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Solute Hardening in Al-Mg: Molecular Dynamics Simulations of Single Dislocations and One-Dimensional Potential Energy Model. DAVID OLMSTED, Div. of Engineering, Brown University, LOUIS HECTOR, JR., GM Research & Development Center, General Motors Corp., W.A. CURTIN, Div. of Engineering, Brown University — Magnesium is used as a substitutional alloying agent to improve the formability, and other properties, of aluminum in alloys such as 5xxx aluminum. Servated flow (Portevin-Le Chatelier effect) in these alloys limit their usefulness in certain automotive applications. These servated flow effects are believed to be dependent on Mg diffusion. In order to establish both a baseline for and a suitable model in which to study the effect of diffusion on dislocation mobility in Al-Mg alloys we have performed molecular dynamics simulations the motion of a single dislocation in Al with randomly distributed 2.5 and 5.0 at% Mg. For a suitable length of dislocation, on the order of the Labusch length, we compare pinning and de-pinning of the dislocation in the molecular dynamics with a model in which a straight dislocation interacts with single Mg atoms, the small Mg-Mg interactions being ignored. We report on the results of the molecular dynamics simulations and the validation of the one-dimensional energy map model.

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