Features of plastic deformation nucleation in the elastically loaded aluminium crystallites during irradiation

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Abstract. The simulation of peculiarities of the surface layer reconstruction in the crystallites of aluminium after the ion bombardment and the copper film irradiated by the electron beam is carried out. The performed calculations are based on the molecular dynamics method. It is shown that the orientation of the irradiated surface and preliminary elastic deformation have a significant impact on features of atomic structure formation in the ion-modified layer in aluminium. Weak structural changes in the surface layer are observed at the irradiation of the \{100\} surfaces. Sufficiently great number of stacking faults is formed under irradiation of the \{111\} and \{110\} surfaces. It is shown that heating by the electron beam of the \{110\} surface in the copper film leads to the formation of stacking faults. It is shown that the preliminary elastic deformation of the material lowers the energy of the irradiation, at which formation of structural defects and fragmentation of crystallites of aluminum and copper will take place.

1.Introduction

Surface treatment by ion and electron fluxes can significantly increase the strength, durability and corrosion resistance of metallic materials, increase their biological compatibility [1-3]. Change of physical-mechanical properties under irradiation is determined by the development of a number of processes. Doping the surface region of the material with chemical elements from the ion beam is performed during ion irradiation. Ion-beam and electronic processing significantly alter the defect system and can lead to fragmentation of the microstructure of the irradiated surface. In this case, the thickness of the fragmented layer essentially depends on the power density, the impact duration and the degree of preliminary elastic deformation of the material. So, the thickness of the fragmented layer can reach several tens of microns under irradiation of the material by energetic ion beams of high energy (>3 MeV). In the case of using ion beams with the energy less than 1 MeV the thickness of the fragmented layer is reduced to a few microns. The thickness of the modified layer (the layer with the changed defect structure) may exceed hundreds of microns. At small values of the ion beam energy due to the effect of the long-range the thickness of the modified surface layer can significantly exceed not only the depth of the mean free path of incident ions, but the average grain size. For the fragmentation of polycrystalline materials under irradiation, in the case of plastic deformation, the occurrence of high elastic stresses which are localized at the grain boundaries and their junctions is necessary [4,5]. It is known that strong elastic fields localized in the surface region are formed upon irradiation of metals and alloys by high energy fluxes of charged particles (ions and electrons). The process of a fragmentation may lead to the formation of the new nonequilibrium micro- and nanoscale
structures in the surface layers of irradiated metals and alloys. Several competing mechanisms for relaxation of the material which are associated with the phase and structural transformations, fragmentation, plastic deformation in the subsurface of the material take place under ion fluxes action [6-9]. Obtaining reliable experimental information about the structural response of the material under irradiation is connected with significant difficulties, due to the small temporal and spatial scales. An effective approach to overcome these difficulties and to obtain detailed information about dynamics of change of the microstructure during irradiation of a material is a computer simulation [10-12].

In this work, the atomic structure changes of the surface layers of aluminum crystallites after bombardment by low-energy particles were studied. Also the influence of the irradiated surface orientation on the peculiarities of the atomic structure formation in the ion-modified layer was revealed. The characteristics of structural changes in a thin film of copper irradiated by the electron beam were also studied in this work.

Formulated problems were solved on the basis of the molecular dynamics method. The simulation was performed using the software package LAMMPS [13]. Interatomic interaction potential for aluminum was described in the framework of the embedded atom method [14]. Crystallite sizes ranged from 75 000 to 1 000 000 atoms. Initial temperature of the crystallites was 300 K. Irradiated surfaces had crystallographic indices \{100\}, \{110\} and \{111\}. Aluminum atoms were used as the incident particles. The velocity of incident atoms was directed normal to the free surface. Its value was equal to 210 Å/ps, which corresponds approximately to 60 eV. The number of incident atoms was 540 (Fig. 1 a). Simulation of structural changes in the surface layers at irradiation was carried out for mechanically unloaded and elastically uniaxially pre-streched in [110] direction crystallites.

A simulated copper film had a form of parallelepiped with a size of 8x8x20 nm. Free boundary conditions were applied in the direction normal to the smallest cross-section, and periodic boundary conditions were set in the other directions. The power density of the electron beam was \( \sim 0.03 \text{ eV/(atom*nsec)} \).

