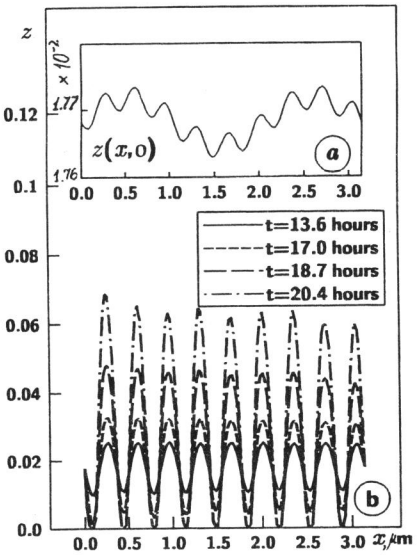

Fig.2. Initial microdamage distribution (a) and its time-related evolution (b).

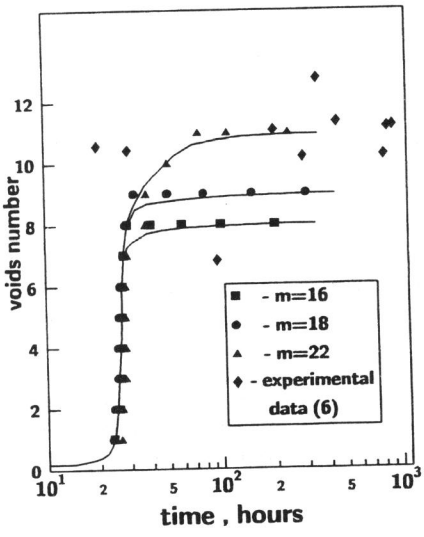

Fig.3. Increase of voids amount in austenitic steel at σ=100 MPa and 600°C.

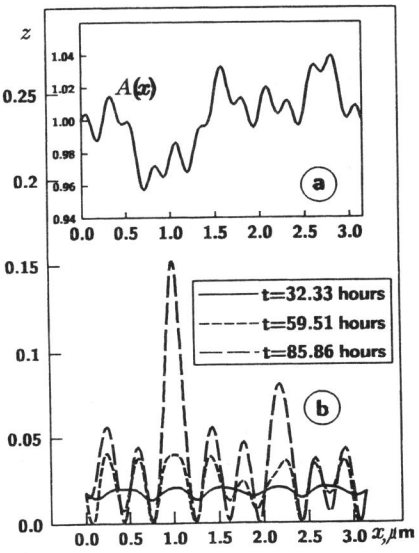

Fig.4.Material inhomogineity (a) effect on microdamage evolution (b).