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Radiation stability of iron nanoparticles irradiated with accelerated iron ions

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ABSTRACT

In the present work the dynamic processes occurring in a nanoscale iron particle exposed to irradiation with iron ions of different energies are studied in detailed. It is shown that the elastic and thermoelastic crystal lattice responses to irradiation form force factors affecting the evolution of defect-impurity system, which, in turn, leads to a decrease in the number of structural defects. Quantitative estimations of the spatial distribution of defects resulting in their migration to the surface were obtained. Such self-organization of nanoparticles exposed to ionizing radiation can be used as a basis for the production of radiation-resistant nanostructured materials capable of sustaining a long-term radiation influence.

1. Introduction

It is well known that the properties of materials irradiated with fluxes of high-energy particles are changed as a result of degradation processes. However, even in the 1960s, it was found that fine-dispersed metal powders have enhanced radiation resistance. In the time of rapidly developing nanotechnologies, such a phenomenon can serve as the basis for the production of nanostructured radiation-resistant materials. Indeed, the opinion that nanoparticles possess the property of enhanced radiation resistance was put forward in a series of papers [1–14].

The number of atoms displaced from lattice sites ranges from tens to thousands in the region of ion deceleration depending on its energy. The thermal heating of materials in the region of the displacement cascade can be from hundreds to several thousands of degrees, the pressure at the front of such waves being very significant. At the primary stage, a hard shock pulse gives rise to dynamic ("flickering") defects whose lifetime significantly exceeds the Debye oscillation period of lattice atoms. Subsequent heating of the deceleration region causes the formation of following elastic perturbation. Elastic acoustic oscillations can also be generated in accordance with some other mechanisms. The existence of such phenomena during ion implantation was established in a series of experimental studies rather long ago. It should also be mentioned that high temperatures in deceleration regions can lead to various phase transformations in them. The described processes pass in a different way when the dimension of the object decreases up to 10–100 nm.

Experimentally revealed data concerning the enhanced radiation stability of nanostructured solids have no any reliable descriptions and the mechanisms of such behavior of nanoparticles under irradiation are not sufficiently studied. In this regard the dynamic processes accompanied by accelerated charged particles penetration into nanoparticles as well as defect system evolution in the irradiated materials are considered in the present work.

The proposed in the work approach for description of radiation stability of nanoparticles is characteristic of any nanoparticle without regard to the material. According to our previous research [15] iron nanoparticles possess a unique ferromagnetic properties that sufficiently depend on their size. Such particles can be served as effective objects for record and storage information in producing of modern electronic systems working including in the extreme conditions. So, the problem of the radiation resistance of iron nanoparticles is sufficiently urgent. Therefore in the present work iron nanoparticles with different sizes were chosen for modeling of radiation defects evolution during the irradiation with iron accelerated ions. The iron accelerated ions were used in the modeling because of excluding from consideration the impurity defects.

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2. Results and discussion

2.1. Formation of elastic perturbations in a nanoparticle under irradiation with ions

When an atom obtains the energy from an implanted ion that exceeds the threshold displacement energy E_d, it leaves its site in the crystal lattice and stops at a distance from it. In this case, a vacancy forms at this site. The total number N of atoms ejected by the impinging ion from sites can be estimated in accordance with the formula proposed by Sigmund:

$$N = \frac{0.84W(E)}{2E_d}, \tag{1}$$

where $W(E)$ is the total energy lost during elastic collisions, E is the energy of the impinging ion, and E_d is the threshold displacement energy (in the case of nanoparticles, it depends on both the nanoparticle size and the atom position inside the volume).

The value N can also be expressed in terms of the cross section S_n of elastic deceleration:

$$N = \frac{0.42n}{E_d}\int_0^l S_n(z)dz, \tag{2}$$

where l is the distance of ion motion in the material and n is the atom concentration in the matrix. For relatively low ion energies, we can set $W(E) = E$. It should be mentioned that these well known concepts in radiation physics [16] can be applied to both macroscopic objects and nanoparticles. However, subsequent processes, which are, in fact, the lattice response to ion implantation, lead to very different final states of the defect-impurity system in macro- and nanoobjects.

One of the ways of formation of elastic perturbation in the matter after the charged particle implantation is generation of unstable Frenkel-pairs. This type of forced impact on the defects existed in the material is characterized by shock mechanism. The dynamic of the formed unstable Frenkel-pairs can be described as a motion of an atom in a matter with dissipation (coefficient of dissipation ξ) when the energy transferred to the atom is less than threshold displacement energy E_d. In this case the atom is displaced to a distance not exceeding the radius of spontaneous recombination R_z and come back to the own vacancy under the Coulomb force and elastic stress of the crystal lattice. The elastic relaxation of the crystal lattice occurs in the area of "flickering" pair localization characterized by the radius R_z of the region of instability. So, the pressure p_0 acting to the lattice from inside of the region of instability can be estimated from the friction force F_{fric} between the matter and the defect moving with the velocity v_d:

$$p_0 = F_{fric}/S_z, \quad (F_{fric} = m\xi v_d, S_z = 4\pi R_z^2), \tag{3}$$

where $v_d \sim 10^4$ m/s, $\xi \sim 2.6 \cdot 10^{12}$ s^{-1}, $R_z \sim 3 \cdot 10^{-9}$ m, and $p_0 \sim 2 \cdot 10^7$ Pa [17].

