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Chemistry of deformation : solid-solution softening from first-principles to dislocation mobility

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Solid solution softening in bcc transition metals has traditionally been attributed to either extrinsic effects (interstitial scavenging) or intrinsic effects (direct solute-dislocation interactions). We investigate intrinsic mechanisms using first principles methods. First, the interaction energy of a transition metal solute with a single straight <111> screw dislocation in Mo and Fe is calculated using density functional theory. Next, the interaction energies and changes in resistance to dislocation motion are incorporated into a mesoscopic double-kink model of dislocation mobility to predict changes in yield stress with temperature and solute concentration. Quantitatively accurate predictions require a model that accounts for clusters of solutes interacting with dislocations.

Previous methods employing the solute response in bulk as an approximation to the solute response in a dislocation lead to incorrect predictions.

Using solute-dislocation interactions coupled with a realistic mesoscopic model, we reproduce the strength behavior of different alloy systems despite the range of intrinsic interactions.

Mardi 26 Juin 2007 à 10h30

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