Effect of Secondary Processes on Material Hardening under Low Temperature Radiation

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Abstract—Evolution of radiation barrier (vacancies and interstitials) clusters is analyzed under low temperature radiation in the presence of the most important secondary effects: recombination and formation of divacancy complexes. It is proposed a barrier hardening model in that mechanisms of mutual annihilation of the vacancy and interstitial barriers and their clusterization play a main role. It is taken into account reducing barrier densities due to barrier mutual annihilation of two different types and developing the large clusters by interconnection of two barriers of the same type.

The construction of physics models to describe analytically dose dependences of irradiated material strength characteristics is very important as well as a theoretical description of their temperature dependences [1–9].

A series of different radiation defects (retardation barriers of dislocations), and their sizes, and a form of their volume distribution contribute into a yield strength increment for all of sorts of irradiation. The contribution of a barrier type is determined by conditions of irradiation and tests. At the low temperature irradiation, interstitial atoms, and vacancies, and their clusters contribute mainly into the hardening.

In this work, it is proposed the model to describe the dose dependence of yield strength increment and to take into account interaction of vacancy and interstitial type barriers.

FORMULATION OF THE MODEL

The base of the model is a barrier mechanism of the radiation hardening [2] according to that the yield strength increment can be represented by the sum of barrier contributions of different types

$$\Delta\sigma = \sum_{i=1}^{N} \Delta\sigma_i, \quad (1)$$

where index i is a barrier type, N is a number of barrier types affecting the yield strength, $\Delta\sigma_i$ is the yield strength increment of i' barrier type.

We consider that the barriers of vacancy and interstitial types make a main contribution to the yield strength increment of a certain material. These barriers play the main role in the hardening at the low temperature irradiation. Therefore, in the proposed model $N = 3$; the index values of $i = 1$ correspond to the vacancy barriers, $i = 2$ do to interstitial ones and $i = 3$ do to more large vacancy complexes. Then in this model Eq. (1) takes the form:

$$\Delta\sigma = \Delta\sigma_1 + \Delta\sigma_2 + \Delta\sigma_3. \quad (2)$$

For all of the obstacle types, the metal yield strength increment conditioned by dislocation deceleration is described by the form (see [1]):

$$\Delta\sigma_i = \alpha_i \mu b (C_i d_i)^{1/2}, \quad (3)$$

where α_i is the parameter characterizing i barrier intensity (a fixed quantity for some of barrier types, material and irradiation condition), μ is the shear modulus, b the Burgers vector length, C_i the volume density of i barrier type, d_i their average size (doesn't depend on dose practically). For instance, the vacancy and interstitial barriers have the average size ≤5 nm, and the parameter characterizing barrier intensity has the value about 0.2 [1].

Under irradiation, development of radiation defect clusters (barriers) of different types occurs in a region of a primary knocked-on atom. It is proposed that the interstitial barriers have considerably smaller sizes and leave the damage region of a sample sooner than the vacancy barriers do. In connection with this, we formulate the phenomenological model that is based on an equation system for volume densities of the radiation-induced non-equilibrium vacancy C_1 and interstitial C_2 barriers and more large complexes C_3 developed by bimolecular mechanism of the vacancy barriers:

$$\begin{cases} \dfrac{\partial C_1}{\partial \tau} = D_1 \Delta C_1 + K_1 - C_1/\tau_1 - \gamma_{12} C_1 C_2 - \gamma_1 C_1^2, \\ \dfrac{\partial C_2}{\partial \tau} = D_2 \Delta C_2 + K_2 - C_2/\tau_2 - \gamma_{12} C_1 C_2 - \gamma_2 C_2^2, \\ \dfrac{\partial C_3}{\partial \tau} = D_3 \Delta C_3 + \gamma_1 C_1^2 - C_3/\tau_3. \end{cases} \quad (4)$$

