Atomic mechanisms of grain structure restructuring in surface of aluminum during ion implantation

D S Kryzhevich, K P Zolnikov and A V Korchuganov
Institute of Strength Physics and Material Science of the Siberian Branch of the Russian Academy of Sciences, Akademicheskii 2/4, Tomsk 634021, Russia
E-mail: kryzhev@ispms.ru

Abstract. The molecular dynamics study of features of structural rearrangements in the surface layer of the aluminum crystallite under ion irradiation was carried out. It is shown that the number of generated defects in the crystallite depends on the irradiation dose and the crystallographic orientation of the irradiated surface. It is revealed that significantly more defects were formed at the irradiation of \{111\} and \{110\} surfaces than of the \{100\} surface. At low irradiation doses the stacking faults were formed only in some grains of the nanocrystalline material. The higher irradiation doses led to grain structure changes in the surface layer. This is connected with melting and crystallization of the surface layer. The grains in the region of the boundary of liquid and crystal phases were centers of crystallization of the liquid surface layer.

1. Introduction

The irradiation of the surface by ion beams is widely used to improve strength characteristics, the corrosion resistance, the biological compatibility of metals and alloys [1, 2]. The change of physico-mechanical properties under irradiation is connected not only with surface alloying of material by chemical elements from the beam, but also with changes of the grain boundary design of the surface layer. Ion irradiation can lead to fragmentation of grains or melting of the surface layer. The thickness of the irradiated layer is largely determined by the intensity of the ion beam. It reaches several tens of microns at the irradiation by ion beams of energy more than 3 MeV. At a beam energy of less than 1 MeV the fragmentation occurs in the layer thickness of a few microns. It should be noted that the thickness of the modified layer with changed defect structure can reach 100 microns and more [3]. Due to the long-range effect the depth of the modified layer significantly exceeds not only the depth of the free path of incident ions, but the average size of the grains. Fragmentation of the surface layer during irradiation is determined by the occurrence of high stresses on boundaries and joints of grains [4–6]. High-energy ion irradiation leads to the generation of high elastic fields, which can form non-equilibrium micro- and nanostructured layers in the near-surface region of metals [7]. A variety of competing mechanisms associated with phase transitions, structural transformations, plastic deformation, fragmentation in the surface region is involved in the relaxation process of the irradiated material [8].

Experimental study of the dynamics of these processes meets the considerable difficulties. Computer simulation allows overcoming them and getting detailed information about the dynamics of structural changes during irradiation and the following relaxation process of the material [9, 10].
The object of this work is investigation of the features of structural transformations in mono- and nanocrystalline surface layers of aluminum under ion irradiation.

2. Formalism
The molecular dynamics method was used to achieve the object. The simulation was performed on the base of the software package LAMMPS [11]. The interatomic potential for aluminum was described in the framework of the embedded atom method [12]. The sizes of the simulated aluminum samples ranged from 75,000 to 1,000,000 atoms. Initial temperature of samples was set to 300 K. The behavior of mono- and nanocrystalline aluminum specimens under different regimes of irradiation was investigated. Structural changes of the \{100\}, \{110\} and \{111\} surfaces were studied under irradiation in the case of single-crystal specimens. Nanocrystalline specimens were consisted of 6 and 10 grains with an average size of 7.5 and 6.5 nm, respectively. The ion irradiation was simulated by collisions of incident atoms with the free surface. The energy of incident atoms was equal to 60 eV and their number was 540. The time step was 1 fs, Both unloaded and elastically deformed crystallites were subjected to irradiation. The number of the incident atoms of energy 1.5 keV ranged from 16 to 80 in the case of nanocrystalline specimens. The time step was 0.01 fs for the first 0.5 ps and then changed to 0.1 fs.

3. Results and discussion
3.1. Monocrystalline specimens
The calculations showed that irradiation of the crystallites is always accompanied by the intense sputtering of atoms and atomic clusters from the irradiated surfaces. The number of sputtered atoms exceeded the number of incident atoms. The process of atom sputtering most actively developed during irradiation of the \{111\} surface. It should be noted that the surface layer temperature exceeded the melting point. Changing of the kinetic temperature for the layer near the \{111\} surface with the thickness of 10 lattice parameters is shown in figure 1. Due to heat dissipation the temperature of the surface layer quickly decreases and is characterized by pronounced oscillations. Temperature oscillations in the surface layer are associated with motion of shock waves generated at irradiation. Note that the period of temperature oscillations is well correlated with the time of shock wave propagation from the top to the bottom surface and back.

It was revealed that the \{100\} surfaces are the most resistant to irradiation. Change of local atomic environment took place only in few atomic layers close to these surfaces. Defects such dislocations, stacking faults, interstitial dumbbells, etc. were not formed as it shown in figure 2(a). The preliminary elastic deformation of the crystallites had no effect on the features of structural changes in the surface layer. Intrinsic and extrinsic stacking faults were formed in the surface region in the \{111\} planes even in the non-deformed crystallite in the case of the \{111\} surface irradiation. In the preliminary deformed crystallites the stacking faults are beginning to nucleate in adjacent planes, see figure 2(b). Irradiation of the \{110\} surface changes the symmetry of local environment of many atoms. These atoms may either restore fcc lattice or form stacking faults (figure 3). The defect size grows with increasing degree of preliminary deformation. It was found in figure 3(b,c) that stacking faults are formed in adjacent planes and their intersection can lead to the formation of vacancy chains.

