SELF-ORGANIZATION PROCESSES AND NANOCLUSTER FORMATION IN CRYSTAL LATTICES BY LOW-ENERGY ION IRRADIATION

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The goal of this paper is to study self-organization processes that cause nanostructural evolution in nonlinear crystal media. The subjects of the investigation were nonlinear homogeneous and heterogeneous atom chains. The method of computer simulation was used to investigate the interaction between low-energy ions and crystal lattices. It was based on the conception of three-dimensional lattice as a nonlinear atom chain system. We showed that that in homogeneous atom chains critical energy needed for self-organization processes development is less than for nonlinear atom chain with already embedded clusters. The possibility of nanostructure formation was studied by a molecular dynamics method of nonlinear oscillations in atomic oscillator systems of crystal lattices after their low-energy ion irradiation.

Introduction

Investigations of nanodimensional systems are most dynamically developing field in the modern physics. 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 papers [4-7] it was shown that nonlinear effects take place during interaction between charged particles and irradiated surface of crystal materials. 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. This modification is strongly observed after low-energy ion irradiation in glow-discharge plasma. A decrease in ion energy up to 1 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]. 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 self-organization processes development in solids caused by low-energy ion irradiation in glow-discharge plasma;
- to show the influence of low-energy ion irradiation on the nanocluster formation process in crystal atom chains.

Experimental and model calculation

Self-organization processes were studied using computer simulation of nonlinear oscillations of atomic oscillators in crystal lattices after their low-energy irradiation.

We chose Morse potential for armco-Fe as the potential of atomic interaction

$$U(r) = J\left\{\exp\left[-2\alpha(r-r_0)\right] - 2\exp\left[-\alpha(r-r_0)\right]\right\} \quad (1)$$

where J and α are parameters of the dissociation energy of a couple of atoms and the degree of the potential unharmonicity, respectively; $\Delta r = (r - r_0)$ is displacement from the equilibrium position. Expanding the 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, D are coefficients of elasticity, quadratic and cubic nonlinearity and coefficients of 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 [9]. 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 time passed after stopping the ion bombardment was investigated.

The main task is to achieve the excitation of nonlinear oscillations in the system and to observe stabilization process of lattices after ceasing of external irradiation. The amount of the energy transferred from the impinging ion to the crystal atom is determined by classic equations given in [10]. Moreover, the initial energy must be less than the energy needed to form point defects in crystals. It is important that the atom chain should not be broken as a condition for excitation of nonlinear oscillations in the chain.

For experimental investigations samples were exposed to the irradiation by ions of residual gases of vacuum (nitrogen, oxygen, hydrogen, etc.). The

ion energy depended on the voltage in the plasmatron and did not exceed 0.8-2.5 keV. Irradiated dose was $2 \cdot 10^{17}$ ion·cm^{-2}. The temperature in the chamber was controlled during the irradiation process and did not exceed 343 K.

The fine structures of materials were studied layer-by-layer using the transmission electron microscopy method [4,9]. The dependences of microhardness and electro resistance on time passed after stopping the irradiation were investigated.

Results and discussion

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

Figure 1 shows the scheme of interaction between a falling ion and crystal lattice. Figure 1a 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). Figure 1b illustrates the initial condition when an arbitrary atom on the surface (N1) was given $m\frac{dx}{dt}$ impulse from a falling low–energy ion. For the convenience we shall refer to the ions in crystal lattices as "atoms" or "atomic oscillators".

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.

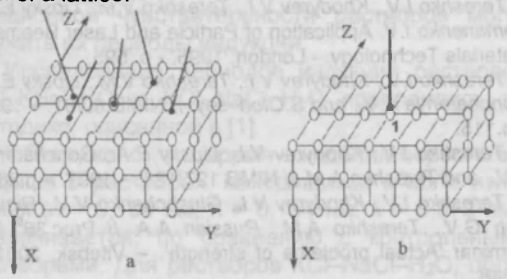


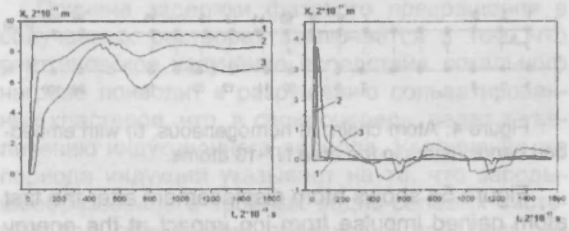
Figure 1. Scheme of interaction between a falling ion and crystal lattice a) random "ions rain", b) single ion impact.

We showed that in the system of coupled oscillators nonlinear oscillations are excited. 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. It specifically depends on rigidity of atomic bonding in lattices (nonlinear coefficients are based on them) and on the value of ion energy of external irradiation. Stabilization should be understood as nonlinear oscillation processes discontinuance and transition of all nonlinear atom oscillators to a stable condition.

Figure 2 illustrates the dependence of atom displacement along the X-axis on the time elapsed after stopping the external influence. The interaction takes place as in figure 1b. The calculation is made for homogeneous nonlinear atom chain consisting of 100 atoms. The main criterion of self-organization processes taking place in crystal lattices is the presence of critical energy transferring from an external falling ion to atom oscillators. Figure 2a shows the displacement of atoms N 1, 25 and 50 at energy more critical one.

