XIV International Conference on Computational Plasticity. Fundamentals and Applications
COMPLAS 2017
E. Oñate, D.R.J. Owen, D. Peric and M. Chiumenti (Eds)

COMPUTER SIMULATION OF SURFACE MODIFICATION OF AL CRYSTALLITE UNDER HIGH ENERGY TREATMENT

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Key words: Ion implantation, Surfaces, Molecular dynamics, Structural defects, Grain Boundaries.

Abstract. The simulation of structural changes in the surface region of Al crystallite during self-ion bombardment was carried out. The calculations were performed on the base of the molecular dynamics method. A many-body potential calculated in the approximation of the embedded atom method was used to describe the interatomic interactions. It is shown that atomic displacement cascades in the near-surface region were generated under ion irradiation. At relatively low energies the impact of the atomic displacement cascades not only lead to the generation of Frenkel pairs, but also to the nucleation of plastic deformation. That is due to the high-rate heating of the grains, causing their expansion and deformation in the stained conditions with the formation of stacking faults. Melting of surface layers takes place at high energies of irradiation. A crystallization process and a formation of a grain structure of the surface layers will be determined by the characteristics of the propagation of the crystallization front, which shape depends on the relative location, size and orientation of grains on the boundary of the liquid and solid phases.

1 INTRODUCTION

Modification of the surface by ion beams is widely used to improve the operating characteristics of metals and alloys [1,2]. The change in physical and mechanical properties is due both to the process of surface alloying of the material by chemical elements from the beam, and to the structural changes of the near-surface layer.

Irradiation by ions can cause not only fragmentation of grains but also lead to melting of the surface layer. The thickness of the modified layer depends on the energy of the ion beam. It may reach to several tens of microns at the irradiation by ion beams with energy of more than 3 MeV. We note that fragmentation takes place in a layer with several micrometers of thickness for beams with energies less than 1 MeV.

In this case, the thickness of the modified layer with the changed defect structure can reach more than 100 μm. Due to the long-range effect, the depth of the modified layer exceeds not only the mean free path of the incident ions, but also the average grain size. The occurrence of high stresses at the boundaries and grain joints causes the fragmentation of the surface layer

upon irradiation [1,3]. Irradiation with high-energy ions leads to the generation of shock waves and strong elastic fields [4-6]. As a result, nonequilibrium micro- and nanostructural layers can form in the near-surface region of metals. Different competing mechanisms connected with phase transitions, structural transformations, plastic deformation, fragmentation in the near-surface region, lay on the base of the relaxation process of the irradiated material.

Experimental study of the dynamics of such processes may face considerable difficulties in view of the small spatial and temporal scales of their occurrence Modeling of these processes allows to overcome these difficulties and to obtain detailed information on the dynamics of structural changes during irradiation and relaxation of the material [7-9]

In this paper, we investigate the features of structural transformations in the surface layer both in single crystals with different orientations of the irradiated surface and in nanocrystalline aluminum samples under ion irradiation.

2 METHODS

The method of molecular dynamics [10,11] was used to solve the problem posed in this paper. The simulation was carried out in the software package LAMMPS [12]. The potential of the interatomic interaction for aluminum was described in the framework of the embedded atom method [13]. The simulated samples contained from 75 000 to 1 000 000 atoms. The initial temperature of the samples was set equal to 300 K. The mono- and nanocrystalline samples of aluminum were subjected to irradiation. The {100}, {110} and {111} surfaces were irradiated in the case of single-crystal samples. The nanocrystalline samples consisted of 6 and 10 grains with an average size of 7.5 and 6.5 nm, respectively. Ion irradiation was simulated by the bombardment of aluminum atoms on a free surface. In the case of a single crystal, the energy of incident atoms on the free surface was 60 eV. Total number of incident atoms was 540. Both mechanically unloaded crystallites and elastically deformed samples were irradiated. In the case of nanocrystalline samples, the number of incident atoms varied from 16 to 80. The energy of each atom was 1.5 keV. Analysis of structural changes in irradiated samples was based on the Common Neighbor Analysis [14] and the Dislocation Extraction Algorithm [15]. Visualization of investigated structures was performed in the OVITO software [16].

