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The paper focuses on the void swelling processes in materials subjected to radiation, that occur due to the formation of the void ensemble in the crystal lattice. According to the theoretical analysis of the kinetics and the pore size distribution with regard to the defect migration, the numerical calculations are performed for void swelling in nickel.

Keywords: defect kinetics, pores, stress, void swelling.

INTRODUCTION

Deformation of materials (void swelling) under irradiation is one of the relevant problems of the radiation materials science. First of all, void swelling is associated with an ensemble of voids with the size ranging from one to tens of nanometers. The void concentration can achieve 10^{23} m^{-3}.

The formation of the porous structure in materials follows certain regularities:

– Voids nucleate in the case of an oversaturation with vacancies. The radius R_m of an individual void can be determined by the number m of vacancies:

$$R_m = R_{m-1} + \frac{V_0}{4\pi R_{m-1}^2}, \tag{1}$$

where $m = n_з + 1, n_з + 2, \ldots, n_з + j$, $n_з$ is the number of vacancies in a stable void nucleus, V_0 is conventionally equal to the atomic volume, *viz.* $R_{n_з} \equiv R_0$.

– Voids do not nucleate in the material's regions without dislocations.

The void nucleation begins when the dislocation density reaches its critical value of ~10^{13} m^{-2} and occurs only on mobile dislocations. Dislocations, which more intensively absorb interstitial atoms, provide an oversaturation with vacancies in the bulk material, that leads to vacancy clustering and then the void formation.

– Internal stresses more likely cause the void nucleation.

– Voids appear within a certain temperature range, which is characterized by the higher mobility of the point defects. The size of voids increases with the temperature elevation.

– Void ordering (the superlattice formation) begins when they reach a certain concentration. The lattice parameter of voids increases with increasing temperature.

– Voids have a similar size in the lattice.

– The lattice parameter of voids decreases with increasing defect generation rate, the temperature being constant.

– The symmetry of the lattice parameter of voids matches the symmetry of the initial crystal lattice.

These regularities represent a "testing ground" for checking the propriety of this or that model description of the formation of voids and their lattices. Gao *et al.* [1, 2] study the void generation and ordering in the superlattice. However, some questions remain unresolved, in particular, the kinetics of the void nucleation and evolution with regard to elastic stresses caused by these defects.

RESULTS AND DISCUSSION

Volume deformation $\varepsilon(t)$ ($\Delta V/V$, where V is the initial material volume) and its rate $d\varepsilon/dt$ in the irradiated material are caused by the formation of voids and described by the following equation [3]:

$$\varepsilon(t) = \frac{4}{3}\pi \int_0^\infty f(R,t) R^3 dR\,, \tag{2}$$

$$\frac{d\varepsilon(t)}{dt} = \frac{4}{3}\pi \left(\int_0^\infty \frac{\partial f(R,t)}{\partial t} R^3 dR + 3 \int_0^\infty f(R,t) R^2 \frac{\partial R}{\partial t} dR \right), \tag{3}$$

where $f(R, t)$ is the density function of the pore size distribution.

The analytical expression for $f(R, t)$ can be derived from the equation of continuity in the size distribution space [4]:

$$\frac{\partial f(R,t)}{\partial t} = W(R,t) - \frac{\partial}{\partial R}\left[f(R,t) \frac{\partial R}{\partial t} \right]. \tag{4}$$

Here $W(R, t)$ is the generation rate of voids with R radius.

For stationary conditions of $W(R, t) = 0$, on the assumption with the void concentration $\left(\int_{R_0}^\infty f(R,t) dR = N_s \right)$, the differential equation (4) can be solved as

$$f(R,t) = N_s \frac{f(R,t_0) e^{\int_{t_0}^{t} A(R,t')dt'}}{\int_{R_0}^{\infty} f(R,t_0) e^{\int_{t_0}^{t} A(R,t')dt'} dR}, \tag{5}$$

where $f(R, t_0)$ is the initial pore size distribution, $A(R,t) = \frac{\partial}{\partial R}\left[\frac{\partial R}{\partial t} \right]$. In the general cease, the function $A(R, t)$ also depends on the spatial value $\bar{r}$.

