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Molecular simulation of dislocation motion in magnesium alloys under high strain rates PENG YI, ROBERT CAMMARATA, MICHAEL FALK, Johns Hopkins University — Dislocation motion of <a>dislocations on the basal and the prismatic planes under simple shear was studied using molecular simulations in Mg/Al and Mg/Y alloys. The critical resolved shear stress (CRSS) was calculated at temperature from 0K to 500K with solute concentrations from 0 to 7 at.%. The strain rates of 10^6-10^8 s^{-1} used in the simulation correspond to experimental strain rates of 10^1-10^5 s^{-1} based on Orowan's equation. Basal slip is dominated by the <a>edge dislocations. Solute hardening to the CRSS follows a power law, c^n, where c is the solute concentration. The exponent n transitions from close to 2/3 at low temperature to close to 1 at high temperature. Temperature and strain rate effects on the CRSS are captured by Kocks model based on thermally activated events. Prismatic slip is controlled by the <a>screw dislocation that cross-slips between the basal and the prismatic planes, in a locking-unlocking pattern. Temperature affects the slip kinetics through the diffusion of the screw dislocation on the basal plane, which leads to vacancy and loop generation. Solute softening was observed for both Mg/Al and Mg/Y alloys. The softening on prismatic slip is due to the solute pinning effect on the basal plane, and Al is more effective in softening.

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