Here $\tau = \Phi t$, Φ is the particle flux, t irradiation time, K_i, $i = 1, 2$, the intensities of forming the radiation - induced vacancy and interstitial barriers, γ_i are the coefficients of barrier recombination and characterize forming the clusters of acceptable barrier type (it can be named as clusterization coefficients), the coefficients τ_i^{-1} can be represented by the form: $\tau_i^{-1} = K_i V_i$, where V_i are the effective volumes of interaction of the certain barriers with each other, γ_{12} the coefficient of mutual recombination of the annihilating vacancy and interstitial barriers. It can be valued as follows [1]:

$$\gamma_{12} = \frac{4\pi r(D_1 + D_2)}{\Omega} e^{-\frac{E_r}{k_B T}},$$

where Ω atom volume, E_r activation energy of recombination of vacancy and interstitial barriers, r recombination radius, T test temperature, k_B Boltzmann constant, D_i diffusion coefficients of the non-equilibrium barriers of the given types: $D_i = D_{i0}\exp(-E_i/k_B T)$, $i = 1, 2$, where E_i energy of activation and migration of respective barriers, $D_{i0} = a^2\nu$, a and ν are length and barrier jumping frequency for migration, respectively.

As material structure changes go under irradiation for times large in comparison with relaxation time of point defects then only diffusion barrier processes are considered to be very slow and therefore we neglect diffusion terms in the equations of the system (4). In addition, we study evolution of barrier volume densities in time considering their distributions are spatially homogeneous. In this case, the system (4) takes the form:

$$\begin{cases} \dfrac{\partial C_1}{\partial \tau} = K_1 - C_1/\tau_1 - \gamma_{12} C_1 C_2 - \gamma_1 C_1^2, \\ \dfrac{\partial C_2}{\partial \tau} = K_2 - C_2/\tau_2 - \gamma_{12} C_1 C_2 - \gamma_2 C_2^2, \\ \dfrac{\partial C_3}{\partial \tau} = \gamma_1 C_1^2 - C_3/\tau_3. \end{cases} \quad (5)$$

The first terms of the equation system (5) describe the intensity of increasing the volume barrier densities of the acceptable type. The second ones correspond to decreasing the volume barrier densities due to absorbing the barriers on natural sinks: voids, dislocations, dislocation network, grain boundaries and so on.

In the proposed model, the mechanisms of the mutual annihilation of vacancy and interstitial barriers and their clusterization are assigned. The third terms of the equation system (5) describe decreasing the barrier densities due to of the mutual annihilation of two different type barriers, and the fourth ones do due to developing the large clusters of two barriers of the same type.

The third equation of the system (5) describes redistribution of divacancy barrier complexes.

Contribution to the hardening due to divacancy barriers is determined by only vacancy barrier density and the kinetic coefficients τ_3^{-1} and γ_1 characterizing intensities of breakdown of vacancy clusters and development of divacancy clusters. Effect of this contribution is appreciable if intensity of secondary processes of developing divacancy complexes predominates over their breakdown.

To find the volume densities of the nonequilibrium barriers it is necessary to set up their initial values:

$$C_i(0) = C_i^{(0)}, \; i = 1, 2, 3. \quad (6)$$

Thus, the mathematical formulation of the model proposed in this work is the Cauchy problem for the system of nonlinear differential Eqs. (5) with initial conditions (6). The volume barrier densities found as a result of solution of the Cauchy problem (5), (6) are to be inserted into Eq. (3) that determines the total yield strength increment (2).

NUMERICAL ANALYSIS OF THE MODEL RESULTS

The model values of parameters (are given in captures of figures) and the initial conditions $C_i^{(0)} = 5 \times 10^{13}$ cm^{-3} are used to fulfill numerical analysis of the Cauchy problem (5), (6). The results of the numerical solution of the Cauchy problem (5), (6) (reduced to the dimensionless form) are represented on Fig. 1 at the indicated parameter values.