If it is assumed that there is only one dynamic defect per a displaced atom [18], then the pressure achieves the values 10^{10} Pa and more. The total quantity of the atoms N displaced by an accelerated charged ion in a nanoparticle with the radius R was estimated by means of SRIM program code. In Fig. 1 the results of modeling the quantity of the displaced atoms N in iron nanoparticle after irradiation with iron ions with different energies are presented.

When propagating in the crystal, the elastic perturbation interacts with the defects and, as a result, changes their positions in crystal lattice and thermodynamic states under certain conditions. In this case, the force F_1 acting on a defect is determined as $P_1\Sigma$. Here, the pressure P_1 is expressed as:

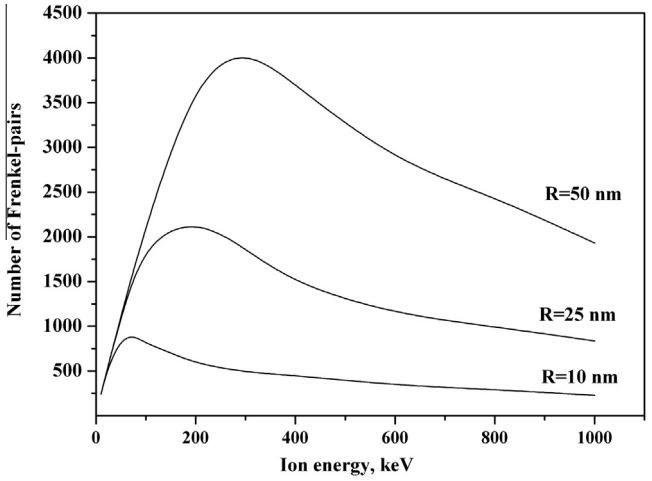

Fig. 1. The dependence of Frenkel-pairs number (N) per ion generated in iron spherical nanoparticles with different sizes on the ion energy.

$$P_1 = P_0^{(1)}\varphi_1(r,t), \tag{4}$$

where $\varphi_1(r,t)$ is an expression for space–time elastic perturbation, and Σ is the interaction cross section, which can be determined using the following equation [19]:

$$\Sigma = \left[\frac{2(1+\nu)V_{dil}G}{3(1-\nu)\pi^2 B}\ln\left(\frac{R_d}{r_d}\right)\right]^2\sum_i k_i^4, \tag{5}$$

where ν is the Poisson coefficient, V_{dil} is the dilatation volume, G is the shear modulus, B is the compression modulus, R_d is the radius of the region deformed by the interstitial atom, r_d is the radius of the interstitial atom, and k_i is the wave vector of the spectral elastic perturbation component.

Another way of the elastic perturbation formation is associated with heat spike which is originated from the displacement cascade. In this case, the force F_2 acting on a defect is described by the similar expression $P_2\Sigma$. The pressure P_2 is, in turn, defined as $P_0^{(2)}\varphi_2(r,t)$. The initial perturbation P_0 does not affect the view of the function $\varphi(r,t)$ (this is abrupt dilatation of the lattice during 10^{-12} s in the vicinity of the heat spike in the both cases); therefore, we can set $\varphi_1(r,t) = \varphi_2(r,t)$.

Taking into account a soliton shape of the elastic perturbation, the function $\varphi(r,t)$ can be expressed as follows [20]:

$$\varphi(r,t) = \frac{u_0}{\delta}\frac{r_c}{r}\frac{1}{\cosh^2[(r - v_w t)/\delta]}, \tag{6}$$

where u_0 is the initial displacement of atoms from equilibrium positions under the elastic perturbation, r_c is the radius of the displacement cascade, v_w is the velocity of the elastic perturbation propagation, and δ is the width of the elastic front. The radius of the displacement cascade can be estimated as a standard deviation of the distribution function for phonons quantity

The estimation of the value of $P_0^{(2)}$ in the thermal spike can be made using the following equation [21]:

$$P_0^{(2)} = \frac{4}{3}\frac{(1+\nu)}{(1-\nu)}G\varepsilon, \tag{7}$$

where ε is the relative deformation in the spike-matrix interface due to differences of temperatures.