3 SIMULATION RESULTS

Calculations showed that ion irradiation with the above energies leads to sputtering of individual atoms and atomic clusters from the irradiated surfaces of the crystallite. Under this irradiation regime, the number of implanted atoms was less than the number of atoms sputtering from the surface. It was found that the process of atom sputtering occurred most intensively at exposing of the {111} surface.

During the irradiation, the temperature of the near-surface layer of the crystallite exceeded the melting point. Temperature dependency on time for the layer with a thickness of 10 lattice parameters near the {111} surface is shown in Fig. 1. After irradiation, the temperature of this layer decreases quite rapidly and is characterized by pronounced oscillations. We note that irradiation of the surface leads to the generation of shock waves in the crystallite. Due to this fact the periodicity of the temperature oscillations correlates well with the time of passage of

the shock waves from the loaded surface to the rear one and back.

Crystallites with the {100} irradiated surfaces are the most stable to structural changes in the near-surface layers. In this case, only a small number of surface layers involved in cascades of atomic displacements locally change the symmetry of the nearest environment (Fig. 2a). It was noted that dislocations, stacking faults, interstitial dumbbells are not formed in crystallites. The elastic deformation of the investigated crystallites before irradiation had little effect on the structural changes in the surface layer.

When the {111} surfaces of the undeformed crystallite are irradiated, the stacking faults are formed in the near-surface region in the (111) planes. If the crystallite is pre-deformed, the stacking faults are also generated in adjacent planes (Fig. 1b). In the case of irradiation of the {110} surface, the local symmetry of the nearest environment changes for many atoms, which can subsequently lead to the generation of stacking faults (Fig. 3). The sizes of the defects increase with the growth of preliminary elastic deformation of the crystallite. In this case, stacking faults are formed in adjacent planes and vacancy chains can be formed at their intersection (Fig. 3b, c).

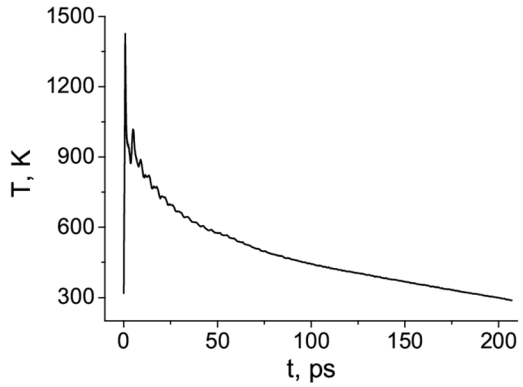

Figure 1: Dependence of the temperature of the surface layer versus time at the irradiation of the {111} surface. Sample was preliminary deformed to 4%

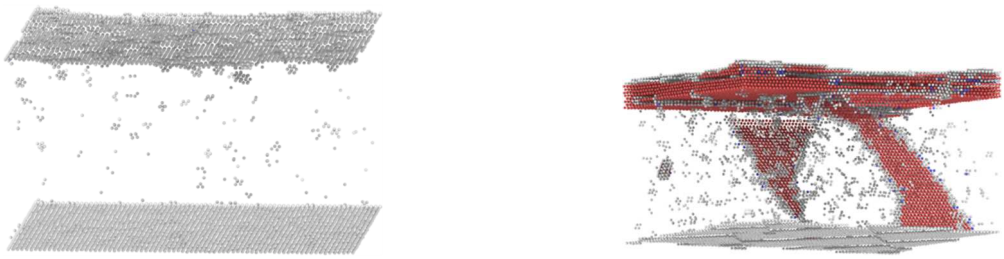

Figure 2: The structure of the samples after irradiation of the {100} (a) and {111} (b) surfaces. Samples were deformed by 4%. Atoms with hcp and an uncertain symmetry of the nearest environment are indicated by pink and gray colors, respectively. Atoms with fcc symmetry of the