Here is shown the specified form of dose dependences of relative densities for vacancy barriers C_1/C_0, and interstitial barriers C_2/C_0, and more large vacancy complexes C_3/C_0 where C_0 is a measure scale of barrier density taken to be equal 10^{15} cm^{-3} in this case on dose τ/τ_0 in units measured by the scale τ_0 (it is convenient to select a minimal fluence of the specific problem as the dose measure scale; for instance, in the ion irradiation the value of τ_0 can be equal 10^{14} ion/cm^2 or

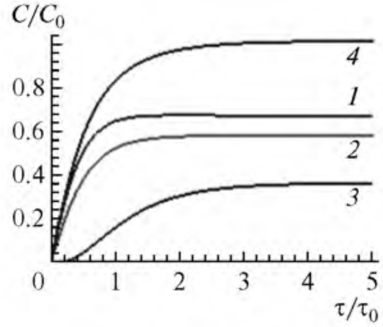

Fig. 1. Dependences of relative barrier density of vacancy type (*1*), interstitial type (*2*), vacancy complexes (*3*) and their total density (*4*) on dose at fixed values of dimensionless parameters $(K_1\tau_0)/C_0 = 1.5$, $(K_2\tau_0)/C_0 = 1$, $\tau_0/\tau_1 = 1$, $\tau_0/\tau_2 = 0.5$, $\tau_0/\tau_3 = 1.25$, $\gamma_{12}C_0\tau_0 = 0.9$, $C_0^2\gamma_1 = C_0^2\gamma_2 = 1$.

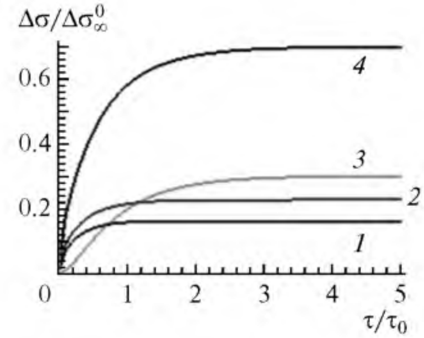

Fig. 2. Dose dependences of barrier contributions of vacancy type (*1*), interstitial type (*2*), vacancy complexes (*3*) and their total density (*4*) to yield strength increment at fixed values of parameters the same as in Fig. 1 and $d_1/d = 0.016$, $d_2/d = 0.035$, $d_3/d = 0.097$.

10^{22} n/m^2 in the neutron irradiation and so on, for the specific problem, respectively). These dependence patterns are universal and independent of the selected measure scales of the specific physics parameters.

It is shown that the saturation of the material by the radiation - induced barriers takes place with increasing dose.

The numerical solution of the Cauchy problem (5), (6) permits to obtain the dose dependences of the total increment of material yield strength increment which is convenient to represent for construction of graph as follows

$$\Delta\sigma = \Delta\sigma_\infty^0 \sum_{i=1}^{3} \sqrt{d_i C_i / dC_0}, \qquad (7)$$

where $\Delta\sigma_\infty^0 = \alpha\mu b(C_0 d)^{1/2}$, d average size of barrier cluster over all of types. The results of numerical modeling the behavior of the yield strength increment are represented in Fig. 2.

The numerical analysis shows that the yield strength increment gets the saturation quickly enough. The typical monotonic form of the dose saturation plots of the yield strength increment does not change virtually in a broad enough interval of the model parameter values satisfying to the existence condition of the Cauchy problem (5), (6) solution.

It is should be noted though the vacancy complexes have lower concentration in comparison with vacancies and interstitial atoms they, due to their larger sizes, contribute more considerably to yield strength increment at dose build-up.

SECONDARY REACTION CONTRIBUTION ANALYSIS

Let us consider the case when secondary reactions play a main role that is barrier recombination goes less intensively than developing barrier clusters. In this extreme case, we consider $\gamma_{12} \ll \gamma_1$ and $\gamma_{12} \ll \gamma_2$. Then the second equation of the system (5) becomes independent and coinciding formally with the first equation. In the result, the system (5) consists of two equations:

$$\begin{cases} \dfrac{\partial C_1}{\partial\tau} = K_1 - C_1/\tau_1 - \gamma_1 C_1^2, \\ \dfrac{\partial C_3}{\partial\tau} = \gamma_1 C_1^2 - C_3/\tau_3. \end{cases} \qquad (8)$$

The first equation of the system (8) doesn't contain C_3. Therefore, it is independent. Its solution with zero initial condition takes the form:

$$C_1(\tau) = C_a \mathrm{th}\left(\frac{\tau}{\tau_c} + \varphi\right) - C_b, \qquad (9)$$

where $\tau_c = 2\tau_1/\kappa$, $C_a = \kappa/2\tau_1\gamma_1$, $C_b = C_a/\kappa$, $\kappa = \sqrt{1 + 4K_1\gamma_1\tau_1^2}$, $\varphi = \mathrm{Arth}(1/\kappa)$. The obtained expression (9) describes the dependence of vacancy barrier volume density on dose $\tau = \Phi t$.