The initial pore size distribution $f(R, t)$ can be represented by the following function:

$$f(R,t_0) = \frac{N_s}{\sqrt{2\pi}\beta} e^{-\frac{(R-R_s)^2}{2\beta^2}}. \tag{6}$$

Here $R_s > R_0$ ($1.5 \cdot 10^{-9}$ and $0.5 \cdot 10^{-9}$ m, respectively), β is very small and fashions Eq. (6) into a narrow normal distribution ($0.5 \cdot 10^{-9}$ m), N_s is the concentration of voids with R_s radius (10^{22} m^{-3}).

It is known, that a void with R radius causes the elastic stress field $\sigma(r, R)$ in the material:

$$\sigma(r,R) = -\gamma \frac{R^2}{r^3}\,, \tag{7}$$

where γ is the energy density of the surface tension (1–15 J/m^2), r is the radius vector modulus.

The size ρ of the elastic stress field (Eq. (7)) can be calculated from $P\Delta\omega \geq U_m$ condition, thus yielding the following relation:

$$\rho(R) = R + \left(\frac{\gamma R^2 \Delta\omega}{3U_m} \right)^{1/3} . \tag{8}$$

Here P is the pressure in the stress field, $\Delta\omega$ is the defect dilatation (~10^{-29} m^3), U_m is the energy of the defect migration (0.1–0.3 eV).

The dependence between the elastic stress field created by one void and its radius is presented in Fig. 1.

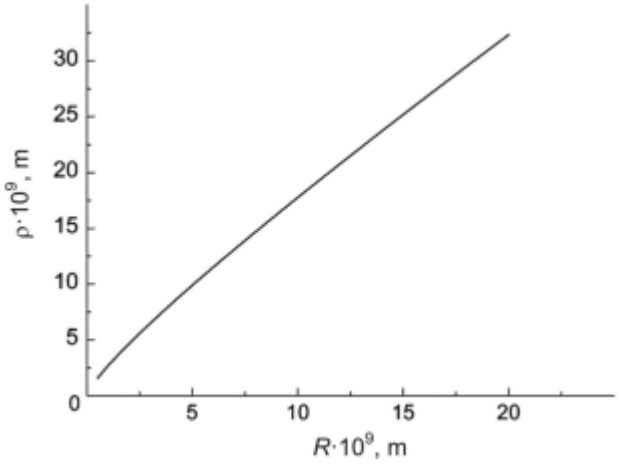

Fig. 1. Dependence ρ(R) between the elastic stress field created by one void and its radius.

With regard to the defect motion $Q_3(\bar{r},t)$ in the elastic stress field (Eq. (7)), the relation is obtained for the growth rate of the individual void:

$$\frac{\partial R}{\partial t} = \left[Q_1(\bar{r},t) - Q_2(\bar{r},t) \right] R^{-1} - Q_3(\bar{r},t) R^{-2/3} , \tag{9}$$

where $Q_1(\bar{r},t) = D_v \left[C_v(\bar{r},t) - C_v^0(\bar{r},t) \right]$, $Q_2(\bar{r},t) = D_i \left[C_i(\bar{r},t) - C_i^0(\bar{r},t) \right]$, $Q_3(\bar{r},t) = Q_2(\bar{r},t) \dfrac{(3U_m)^{4/3}}{k_B T (\gamma\Delta\omega)^{1/3}}$; D_v and D_i are the diffusion coefficients of vacancies and interstitial atoms, respectively (10^{-13} and 10^{-8} m^2/s [5]); $C_v(\bar{r},t)$ and $C_i(\bar{r},t)$ are concentrations of vacancies and interstitial atoms, respectively; $C_v^0(\bar{r},t)$ and $C_i^0(\bar{r},t)$ are equilibrium concentrations of vacancies and interstitial atoms, respectively (10^{-4} and 10^{-9}); k_B is the Boltzmann constant; T is the absolute temperature.

Using Eqns (5), (6) and (9), we plot the functions $f(R, t)$ in the approximation of a homogeneous defect distribution at different ratios between $Q_1(\bar{r},t) = Q_1(t)$ and $Q_2(\bar{r},t) = Q_2(t)$ terms, as illustrated in Fig. 2.

