CHANGE IN PORE SIZE DURING RELAXATION OF THE THERMAL STAGE OF A CASCADE

N. P. Reznikova

On the basis of the solution of the thermoelasticity problem, an analysis is given on the temperature and force fields in the cascade region in the presence of a pore and the change in the size of a small pore is estimated from the balance of point defects on it.

It is known that neutron irradiation of materials is accompanied by the formation of cascades of atom-atom collisions. The specific features of these cascades are associated with the high concentration of defects and thermal energy in the cascade region. Several aspects of the action of the temperature field of a cascade should be considered. First, intensification of the diffusion processes can lead to both a growth of defects and to the reverse process. Second, the formation of a field of thermoelastic stresses can not only organize diffusion flows, but also to change the type of defect (e.g., collapse a pore into a loop). We shall consider the first of these aspects in relation to a pore.

The presence of a pore causes local changes in the temperature field around it. The solution of the heat-conduction problem for an unbounded space with a pore can be written as

\[ T = T_0 + T_p, \]

where \( T_0 \) is the temperature field in the absence of a pore and \( T_p \) is the local temperature change in the vicinity of a pore, with

\[ T_0 = \frac{\omega \eta}{\chi(1 + 4\omega b t)^1.5} \exp \left[ -\frac{b(r^2 + a^2 - 2ra \cos \Theta)}{1 + 4\omega b t} \right], \]

\[ T_p = \sum_{n=1}^{\infty} f_n \cdot P_n \cdot \tilde{W}_n. \]

Here, \( \omega \) and \( \chi \) are the coefficients of thermal diffusivity and thermal conductivity, \( \eta \) and \( b \) are parameters describing the energy release in a cascade, \( a \) is the distance between the center of the pore and the cascade, \( P_n \) is a Legendre polynomial dependent only on the coordinate \( \Theta \), and \( f_n \) are the coefficients of the Legendre-polynomial expansion of the function describing the energy distribution in the cascade by the time the dynamic stage is completed. The function \( \tilde{W}_n \) is determined by the inverse Laplace transform with respect to time. The transform of this function can be written as

\[ \tilde{W}_n = \left( \frac{\pi V_0}{2r V_s} \right)^{0.5} \cdot K_{n+1/2} \left( V_s \sqrt{\frac{\pi}{\omega}} r \right). \]

Here, \( K_{n+1/2}(z) \) is a spherical Bessel function.

Calculation of the temperature fields from formulas (1)-(4) revealed the existence of considerable temperature concentrations on the surface of pores of 10-20 nm, which causes considerable stresses in the vicinity of a pore.

The approximating solution for regions in which the temperature gradient is nearly linear was chosen for the investigation of small pores (\( R \approx 1-2 \) nm). In this case the temperature...
field can be described by

\[ T = T_0 + f \cos \Theta \left( r + \frac{R^2}{2r^2} \right), \]  

where \( T_0 \) is the temperature of the point in continuous space that corresponds to the center of the pore in the case of discontinuous space. The function

\[ f = f_0 (\omega t/R^2)^{\gamma} \exp \left[ -c_2 \omega t/R^2 \right] \]

describes the time variation of the temperature gradient.

The given temperature field gives rise to corresponding fields of thermoelastic stresses:

\[ \sigma_{rr} = 2A (R^2/r^2 - R_0^2/r_0^2) \cos \Theta, \]
\[ \sigma_{\varphi\varphi} = \sigma_{\varphi z} = -A (R^2/r^2 + R_0^2/r_0^2) \cos \Theta, \]
\[ \sigma_{\varphi z} = -A \left( R^2/r^2 - R_0^2/r_0^2 \right) \sin \Theta. \]

The coefficient \( A \) in formula (7) takes account of the thermal and mechanical properties of the material and depends on the pore size.

The existence of temperature and stress concentration alters the balance of point defects at a pore since in this case the rate of the reaction of the pore with the respective defect depends on the coordinates:

\[ K_s = \frac{1}{2} \int_D \rho_s \langle \tau \rangle_{r-R} ds. \]

When the boundary conditions at the pore are taken into account the expressions for the rates of the reactions of the pore with vacancies \( K_v \) and interstices \( K_i \) are written in the form

\[ K_v = -2\pi R c_v D_{ov} \int \exp \left[ -\frac{U^m_v}{\kappa (T + T)} \right] s^{-1} \exp \left[ \frac{2\Omega_1}{R \kappa (T + T)} \right] \frac{1}{3\kappa (T + T)} d (\cos \theta), \]
\[ K_i = -2\pi R c_i D_{oi} \int \exp \left[ -\frac{U^m_i}{\kappa (T + T)} \right] d (\cos \theta). \]

Here, \( s \) denotes the degree of supersaturation with vacancies in comparison with the equilibrium values for the given temperature, \( U^m_v \) and \( U^m_i \) are the migration activation energies of vacancies and interstices, \( c_v \) and \( c_i \) are the concentrations of defects, \( \gamma \) is the surface tension energy, \( \Omega \) is the atomic volume, \( \sigma_1 \) is the first invariant of the stress tensor, \( R \) is the pore radius, and \( D_{ov} \) and \( D_{oi} \) are the preexponential diffusion coefficients.

Since \( T/T < 1 \), the denominators of the exponential factors in expressions (9) and (10) can be expanded in a series and, limiting ourselves to linear terms, we can integrate these expressions.

As a result of mathematical rearrangements the balance equation for point defect at a pore,

\[ \frac{dV_R}{dt} = \sum K_s (R, t), \]

in which \( V_R \) is the pore volume \( V_R = 4\pi R^3/3 \Omega \), can be written as

\[ \frac{dR}{dt} = \frac{D_{ov} c_v}{R} \left( \exp \left[ \frac{U^m_v T_0^2}{\kappa T^2} \right] - \gamma \exp \left[ \frac{U^m_i T_0^2}{\kappa T^2} \right] - s^{-1} \exp \left[ \frac{U^m_v - 2\Omega_1 R}{\kappa T^2} \right] T_0 + \frac{2\Omega_1}{R \kappa T} \right). \]

The parameter \( \eta \), which is associated with the value of the diffusion flows of interstices and vacancies and depends on the defect structure of the material and the rate \( G \) of generation.