3.2. Nanocrystalline specimens
Calculations have shown that the structural response of the nanocrystalline sample essentially depends on the irradiation dose. At low doses (16–40 incident atoms) the grain size and their position are not changed. During irradiation stacking faults nucleate in the grain boundary region and begin to propagate into the body of a grain. This is due to the fact that the incident
Figure 1. Temperature versus time for the \{111\} surface layer of the single crystal preliminary deformed to 4%.

Figure 2. Structure of the single crystal preliminary deformed to 4% after irradiation of the \{100\} (a) and \{111\} (b) surfaces. Atoms with fcc, hcp and uncertain symmetry of local environment are marked in green, pink and grey, respectively. Atoms with fcc symmetry of local environment are not shown.

Atoms generate atomic displacement cascades as it shown in figure 4(a, c), which lead to high-rate local heating of the grains and the formation of shock waves [13,14]. In turn, the local stress growth and the nucleation of stacking faults occur as a result of the interaction of shock waves with grain boundaries. The density of stacking faults in the grains increases with an increasing number of incident atoms (figure 4). Note that at the irradiation by 16 atoms the stacking faults are formed only in some grains. They were generated in the parallel slip planes in each grain as it shown in figure 4(b). With increasing irradiation dose (to 40 incident atoms) the number of generated stacking faults increases, they are formed in all grains. In this case, the indices of their slip planes in the grain may have different signs, see figure 4(d).
Figure 3. Structure of the single crystals after irradiation of the \{110\} surface preliminary deformed to 0\% (a), 4\% (b) and 5\% (c). Pink 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 4. Structure of the irradiated nanocrystalline specimen with 6 grains at different time moments: the end of irradiation (a, c), after relaxation (b, d). The upper and lower rows correspond to 16 and 40 incident atoms, respectively. Grey, yellow and pink colors denote grain boundaries, defects formed by atomic displacement cascades and stacking faults, respectively. Atoms with the fcc symmetry of local environment are not shown.

The surface layer is melted at higher irradiation doses. The crystallization front begins to propagate from the boundaries of the liquid and crystal phases after irradiation. Each grain on
this boundary is enlarged by the atoms of the liquid phase. The newly formed grain structure of the surface layer differs substantially from the one that was before irradiation. Calculations show that the crystallization results in the decrease of the grain number in the simulated sample (figure 5). The histogram shows the grain size distribution before and after irradiation of the specimen with 80 atoms of 1.5 keV energy. The average grain size in the surface region is increased. This was due to the fact that the atoms of the molten region adjusted to the structure of the underlying grains, increasing their size. Note that craters are formed on the specimen surface during its irradiation and relaxation. Their size increases with increasing the irradiation dose.

Figure 5. Grain size distribution before (black columns) and after (red columns) irradiation of the specimen.

4. Summary
On the base of simulation results it is possible to conclude that the nature of structural changes in the aluminum single crystal essentially depends on the crystallographic orientation of the irradiated surface. The \{100\} surfaces are the most resistant to ion irradiation. A large number of stacking faults is formed at the irradiation of the \{111\} and \{110\} surfaces. On the basis of the results obtained it can be assumed that increase of the dose may lead to a fragmentation of the irradiated aluminum crystallites. Stacking faults nucleate at irradiation of the nanocrystalline specimen by small doses. Their number increases with increasing the irradiation dose. The surface layer melts at higher doses. The grain size increases in the surface region of irradiated specimens after the crystallization of irradiation-damaged zone. This is due to the fact that the atoms of the molten layer adjust to crystal structure of grains and increase their size at the boundary of liquid and crystal phases.

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

[1] Gleiter H 1989 *Prog. Mater. Sci.* **33** 223–315
[2] Psakhie S G, Zolnikov K P, Kryzhevich D S, Zheleznyakov A V and Chernov V M 2009 *Crystallogr. Rep.* **54** 1002–10
[3] Meisner S N, Meisner L L, Lotkov A I and Tverdokhlebova A V 2015 *Steel Transl.* **45** 258–61
[4] Meisner S N 2014 *Russ. Phys. J.* **57** 403–10
[5] Zolnikov K P, Psakh’e S G and Panin V E 1986 *J. Phys. F: Met. Phys.* **16** 1145–52
[6] Psakhie S G, Kryzhevich D S and Zolnikov K P 2012 *Tech. Phys. Lett.* **38** 634–7
[7] Korchuganov A V, Zolnikov K P, Kryzhevich D S, Chernov V M and Psakhie S G 2016 *Phys. At. Nucl.* **79** 1193–8
[8] Psakhie S G, Zolnikov K P, Kryzhevich D S, Abdrashitov A V and Lerner M I 2010 *Phys. Mesomech.* **13** 184–8
[9] Psakhie S G, Korostelev S Yu, Negreskul S I, Zolnikov K P, Wang Z and Li S 1993 *Phys. Status Solidi B* **176** K41–4
[10] Psakh’e S G and Zol’nikov K P 1998 *Combust., Expls. Shock Waves* **34** 366–8
[11] Plimpton S 1995 *J. Comput. Phys.* **117** 1–19
[12] Mendelev M I, Kramer M J, Becker C A and Asta M 2008 *Philos. Mag.* **88** 1723–50
[13] Zol’nikov K P, Uvarov T Yu, Lipnitskii A G, Saruev D Yu and Psakh’e S G 1999 *Tech. Phys. Lett.* **25** 936–7
[14] Korchuganov A V, Zolnikov K P, Kryzhevich D S and Psakhie S G 2017 *Russ. Phys. J.* **60** 170–4