It is seen that atoms mentioned above which initially received a small displacement by the external low-energy influence, as a result of collective nonlinear oscillations of all atom oscillators of the crystal lattice displaces very far from the initial equilibrium position. Our calculation experience allows us to conclude that it will never return to its initial state and it is an element of new structures in crystal (probably with nanodimentions). Figure2a underscores that the time elapsed after stopping the irradiation of crystal is by three orders higher than that of ordinary relaxation but the lattice has not been stabilized yet.

Figure 2b represents atom displacement of the same nonlinear atom chain at excitation energy less than critical one. In this case atoms return to the equilibrium position and nonlinear oscillation process takes place near initial positions of the atoms.



a) b)

Figure 2. Dependence of atom displacement (1- atom N1, 2 - atom N25, 3 - atom N50) along the X-axis on the time elapsed after stopping the external influence: a – at the energy more than critical one; b – at the energy less than critical one.

Figure 3 illustrates the results of a numerical experiment in the investigation of a relaxation process in one-dimensional nonlinear atomic chain consisting of 100 atoms in the case that its first atom receives an impulse from an external ion impact at the energy more than critical one.

Nonlinear oscillations become excited in the chain along the X axis and as a result of them the whole atoms become stabilized in new positions, which results in the formation and development of new metastable atomic groups (nanoclusters). The calculation for figure 3 was made at increase of damping coefficient in 2 times in comparison with the data presented in figure 2 and by using the scheme shown in figure 1b.

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, N10 and N11, N93 and N94 atoms). It is clusters that provide new complexes of physical and mechanical properties for lattices (irradiated materials).

We also focused our attention on initial processes In nonlinear atom chains after the first atom gained impulse from ion impact. The calculation was also made for nonlinear atom chain with already embedded cluster in the area of N7-13 atoms (figure 4) that was exposed to the low-energy ion irradiation. Figure

5a, b illustrates the displacement of atoms N1, 10 and 50 of the chain with already embedded cluster.

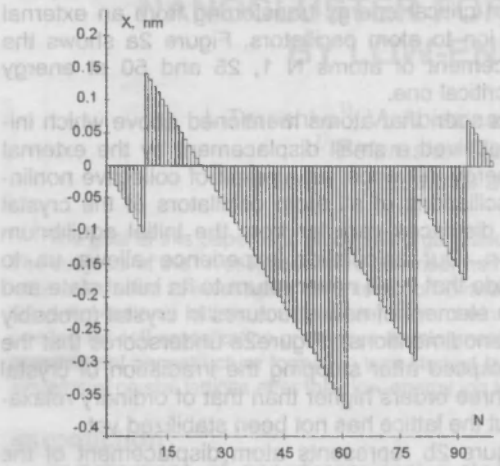


Figure 3. Displacement of 100 atoms of the excited nonlinear atomic chain along the X axis at the time of stabilization. Y-axis represents atom displacement, X-axis shows atom number in the nonlinear chain.

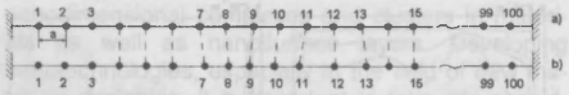


Figure 4. Atom chain: a) homogeneous, b) with embedded nanoclusters in the area N7-13 atoms.

Figure 5a shows atom displacement after the first atom gained impulse from ion impact at the energy equals critical one for homogeneous chain (as used for figure 2a).

It is seen that in this case atoms stabilize in initial positions that corresponds to the increase in critical energy in nonlinear atom chains in comparison with homogeneous ones. Figure 5b shows the displacement of atoms N1, 10 and 50 in case when atom N10 (inside the cluster) is exposed to single ion impact from external ions at the energy more critical one (scheme of irradiation mentioned in figure 1a). It is seen that atom N1 (out of the cluster) stabilizes in initial position and atoms N10 and 50 – in new ones. In this case nanocluster becomes active zone determining further self-organization processes.

The transmission electron microscopic results confirm the nanocluster formation process in armco-iron [11]. Changes in mechanical and electrical properties of metals after their low-energy ion irradiation in glow-discharge plasma are presented in [6, 7].

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 their nanocluster evolution.

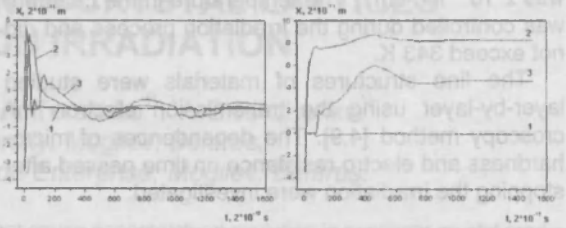


Figure 5. Dependence of atom displacement (1- atom N1, 2 - atom N10, 3 - atom N50) along the X-axis on the time elapsed after stopping the external influence: a – at the energy equals critical one for homogeneous chain; b –when atom N10 is exposed to single ion impact at the energy more critical one for homogeneous nonlinear atom chain.

2) It was shown that in nonlinear homogeneous atom chains critical energy needed for self-organization processes development is less than for nonlinear atom chain with already embedded clusters.

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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