nearest environment are invisible

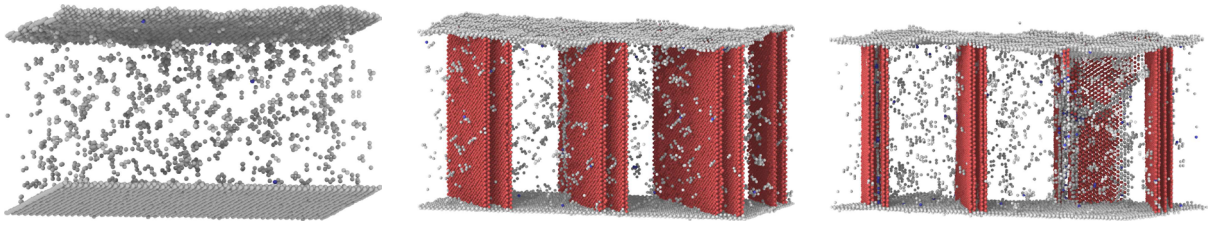

Figure 3: Structure of the crystallite after irradiation of the {110} surface. The value of the preliminary deformation is: a) 0%; b) 4%; c) 5%. Atoms with fcc symmetry of the nearest environment are not shown. Pink and gray spheres are atoms with a hcp and an uncertain symmetry of the nearest environment, respectively

Irradiation dose have a significant effect on the structural changes in a nanocrystalline sample. Small dose of irradiation (16-40 atoms with energy of 1.5 keV) do not change the sizes and positions of grains in the sample. At the irradiation of the nanocrystalline samples stacking faults are generated in grain boundary regions and begin to propagate into the grain interior. This is due to the fact that the incident atoms generate cascades of atomic displacements (Fig. 4a, c). This leads to high-rate local heating of the grains and the formation of shock waves [4,17]. As a result, the interaction of shock waves with grain boundaries causes a local increase in stresses and generation of stacking faults. At the same time, the density of stacking faults in grains increases with increasing number of incident atoms (Fig. 4). The stacking faults locating in parallel slip planes were formed only in few grains at irradiation by 16 atoms (Fig. 4b). When the irradiation dose was increased to 40 atoms with energy of 1.5 keV, the stacking faults are formed in all grains in a larger number. In this case, their slip planes have indices of different signs (Fig. 4d).

If the radiation dose is increased, the surface layer will melt. At the stage of relaxation, the crystallization front propagates from the boundary of the liquid and crystalline phases. As a result, the formed grain structure in the surface layer differs significantly from the structure before irradiation. Analysis of the calculation results shows that after crystallization, the number of grains in the simulated sample is changed (Fig. 5). This is clearly seen in the histogram, which shows the change in grain size distribution after irradiation of the sample with 80 atoms with energy of 1.5 keV. The grain sizes in the near-surface layer of the sample are increased. This is due to the fact that the atoms of the molten region were adjusted to the grain structure at the crystallization front and increased their size. Note that craters formed on the surface of the irradiated sample, which size increases with increasing radiation dose.

