Computer Simulation of Self-Organization Processes Leading to Nanostructure Formation in Nonlinear Crystal Media

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Abstract – The present paper is aimed at studying nonlinear effects in solids induced by the interaction of low-energy ions with the surface of crystal lattices as well as self-organization processes that cause nanostructural evolution in nonlinear crystal media. The computer simulation was used to investigate the interaction between low-energy ions and nonlinear crystal lattices. Energy transmitted to target atoms was less than the threshold needed to form point defects but sufficient for nonlinear oscillation excitation in ion subsystem of a lattice. A molecular dynamics method was applied for calculating the evolution of atom ensembles in lattices of different dimensions using the equations of classical dynamics. We have showed that nonlinear oscillations become excited in the atomic chains of crystal lattices after low-energy ions irradiation and as a result of them the whole atoms become stabilized in new positions, which results in the formation and development of new metastable but long-lived atomic groups (nanoclusters).

1. Introduction

Effective increase in operating characteristics and functional complexity of constructional materials is possible on the basis of the formation of nanodimensional complexes and clusters in materials as well as nanosurface layers. Developing nanotechnologies, especially in the field of new materials designing, it is important to take into consideration that many problems may be solved on the basis of well studied and widely used methods of modification of solid structures by charged accelerated beams [1–3]. In [4–7], it was shown that a decrease in ion energy up to 1–3 keV leads to a great increase in the depth of modified layer of the irradiated materials. In fact, related to long-range effect bulk modification occurs [8]. It should be noticed that this modification is strongly observed after low-energy ion irradiation in glow-discharge plasma.

These effects become one of underlying reasons for self-organization of irradiated materials that results in their deep modification, often unexplained in the course of classic solid-state physics. Bombardment of solid surfaces by low-energy ions leads to nonlinear oscillations of atom oscillators of crystal lattices. As a result, new metastable and long-lived structures form and nanodimensional structures deserve more attention among of them [9].

The main aims of this paper are the following:

– to investigate the nanocluster formation by the development of self-organization processes in solids caused by low-energy ion irradiation in glow-discharge plasma;

– to show the difference between the impact of directed low-energy ion irradiation and low-energy ion irradiation in glow-discharge plasma.

2. Model of calculation

In the present paper, using computer simulation the possibility of nanostructure formation in metals exposed by low-energy ion irradiation in glow discharge plasma is shown and self-organizing processes caused by this interaction have been studied.

Figure 1 shows the scheme of interaction between a falling ion and crystal thin film. Fig. 1, *a* shows the diagram of external disturbances as the result of interaction between accidental "ions rain" (plasma) and the surface of the thin film (target atoms were given random impulses from falling ions and they displaced along *X*-, *Y*-, *Z*-axes).

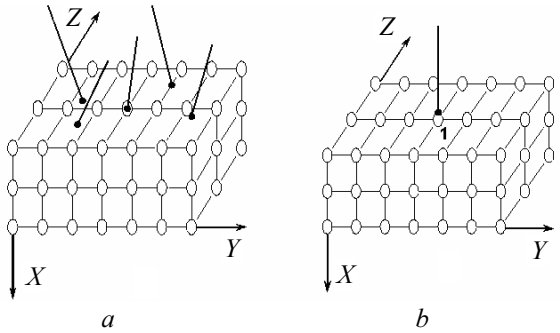


Fig. 1. Scheme of interaction between a falling ion and crystal thin films: *a* – random "ions rain"; *b* – single ion impact

Figure 1, *b* illustrates the initial condition when an arbitrary atom on the surface (N_1) was given $m(dx/dt)$ impulse from a falling low–energy ion.

For the convenience, we shall refer to the ions in crystal lattices as "atoms" or "atomic oscillators". In the computer simulation energy transmitted to target atoms is less than the threshold needed to form point defects but sufficient for nonlinear oscillation excitation in ion subsystem of a lattice.

Self-organization processes have been studied using computer simulation of nonlinear oscillations of atomic oscillators in crystal lattices after their low-energy irradiation. We have chosen Morse potential for metals as the potential of atomic interaction:

$$U(r) = J\left\langle \exp\left[-2\alpha\left(r-r_0\right)\right] - 2\exp\left[-\alpha\left(r-r_0\right)\right]\right\rangle, \quad (1)$$

where J and α are the parameters of the dissociation energy of a couple of atoms and the degree of the potential unharmonicity, respectively; $\Delta r = (r - r_0)$ is the displacement from the equilibrium position. Expanding potential (1) in a Taylor series and taking advantage of the well-known relationship, we obtain:

$$F = -\frac{dU(r)}{dr} = -K\Delta r + A\Delta r^2 - $$

$$-B\Delta r^3 + C\Delta r^4 - D\Delta r^5, \quad (2)$$

$$K = 2\alpha^2 J\ ,\ A = 3\alpha^3 J\ ,\ B = 2.3\alpha^4 J\ ,$$

$$C = 1.25\alpha^5 J\ ,\ D = 1.1\alpha^6 J\ ,$$

where K, A, B, C, and D are the coefficients of elasticity, quadratic and cubic nonlinearity, and nonlinearity of the fourth and fifth orders, respectively.