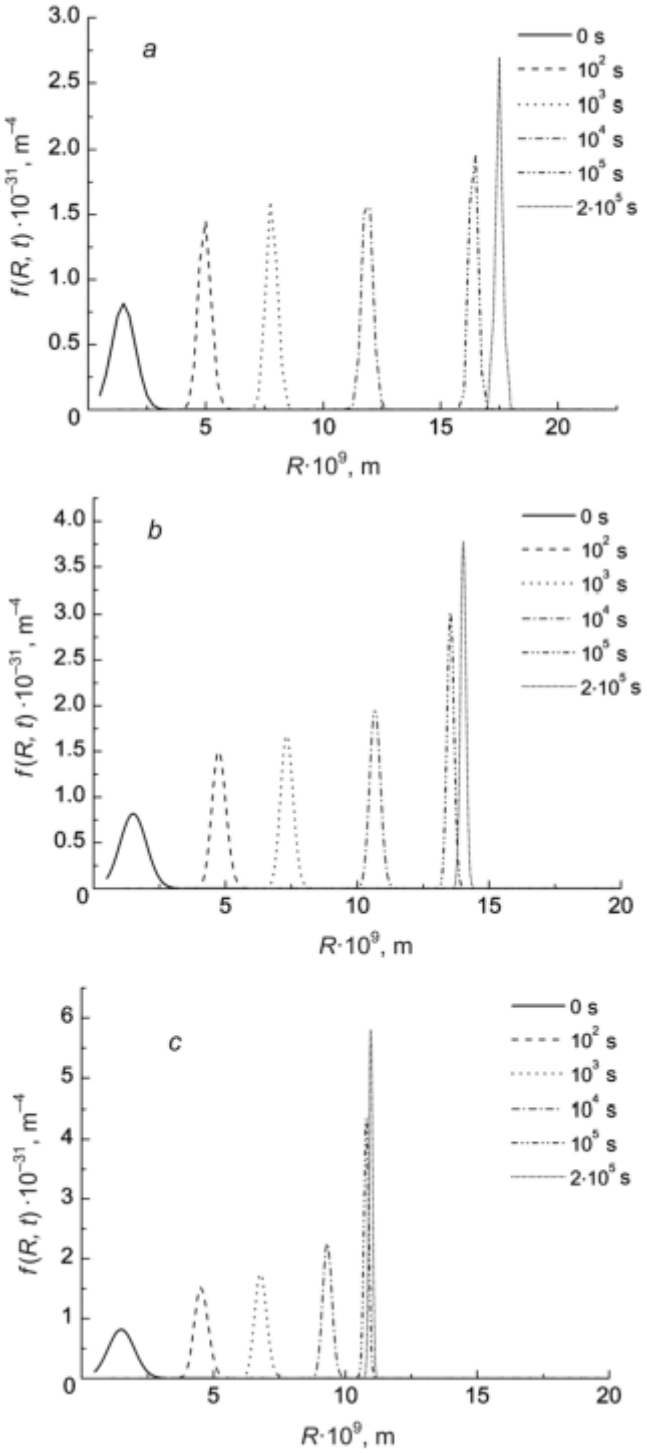

Fig. 2. Density functions of the pore size distribution at T = 900 K and different ratios between $Q_1(t)$ and $Q_2(t)$: *a* – $Q_1/Q_2 \approx 4.46$, *b* – $Q_1/Q_2 \approx 4.14$, *c* – $Q_1/Q_2 \approx 3.87$.

As can be seen from Fig. 2, the void growth occurs over time. With increasing Q_1/Q_2 ratio, the average pore size also increases, which can be explained by the greater degree of the oversaturation with vacancies.

The growth in the individual void can be obtained from Eq. (9):

$$\int_{R_0}^{R} \frac{R'}{Q_1(\bar{r},t) - Q_2(\bar{r},t) - Q_3(\bar{r},t)R^{1/3}} dR' = t - t_0, \tag{10}$$

provided that the radius of the stable void nucleus is R_0 at time t_0.

Figure 3 presents the growth rate of the individual void at T = 1000 K and different ratios between $Q_1(t)$ and $Q_2(t)$.

