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Abstract

Solute drag in solute-strengthened alloys, caused by diffusion of solute atoms around moving dislocations, controls the stress at deformation rates and temperatures useful for plastic forming processes. In the technologically important Al–Mg alloys, the solute drag stresses predicted by classical theories are much larger than experiments, which is resolved in general by eliminating the singularity of the dislocation core via Peierls–Nabarro-type models. Here, the drag stress versus dislocation velocity is computed numerically using a realistic dislocation core structure obtained from an atomistic model to investigate the role of the core and obtain quantitative stresses for comparison with experiment. The model solves a discrete diffusion equation in a reference frame moving with the dislocation, with input solute enthalpies and diffusion activation barriers in the core computed by or estimated from atomistic studies. At low dislocation velocities, the solute drag stress is controlled by bulk solute diffusion because the core diffusion occurs too quickly. In this regime, the drag stress can be obtained using a Peierls–Nabarro model with a core spreading parameter tuned to best match the atomistic models. At intermediate velocities, both bulk and core diffusion can contribute to the drag, leading to a complex stress–velocity relationship showing two peaks in stress. At high velocities, the drag stress is controlled solely by diffusion within and across the core. Like the continuum models, the drag stress is nearly linear in solute concentration. The Orowan relationship is used to connect dislocation velocity to deformation strain rate. Accounting for the dependence of mobile dislocation density on stress, the simulations are in good agreement with experiments on Al–Mg alloys over a range of concentrations and temperatures.

Keywords

Aluminum alloys, Solute diffusion, Dynamic strain aging, Dislocations