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FEATURES OF STRUCTURAL TRANSFORMATIONS OF NANOCRYSTALLINE METALS UNDER SHEAR DEFORMATION

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Due to nanoscale and interface effects, nanocrystalline metallic materials possess unique physical, mechanical and chemical properties, in particular, high strength, hardness and wear resistance. They are characterized by good ductility and toughness, which makes them promising materials for many practical applications. High performance characteristics of these materials are largely due to the small grain size.

This work is aimed at studying the features of the nucleation of plastic deformation in nanocrystalline iron under shear loading. The simulated sample had grains of approximately the same size with large misorientation angles relative to each other. Periodic boundary conditions were set along two directions of the sample and a shear load was applied in the third direction. The calculations were carried out on the basis of the molecular dynamics method using manybody interatomic potentials. The elastic limit and the effect of shear loading rate on the features of the nucleation of plasticity in a nanocrystalline sample are determined. Based on the calculations, the features of the grain boundary migration, grain boundary sliding, changes of grain sizes and grain fragmentation are revealed.

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