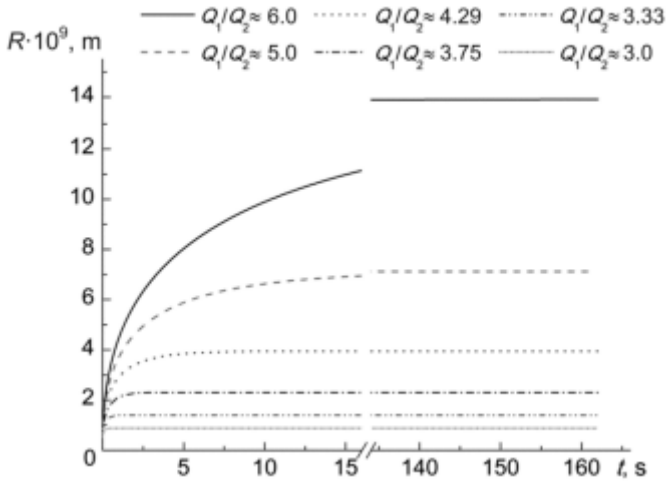

Fig. 3. Growth rate of individual voids at T = 1000 K and different $Q_1(t)/Q_2(t)$ ratios.

The dependences shown in Fig. 3 can be explained by the fact that the void radius increases with increasing oversaturation with vacancies.

The spatiotemporal distribution of $C_v(\bar{r},t)$ and $C_i(\bar{r},t)$ concentrations in equations for and is derived from a solution of the system of kinetic balance equations [6] subject to the defect motion in the elastic stress field created by the voids:

$$\frac{\partial C_v(\bar{r},t)}{\partial t} = \Theta - \kappa_v D_v \left[C_v(\bar{r},t) - C_v^0(\bar{r},t) \right] - \lambda \left[C_v(\bar{r},t) C_i(\bar{r},t) - C_v^0(\bar{r},t) C_i^0(\bar{r},t) \right] + \nabla \left[D_v \nabla C_v(\bar{r},t) \right], \tag{11}$$

$$\frac{\partial C_i(\bar{r},t)}{\partial t} = \Theta - \kappa_i D_i \left[C_i(\bar{r},t) - C_i^0(\bar{r},t) \right] - \lambda \left[C_v(\bar{r},t) C_i(\bar{r},t) - C_v^0(\bar{r},t) C_i^0(\bar{r},t) \right] + \nabla \left[D_i \nabla C_i(\bar{r},t) - \frac{D_i C_i(\bar{r},t)}{k_B T} \overline{F}_i \right]. \tag{12}$$

Here $\lambda = 4\pi r_{\text{рек}} (D_v + D_i)/V_0$ рек – rec is the recombination coefficient; r_{rec} is the radius of spontaneous recombination ((3–4)·a_0, where a_0 is the lattice parameter); $\kappa_{i,v} = 4\pi \langle R \rangle N_p$ is the sink-void strength; $\langle R \rangle$ is the mean void radius; N_p is the void concentration; $\overline{F_i} = \Delta\omega\nabla\sigma$; Θ is the generation rate of vacancies and interstitial atoms or a 10^{-10}–10^{-2} dpa/s dose rate.

In this work, we do not consider a certain type of radiation. The radiation parameters are set through the generation rate of the point defects and the radiation temperature.

Figure 4 contains the time dependences of void swelling in nickel at different temperatures.

