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CONSTRAINED CONDITIONS INFLUENCE ON THE FEATURES OF NUCLEATION AND EVOLUTION OF PLASTIC DEFORMATION OF NANOCRYSTALLINE METALS

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At present, gradient metallic materials are of considerable interest for scientific research and for various practical applications. The structure, physical and mechanical properties of these materials uniformly or jumplike change at least in one direction. In the process of formation of such materials, a substantial redistribution of normal and tangential stresses occurs in the region with a gradient structure. These features of the internal structure and stress distribution lead to the fact that gradient metallic materials simultaneously have high hardness and high ductility. The study of behavioral features, in particular, mechanisms of plasticity nucleation and fracture of such materials under extreme conditions, is an urgent task.

In the present work, molecular dynamics simulation of behavior of nanocrystalline iron with a gradient structure under mechanical loading was carried out. The gradient structure was formed by changing the grain size in the selected direction. The role of the character of the stress distribution in the nucleation of plasticity in the simulated material was studied. The effect of the gradient change in the grain size on the mechanical properties of the sample was investigated. The features of grain boundary migration and the evolution of dislocations in the iron sample with a gradient structure were studied.

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