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Molecular dynamic modeling of plasticity of Al and Al-Cu alloys under dynamic loading VLADIMIR STEGAILOV, ALEXEY KUKSIN, GENRI NORMAN, ALEXEY YANILKIN, Joint Institute for High Temperatures of RAS, Moscow, Russia — The molecular dynamic (MD) simulations are carried out to study the mechanisms and kinetics of plasticity of Al and its alloys. The mobility of dislocations is evaluated from non-equilibrium MD simulations. The influence of temperature, presence of Cu precipitates and voids on dislocation motion is analyzed. Temperature dependence of the phonon drag coefficient on dislocations is calculated for Al. The drag coefficient increases linearly in all the temperature range (except the region near the melting point). It leads to an anomalous increase of the yield stress of single crystal Al with growing temperature. Critical resolved shear stresses required for dislocation to penetrate obstacle (precipitate or void) are calculated. Critical stress decreases with temperature, while pinning time increases. The following mechanism of the dislocation depinning is observed for cluster sizes (0.5–3 nm) and distances between them (10–60 nm) studied: strong bowing of the dislocation line with subsequent formation of the local shear plane cutting the cluster. A climb of the dislocation segment can be observed during depinning. The value of the dynamic yield stress of single crystal Al and Al-Cu alloy is estimated. Possible interpretation of the experimental data [G.I.Kanel et al., 2001,2008] on dynamic yield stress is discussed.

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