When the processes of vacancy barrier clusterization are absent overall ($\gamma_1 = 0$) it results from (8) $C_1(\tau) = K_1\tau_1(1 - e^{-\tau/\tau_1})$ whence the well known contribution to yield strength increment follows in the case of hardening by the barrier of a single type:

$$\Delta\sigma_1 = \Delta\sigma_\infty^0 \left\{ d_1 K_1 \tau_1 (1 - e^{-\tau/\tau_1}) / dC_0 \right\}^{1/2}. \qquad (10)$$

Substituting Eq. (9) into the second equation of the system (8) its solution can be written as

$$C_3(\tau) = \gamma_1 \int_0^{\tau} e^{(s-\tau)/\tau_3} C_1^2(\tau)\, ds. \qquad (11)$$

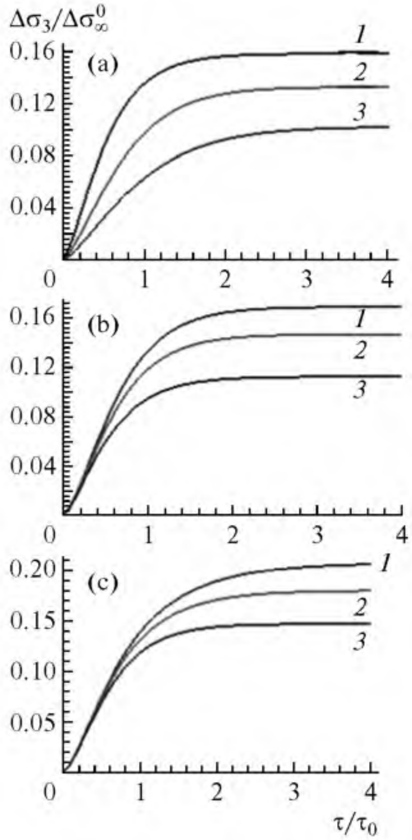

Fig. 3. Dose dependences of vacancy complex contribution to yield strength increment at fixed values of parameters $(K_1\tau_0)/C_0 = 1$, $d_3/d = 0.097$: (a) (*1*) $\tau_1/\tau_0 = 1$, $\tau_3/\tau_0 = 0.4$, $C_0^2\gamma_1 = 5$; (*2*) $C_0^2\gamma_1 = 1.5$; (*3*) $C_0^2\gamma_1 = 0.5$; (b) (*1*) $\tau_3/\tau_0 = 0.4$, $C_0^2\gamma_1 = 3$, $\tau_1/\tau_0 = 2$; (*2*) $\tau_1/\tau_0 = 1$; (*3*) $\tau_1/\tau_0 = 0.5$; (c) (*1*) $\tau_1/\tau_0 = 1$, $C_0^2\gamma_1 = 3$, $\tau_3/\tau_0 = 0.8$; (*2*) $\tau_3/\tau_0 = 0.6$; (*3*) $\tau_3/\tau_0 = 0.4$.

Further, this expression is used to analysis the vacancy complex contribution to yield strength increment:

$$\Delta\sigma_3 = \Delta\sigma_\infty^0(d_3C_3/dC_0)^{1/2}. \quad (12)$$

The increasing of saturation quantity of yield strength increment goes with increasing intensity of the clusterization processes that is with increasing parameter γ_1 (Fig. 3a).

This increasing is nonlinear, enlargement of yield strength increment saturation going less and less considerably with increasing intensity of the clusterization processes.

Growth of saturation quantity of yield strength increment goes with increasing specific times τ_1 and τ_3 as well (Figs. 3b and 3c).

CONCLUSION

In the frame of the proposed model, it can be estimated both contributions to yield strength increment from different type barriers and its total value in dependence on dose.

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