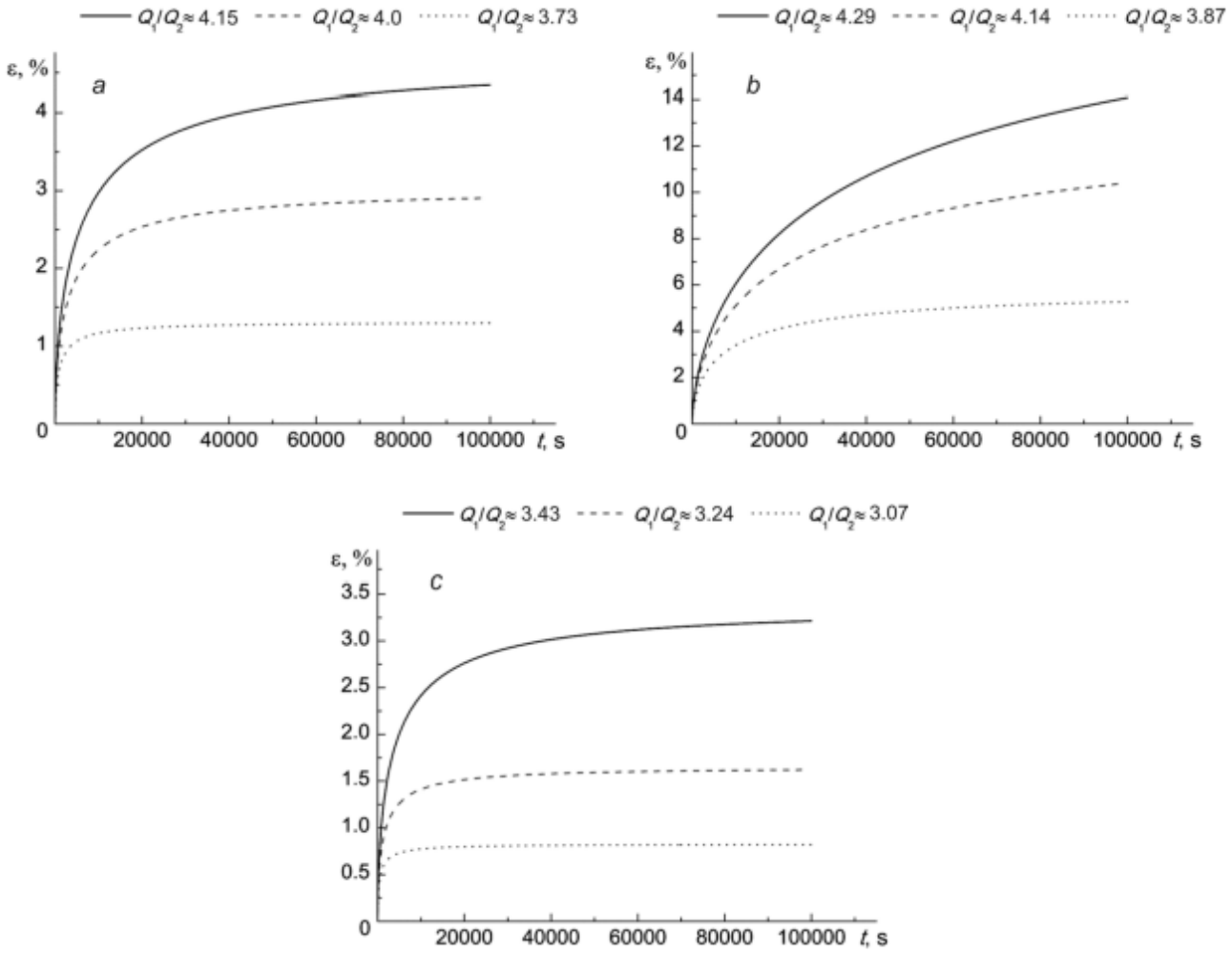

Fig. 4. Time dependences of void swelling in nickel at different temperatures: *a* – 800 K, *b* – 900 K, *c* – 1000 K.

According to Fig. 4, the lower Q_1/Q_2 ratio the lower void swelling. In other words, during the activation of the kinetics of the interstitial atoms, void swelling decreases, which is also associated with the reduction in the average pore size (see Fig. 2*b*, *c*). The obtained results are in good agreement with, for example, the experimental data on Ni+ ions irradiation with energy of 500 keV up to a fluence of 25 dpa [7]. It should be noted that the theoretical analysis and numerical simulation of the void formation and evolution are rather difficult because of the lack of reliable data in the literature on the relevant coefficients and parameters of the radiation process, that may also depend on time.

Thus, practical implications of the void swelling reduction in materials subjected to radiation can be provided by the certain radiation conditions.

CONCLUSIONS

The theoretical analysis of the void swelling process in irradiated materials allowed us to determine the main regularities of the void generation and obtain the analytical expression for the pore size distribution density. For the first time, the influence of void-induced elastic stresses was considered in these processes, in the vicinity of a void. With regard to the defect motion, the kinetics of the void nucleation and the evolution of both the individual void and void ensemble were described more adequately. It was shown that the ratio between the concentration of vacancies and interstitial atoms contributed much to the void swelling process. The analysis and regularities of the void swelling

process in nickel were presented and described using the pore size distribution density function close to the Gaussian function.

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