

# Molecular dynamics simulation of symmetric tilt grain boundary (110) response in fcc metals on shear deformation

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## ABSTRACT

The continual models of the dislocation nucleation at the grain boundary (GB) and the low-angle GB migration are developed based on the data of molecular dynamics (MD) simulation [1] of shear deformation of aluminium and copper bicrystals with the embedded atom potentials [2-3]. The progress of several papers is chosen to construct these models: the equations of dislocation motion and the equations of dislocation plasticity from works [4-5] and the criterion of the homogeneous nucleation of dislocations in paper [6] are taken. MD simulation shows the presence of three types of dislocation boundaries in symmetric tilt GBs relative to the axis (110) in the range of misorientation angles from 0 to 90 degrees. These boundaries have different structures and ways of dislocation nucleation from GBs and the possibility of boundary migration (the simulation data correspond to the experimental and theoretical data in studies [7-8] and the MD simulation data in other works [9-11]). The continuum model takes into account of different types of GBs and methods of dislocation nucleation for each GB according to MD simulation data. In addition, the boundary migration in the first type of GB (low-angle) is estimated using the equations of dislocations motion, since the data of MD simulation shows that the boundary migration is the main effect and the large part of dislocations nucleation occurs on residual defects after GB migration. The work is supported by the ministry of education and science of the Russian Federation, state task no. 3.2510.2017/4.6.

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