Molecular dynamics simulation of nucleation and growth of defects in the alloy Fe-Cr in the conditions of high-energy loading

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ABSTRACT

Free surfaces and grain boundaries determine the features of nucleation and development of plastic deformation, the number and type of surviving defects under external influences. The irradiation of material by beams of high energy particles leads to the generation of atomic displacement cascades in the free surface region. The defects formed by such cascades have the features of evolution, due to their proximity to the free surface. The nucleation and evolution of structural defects in the Fe-Cr crystallite at the bombardment of its free surfaces by high energy particles was carried out in this work. The calculations were based on the molecular dynamics method. It was found that the number of surviving defects at the generation of atomic displacement cascades near the free surfaces is almost twice their number than in case of cascade generation far away from the various interfaces. Besides it the cascades can knock out some atoms from the free surfaces and form some specific structural defects: craters, adatom islands, dislocation loops of vacancy type. The crystallographic orientation of the irradiated surfaces has a significant influence on the features of the material damage. In particular, craters are much more frequently formed at the irradiation of the (111) surface. It was revealed that there is a correlation between the size of the vacancy loops and the number of adatoms on the free surface. The size of the vacancy loops formed by the irradiation of the (111) surface is slightly larger than the number of adatoms. The inverse relationship was found at the irradiation of the (110) surface of Fe-Cr crystallite.

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