Within the investigation a special model for calculating the atom displacement of the crystal lattice under the influence of external low-energy ion irradiation was developed. It was based on the conception of three-dimensional lattice as a nonlinear atom chain system. The accuracy of this model and the results of calculations were checked during extracting from three-dimensional lattice one atom chain which can be described by the equations given in [9] and in which errors in calculations were minimal.

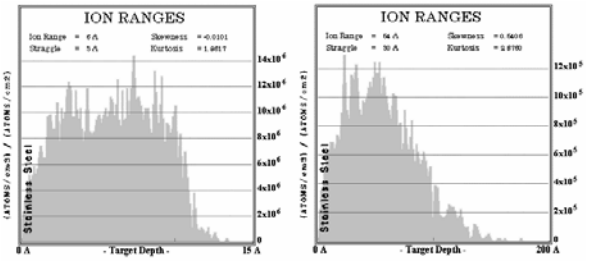
A molecular dynamics method has been applied for calculating the evolution of atom ensembles in lattices of different dimensions using the equations of classical dynamics. The dependence of each atom displacement on the time passed after stopping the ion bombardment was investigated.

Dimensions of the model crystal, boundary conditions, energy transmitted from falling ion, time of irradiation, impact frequency in the case of "ion rain", as well as nonlinear coefficients determining multi-valleys of the potential varied in this computer simulation.

Simulation of ion interaction with crystalline solids was also carried out using TRIM/SRIM 2006 programs. The scheme of interaction shown in Fig. 1, *a* was used for simulation of plasma impact. Ions fell on the target surface at different angles and had different energy not exceeding 3 keV. Interaction of nitrogen ions with stainless steel was simulated. Similar simulation was carried out for the case of ion interaction with 3 keV energy directed perpendicular to the surface (Fig. 1, *b*). Irradiation dose was the same for both cases. Plasma irradiation and ion beam impact on crystalline solids were compared.

3. Results and discussion

Figure 2 shows the distributions of nitrogen ions embedded in the stainless steel target in case of plasma irradiation (ion energy randomized and did not exceed 3 keV) and 3 keV ion beam. Data were obtained using TRIM/SRIM 2006 programs.



a *b*

Fig. 2. Distribution of nitrogen ions into stainless steel: *a* – plasma irradiation (ion energy randomized and did not exceed 3 keV); *b* – 3 keV ion beam

One can see in Fig. 2, *a* that the depth of nitrogen ion penetration in case of plasma treatment does not exceed 15 Å.

In case of ion beam (Fig. 2, *b*) the depth of ion penetration is up to 200 Å and ion ranges are more considerable in comparison with plasma treatment. Maximum concentration of nitrogen in case of plasma treatment is equal to $4 \cdot 10^{24}$ atom/cm^3 at the depth of ~8 Å from the irradiated surface. In case of nitrogen ion beam maximum concentration is by an order less and equal to $4 \cdot 10^{23}$ atom/cm^3 at the depth of ~60 Å from the irradiated surface. Thus, in case of plasma treatment maximum concentration of nitrogen accumulates in thinner layer in comparison with ion beam treatment.

Using details calculation when all collisional damage to the target is analyzed, it was shown that in case of plasma treatment incident ions spend 64% their energy (max 1.9 keV) for atomic vibrations in a crystal and recoil atoms – 18% of their energy (max 0.5 keV). In case of ion beam treatment, incident ions spend 6% of their energy (180 eV) for atomic vibrations in a crystal and recoil atoms – 57% of their energy (1.71 keV).

Thus, in case of plasma treatment incident ions are more important for the process of atom oscillations in a crystal.

TRIM/SRIM programs study elastic collisions, which do not describe real interaction of ions with a solid; therefore, it is necessary to take into consideration nonlinearity of materials under bombardment. In this work, we have used computer simulation based on nonlinearity of materials.

