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Chemistry and Deformation: First Principles Studies of Local Plasticity

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In order to understand the how chemistry influences deformation, an adequate description of the strain field near the center of dislocations (i.e. the core) is required. Continuum level descriptions of deformation ignore this short-range coupling between dislocations and the local atomic lattice. Interactions at this scale are non-linear and can strongly influence plastic deformation in fcc and bcc metals. Here, density functional theory is used in conjunction with a flexible boundary condition method to calculate the equilibrium dislocation core structure in a variety of bcc and fcc metals. The problem is divided into two parts: a solution for the nonlinear dislocation-core region and a solution for the long-range elastic response. Solving these individual problems is straightforward and by iteratively coupling the two solutions we can efficiently solve for the strain field in all space. Chemical effects, in the form of local solute-dislocation interactions, can also be calculated using this method. Derived solute-dislocation interactions are used to inform new models of solution hardening (and softening) in bcc Mo-X (X=Re, Pt) and fcc Al-X (X=Mg, Cr, Si, Cu) alloys. Currently, solute dislocation interactions are being assessed in bcc Fe-H alloys using this first principles technique.