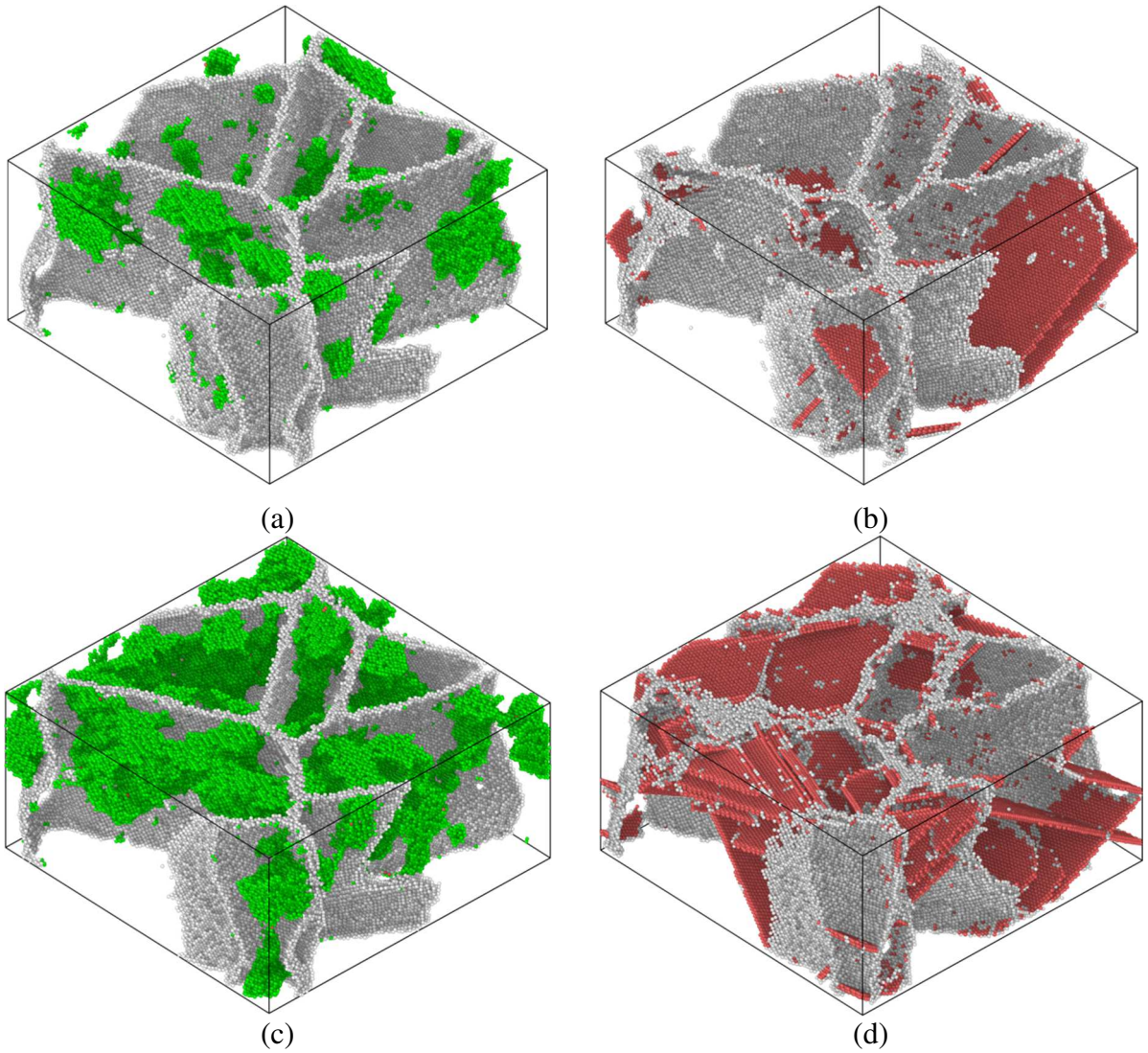

Figure 4: Structure of irradiated sample with 6 grains before (a and c) and after relaxation (b and d). The upper and lower rows of figures refer to the irradiation by 16 and 40 atoms, respectively. The grain boundaries, defects formed by cascades and stacking faults are shown in gray, green and pink, respectively. Atoms with fcc symmetry of the nearest environment are invisible

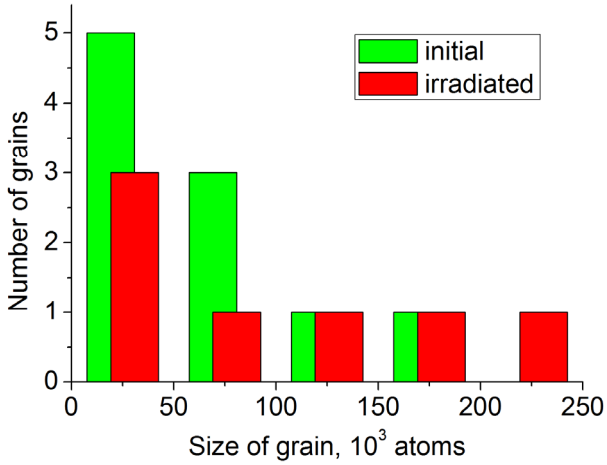

Figure 5: Distribution of grains in size before (green bars) and after irradiation (red bars) of the sample

4 SUMMARY

It is shown that the nature of structural changes in the surface layer of an aluminum single crystal upon irradiation is largely determined by the crystallographic orientation of the irradiated surface. The {100} surfaces undergo the smallest structural changes under irradiation. Irradiation of the {111} and {110} surfaces results in formation a large number of stacking faults in the surface layer. On the basis of this, it can be assumed that an increase in the irradiation dose can cause fragmentation of the surface layer of the crystallite. Irradiation of a nanocrystalline sample with small doses leads to the formation of stacking faults in grains. Their number increases with increasing radiation dose. At higher doses, the surface layer melts. Crystallization of the molten layer increases the grain size in the near-surface region. This is due to the fact that the atoms of the molten layer are adjusted to the crystal structure of grains at the boundary of the liquid and crystalline phases.

ACKNOWLEDGMENTS

The work is supported by the Programme of Presidium of Russian Academy of Sciences No 13 “Thermophysics of high energy densities”.

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