We have shown that in the system of coupled oscillators nonlinear oscillations are excited. Energy transmitted to target atoms is less than the threshold needed to form point defects but sufficient for nonlinear oscillation excitation in ion subsystem of a lattice

(for the convenience we shall refer to the ions in crystal lattices as “atoms” or “atomic oscillators”).

The process of the propagation of nonlinear oscillations embraces the whole nonlinear atom chain. The calculation showed that the time of stabilization is almost by 3–4 orders higher than that of ordinary atom relaxation. Stabilization should be understood as nonlinear processes stop and transition of all nonlinear atom oscillators to stable condition.

Figure 3 illustrates the dependence of atom displacement along the X-axis on the time elapsed after stopping the external influence from incident ion (interaction takes place as in Fig. 1, *b*). The calculation is made for homogeneous nonlinear atom chain consisting of 50 atoms.

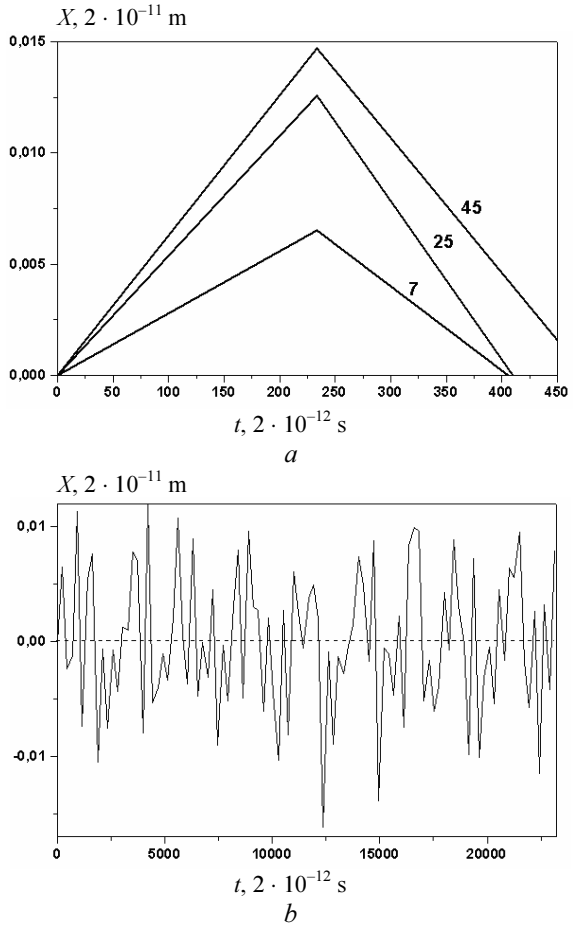


Fig. 3. The displacement of atoms N7, 25 and 45 at energy more critical one: *a* – atom displacement at initial time; *b* – oscillations of atom N7 for long observation period

Figure 3, *a* shows initial displacement of atoms N7, 25 and 45 from equilibrium positions. Fig. 3, *b* represents the displacement of atom N7 within long period of time considerably exceeding the time of standard atom relaxations. This condition can be described as long-lived oscillating one.

The main criterion of self-organizing processes taking place in crystal lattices is the presence of critical energy transferring from incident ions to atom oscillators. As a result of collective nonlinear oscillations, all atom oscillators of the crystal lattice displace very far from the initial equilibrium position at the time considerably exceeding the time of standard atom relaxations of metastable long-living structures in the former target ordered structure.

We have shown that an increase of damping coefficient in 2 times leads to the fact that all atoms become stabilized in new positions, which results in the formation and development of new metastable atomic groups (nanoclusters).

Figure 4 shows that the period of the lattice inside the clusters does not correspond to the initial one; some clusters are separated with areas having negative atom density (for example, N1 and N2, N3–5 and N7–21 atoms). It is clusters that provide new complexes of physical and mechanical properties for lattices (irradiated materials).

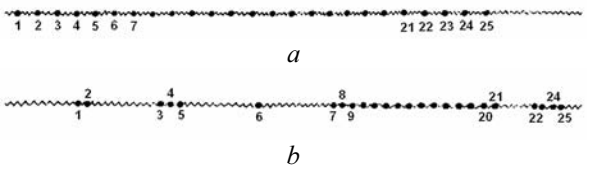


Fig. 4. One-dimensional lattice: *a* – initial state; *b* – new stable state

The time of stabilization is very long. It specifically depends on rigidity of atomic bindings in lattices (nonlinear coefficients are based on them) and on the value of ion energy of external irradiation. For absolute interpretation, it is desirable to take into consideration that the initial potential of the lattice is also constantly “deformable”, i.e., new long-lived structures do not correspond to the “old” potential, therefore new lattice “periods” appear inside clusters.

