Elastic-plastic transition in nanocrystalline aluminum with various grain boundaries

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Effect of GB structure and specific energy on mechanical response and elastic-plastic behavior of Al was investigated. Tilt and twist [100] GBs with various misorientation angles were considered. HAGBs with different specific energy demonstrate a significant spread of critical stresses, differing up to 3 times in the case of tilt GBs. For LAGBs, there was no spread of results. The smallest activation stress for tilt GBs was about 200 MPa, the largest – 1800 MPa. For tilt HAGBs, the predominant plasticity mechanism is GB sliding, while for LAGBs, it is GB migration. The transition from HAGBs to LAGBs is accompanied by gradual increase in the number of systems in which GB migration is observed. For twist GBs, a similar tendency to critical stress decrease with an increase in the GB misorientation angle was observed. The results of MD are generalized with ANN, which is used in continuum approach as constitutive relations for elastic-plastic behavior of Al. Using SPH with ANN, the deformation of a representative volume with different GBs was simulated. In the case of one type of GBs, the stress evolution largely repeats MD system. With random GB distribution, an averaged and fairly stable stress-strain curve is obtained. Inclusion of only GBs with maximum or minimum energy for a given type GBs has little effect on the stress-strain curve. Twist HAGBs significantly reduce the flow stress at the initial stages of shear. Random distribution of GBs leads to plastic localization.

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