2. Computational results and discussion

The calculations have shown that as in the case of mechanical loading [15] the orientation of the irradiated surface has a significant effect on the characteristics of structural changes in the surface layer of aluminum crystallite. So, the \{100\} surfaces were the most resistant to structural rearrangements upon irradiation. A local change of atomic environment symmetry took place only for the individual atoms of the \{100\} surface layers, which were involved in the atomic displacement cascades (Fig. 1 b). However, such rearrangements of atomic configurations did not lead to the formation of structural defects (dislocations, stacking faults, interstitial dumbbells, etc.). Note that pre-elastic deformation of the samples prior to irradiation had no significant effect on the character of the structural changes in the surface layer. In the case of the \{111\} surface irradiation the intrinsic and extrinsic stacking faults were formed in the surface region in the (111) planes even in the undeformed crystallites.

Preliminary deformation led to the formation of stacking faults in adjacent directions (Fig. 1). At the irradiation of the \{110\} surface there were atoms with changed symmetry of their atomic environment, some of which restored the symmetry of local environment, and the other part formed the stacking faults (Fig. 2 a). The size of the defects grows with the increase of the specimen elastic pre-streching. Stacking faults were formed in adjacent planes and interacted with each other forming vacancy chains (Fig. 2 b, c). This process slowed down the accumulation of defects. Fig. 3a, b clearly shows how the structural response of the irradiated crystallite changed with increasing degree of the sample elastic pre-streching from 4 to 5%.

The simulation results showed that irradiation of the crystallites was accompanied by intensive sputtering of atoms and atomic clusters away from the irradiated surface. The total number of sputtered atoms exceeded the number of implanted atoms. Note that under the same irradiation conditions the process of sputtering was the most active for the \{111\} surface.
Figure 1. The initial structure of the simulated system (irradiated sample and incident atoms) (a). Structure of the samples deformed to 4\% after irradiation of \{100\} (b) and \{111\} (c) surfaces. The blue color indicates incident atoms; atoms with fcc, hcp and uncertain symmetry of local environment are marked in green, red and grey, respectively. Atoms with fcc symmetry of local environment are not shown in Fig. (b) and (c).

Figure 2. Structure of the simulated samples after irradiation of the \{110\} surface. Pre-stretching: a) 0\%; b) 4\%; c) 5\%. Red and grey colors indicate atoms with hcp and uncertain symmetry of local environment, respectively. The atoms with fcc symmetry of local environment are not shown.

Figure 3. Projection of defect structure of the sample with irradiated \{110\} surface on (110) plane. Pre-stretching: a) 4\%; b) 5\%.

Kinetic temperature calculation showed that for the given irradiation intensity the surface layer may be heated to a temperature above the melting point. Kinetic temperature versus time for the \{110\} surface layer with thickness of 8.5 lattice parameters is shown in Fig. 4. After irradiation the temperature of the surface layer quickly decreased due to the applied thermostat and was characterized
by well-pronounced oscillations. The nature of the temperature oscillations in the surface layer as well as the sputtering of atoms and atomic clusters from the irradiated surface is associated with the generation of shock waves caused by rapid heating of the surface layer [12]. The frequency of the oscillations well correlates with the time of the passage of shock waves of the distance from the loaded face to the back surface (from which they are reflected) and backwards.

![Figure 4](image)

**Figure 4.** The temperature versus time for the \( \{110\} \) surface layer of the sample pre-stretched to 4%.

The simulation results of the electron beam impact on the copper film show that up to the melting point the heating rate was proportional to the density of the heat source power. The spatial distribution of temperature was homogeneous in the sample. Further heating of the material leads to a change in the spatial distribution of temperature in the sample. This is due to the fact that the liquid phase starts to nucleate in the region of the free surfaces. The analysis of the change of the phase state of the film allows allocating two regions: the region with the crystalline state and the region with the liquid phase separated by interphase boundary, consisting of 4-6 atomic planes. The local environment of individual atoms changes its fcc symmetry on the hcp one at the process of heating of the film with the \( \{110\} \) free surface. As a result stacking faults are formed in the film. The material structure after such local transformation is shown in Fig.5.

![Figure 5](image)

**Figure 5.** Relaxed structure of copper film after the impact by an electron beam. Red color corresponds to stacking faults, grey – atoms with undefined symmetry of the local environment. Atoms with local fcc symmetry are not shown.
3. Conclusion
The simulation results showed that the formation of defects during ion irradiation of crystalline aluminium and electronic heating of a copper crystalline film largely depends on the crystallographic orientation of the irradiated surface. It was revealed that the \{100\} surfaces are the most resistant to structural changes. A large number of stacking faults are formed at the irradiation of the \{111\} and \{110\} surfaces. The increase in the energy of the incident beams and the preliminary elastic deformation can lead to fragmentation of the surface layers of irradiated materials. The grains in the surface layer having the above mentioned crystallographic orientation to the direction of irradiation and excess elastic stress will be subjected to fragmentation.

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