It should be noticed the following peculiarities of self-organization processes development in case of “ion rain” (interaction takes place as in Fig. 1, *a*) in comparison with ion beam treatment:

1) less critical energy is required for self-organization processes development,

2) time of transition to stable state of lattice decreases considerably,

3) three dimensional nanoclusters form,

4) formed nanoclusters as a rule are long-lived pulsating elements of crystal lattice.

These peculiarities are shown in Fig. 5.

Figure 5, *a* shows that oscillations become earlier than in case of ion beam treatment (Fig. 3, *a*). Figs. 5, *b* and *c* represent displacement of atom N7 on *YX* and *ZX* planes correspondingly. It is seen that oscillations take place on three planes.

After stabilization, all atoms will be in new stable positions forming three-dimensional clusters as it was observed experimentally in [10]. That is achieved by a fast transition: chaos of incident ions → local chaos in the former ordered structure → the formation of

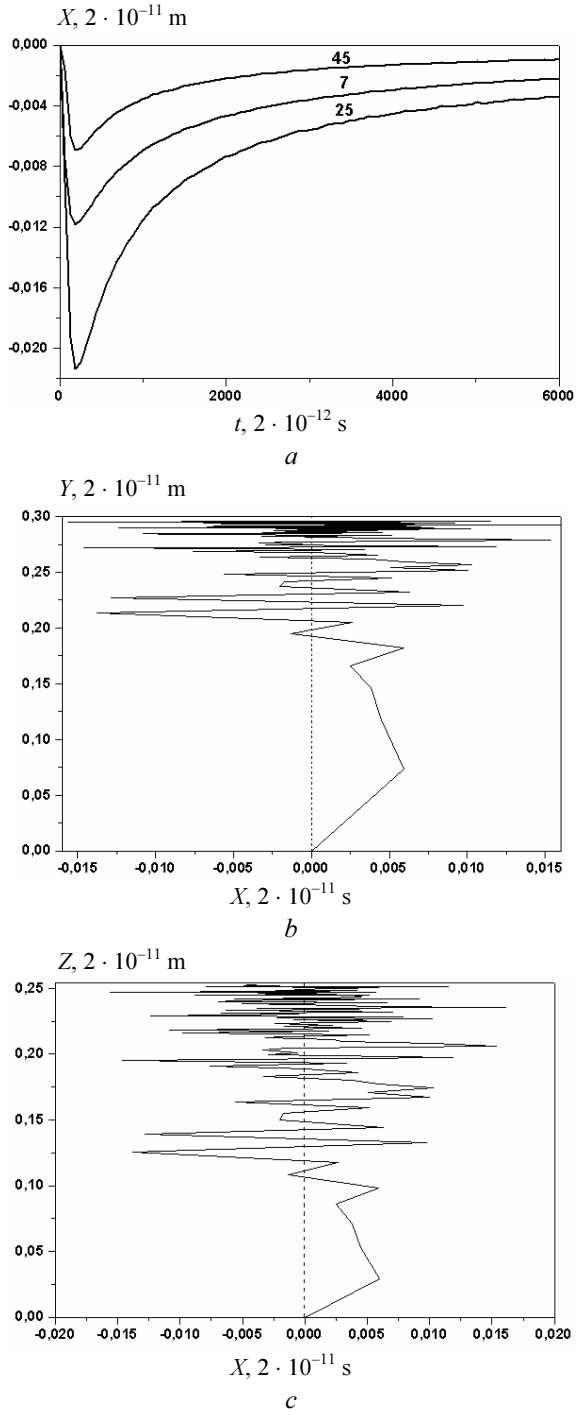


Fig. 5. The displacement of atoms N 7, 25 and 45 in case of plasma treatment: *a* – displacement of atoms at initial time; *b* – displacement of atom N7 on the *YX* plane; *c* – displacement of atom N7 on ZX plane

new metastable long-lived structures in the former ordered structure of the target. In this case, nanocluster becomes active zone that determines further self-organizing processes.

4. Conclusions

1. Computer simulation (using a molecular dynamics method) of nonlinear oscillations in atom oscillator systems of crystal lattices after their low-energy ion irradiation showed the possibility of nanostructures formation and their stability.

2. It was shown that in homogeneous atom chains critical energy needed for self-organizing processes development after plasma irradiation is less than for nonlinear atom chain after ion beam treatment.

3. Low-energy ion irradiation in glow-discharge plasma may be used to develop new hardening technologies of metals and alloys on the basis of the formation of nanoelements in them.

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