Solute interactions with dislocations in BCC Fe

Dallas R. Trinkle[1], Anne Marie Z. Tan[1], Michael R. Fellinger[1], Louis G. Hector, Jr.[2]

[1] *Materials Science and Engineering, Univ. Illinois, Urbana-Champaign, USA;*
[2] *General Motors R&D Center, Warren, MI, USA.*

Integrated computational materials engineering of third-generation steels requires a multiscale approach that passes first principles data to mesoscale (e.g. microstructural) models. In particular, we are interested in the effects of solutes on mechanical behavior—both elastic and plastic. The challenge of lattice constants can be computed efficiently using density-functional theory from the elastic dipole tensor that quantifies how solutes induce stress in the host crystal. The changes in elastic constants can be similarly computed from changes in the elastic response of the unstrained cells combined with higher order elastic constant data. To model solid solution strengthening, however, we require not just misfit data that captures the long-range interaction, but the quantification of solute interaction with the dislocation core.

Modeling isolated dislocations is challenging due to their long-ranged strain fields. While there are a variety of possible coupling or "multiscale" techniques available, I will focus on flexible boundary conditions, which use the lattice Green's function to couple electronic structure to an infinite harmonic bulk; this approach greatly simplifies many "hand-shaking" problems, and generally provides a computationally efficient approach. This methodology has explained solid-solution softening in molybdenum (explaining a 50-year-old mystery of metallurgy), dislocation cores in aluminum and titanium, and provided a wide range of mechanical behavior predictions for magnesium alloys. I will discuss our recent work improving the accuracy and efficiency of flexible boundary condition methods specifically for a dislocation geometry, and the application to dislocations cores in BCC Fe.

These results provide the starting point for direct calculation of solute-dislocation interactions in BCC Fe. We start with relaxed dislocation core geometries, introduce solutes at different locations in and around the core, and relax to map out the interaction energy landscape. I will conclude with our results for Al, B, Cu, Mn, Si substitutional solutes and C and N interstitial solutes in BCC Fe, their interactions with dislocations, and comparisons with experimental data.