Topic 6: How do point defects and dislocations interact?

Overview

Solutes, whether substitutional or interstitial, interact with dislocations in materials. The interaction is due to a combination of effects: solutes introduce local strains, changes in bonding, and even different charge states, while dislocations have both long-range strain fields, large distortions in the core including regions of stacking faults. This interaction causes numerous material effects: solid solution strengthening and softening, segregation to and precipitation at dislocations, formation of Cottrell atmospheres, pipe diffusion, strain aging, and dynamical strain aging. In the past decade, computational studies have vastly improved our understanding of dislocations and specifically their interactions with solutes. This includes accurate computation of solute misfits (strains induced by solutes) and their interactions with stacking faults, as well as direct solute-dislocation interaction calculations using both density-functional theory and empirical potentials. At the same time, measurement techniques like atom-probe tomography have been used to demonstrate Cottrell atmospheres and other solute segregation to dislocations. These development simultaneously push the theoretical developments of models; in the case of solid-solution strengthening and softening, the introduction of new, accurate solute-dislocation interactions have forced improved models that can be compared with careful experimental measurements. As is often the case, isolating what effects are important–core vs. long-range interactions, dilute vs. non-dilute, solid-solution vs. precipitation–makes any study of solute-dislocation interaction complex.

Reading

For this topic, we'll look at measurements of solid-solution strengthening, followed by two different types of computational studies: one based on density-functional theory, and another based on empirical potentials, to get an idea of what we can successfully quantify.

- Ø. Ryen, B. Holmedal, O. Nijs, et al., "Strengthening mechanisms in solid solution aluminum alloys." *Metall and Mat Trans A* **37**, 1999 (2006): doi:10.1007/s11661-006-0142-7
- J. A. Yasi, L. G. Hector, Jr., and D. R. Trinkle, "First-principles data for solid-solution strengthening of magnesium: From geometry and chemistry to properties." *Acta mater.* **58**, 5704-5713 (2010): doi://10.1016/j.actamat.2010.06.045
- L. Proville and S. Patinet, "Atomic-scale models for hardening in fcc solid solutions." *Phys. Rev. B.* **82**, 054115 (2010): doi:10.1103/PhysRevB.82.054115

Team assignment

Your research group-mate from Topic 1 is back, and she's successfully demonstrated that Al, when alloyed with Sb (1at.%) shows increased radiation resistance. You decide that the next step will be to look into the mechanical behavior of possible solid-solution Al-Sb alloys. Your team is interested in yield strength from room temperature up to 400°C.

1. Is there any computational or experimental values that you would trust to make an *estimate* of the strength?
2. If you need additional data, how could you get it?

Prelecture questions

1. Consider a long, straight edge dislocation. For a solute at a position $\mathbf{r}$ from the dislocation, the interaction energy can be estimated as $p(\mathbf{r})\Delta V$ where $p(\mathbf{r})$ is the hydrostatic pressure at the position $\mathbf{r}$ from the dislocation, and ΔV is the solute's size misfit (change in lattice constant with concentration due to the solute). What is the strongest interaction energy you would estimate, and where is the solute relative to the dislocation where this interaction occurs?

2. How would you estimate the interaction energy of solutes with screw dislocations in a material?

3. Pipe diffusion is where solutes find a short-circuit diffusion pathway along dislocations, as dislocation cores attract solutes and lower the activation barrier for diffusion. If a solute has a diffusivity D_0 in the absence of dislocations, develop an expression for the diffusivity in a crystal with a dislocation density $\rho_\perp$, if the dislocation-solute binding energy is E_{bind} and the activation energy for diffusion in the dislocation is lower by Q_{pipe}.

Suggested background

These may help you think about the papers and questions raised; you may want to look beyond these, too.

- Ali Argon, *Strengthening Mechanisms in Crystal Plasticity* (Oxford, 2007). Chapter 5: doi:10.1093/acprof:oso/9780198516002.003.0005
- D. Hull and D. J. Bacon, *Introduction to Dislocations.* Fifth ed. (Elsevier, 2011): doi:10.1016/B978-0-08-096672-4.00010-4 Chapter 10.
- Slides (on Google Drive):
    - Dislocation Energy

Discussion: Nov. 1-3, 2022