

Computer simulation of surface modification of Al crystallite under high energy treatment

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ABSTRACT

The surface treatment by different beams of energy widely used to improve functional properties of materials. The particle irradiation can lead to such processes like melting or a reconstruction of a grain structure in the surface layers of the material. Dynamics of structural transformations under such impacts is not studied enough due to the small space-time scales of the processes and a wide variety of materials. In this work, 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 strained 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.

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