Plastic deformation in nanocrystalline aluminum at twist grain boundaries

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MD study of mechanical response and elastic-plastic behavior of Al with different grain boundaries (GB), misorientation angles, specific energies, and Cu atom concentrations is performed. Systems containing symmetrical twist GBs with misorientation angles of 4°, 12.68°, 36.87° and 43.61° with a misorientation axis [100] were considered. For each angle, several GBs were created, differing in structure and specific energy. For angles of 4° and 18.435°, systems containing Cu atoms segregated at GB in different concentrations were considered. Depending on angle, specific energy and the Cu atom concentration various critical shear stresses and relaxation mechanisms (grain rotation and dislocation processes) were observed. Rotation occurs in all systems when the shear stress exceeds a threshold value specific to a given boundary and is accompanied by an increase in Sxx and Szz stresses in the system, which leads to the shear stress increase due to change in the elastic constants of the lattice. Dislocation nucleates at a relatively low shear stresses in the systems. For 4.00° and 12.68° angles, there is average shear stresses increase after dislocation formation without their motion. The reason for dislocation loop formation in this case is the local stresses formed at the GB due to the contact of grain parts. The nucleated dislocations can be absorbed by the opposite GB, after that there are no mobile dislocations in the system and grain rotation continues. The average shear stresses after the recession associated with dislocation processes continue to grow with characteristic dependence.
The work is supported by the RSF, project №. 24-11-20031.