Multiscale modeling of dynamical plasticity in Al–Cu alloy

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We combine molecular dynamics, theoretical model and discrete dislocation dynamics to investigate the dynamical plasticty of Al–Cu alloy. At the first stage we study the interaction of edge dislocation with various types of hardening inclusions of second phase in Al–Cu system, which are solute atoms, Guinier–Preston (GP) zones, θ'', θ' and θ phases. The main mechanisms of interaction between dislocation and different types of inclusions are established. It is shown that with an increase in the thickness of the hardening inclusion from one layer of copper atoms in the case of GP zones, the mechanism of the first interaction changes from cutting to the formation of Orowan loop. The accumulation of lattice incompatibilities upon repeated overcoming of an obstacle by a dislocation nevertheless leads to the gradual damage of inclusions. phase inclusions are the most stable. The parameters of the inclusion softening during long-term deformation are determined. Secondary, the model of dislocation-obstacle interaction is offered based on the concept of Orowan loop formation. The interaction energies for nanoscale hardening phases are determined by fitting to the moleqular dynamic data both for dislocation position and average stress in the systems. Inclusion softening is empirically taken into account by introducing an effective interaction radius that decreases with deformation. At the third stage, a discrete dislocation technique is formulated for plasticity modeling. Equation of dislocation motion accounts both dynamical effects and interaction with inclusions. The experimental data on size distribution of inclusions are introduced into the model. The obtained values of flow stress for alloy demonstrate good agreement with experimental results, also, calculations well predict the thermal softening of alloy.