Topic 8: How do dislocations interact?

Overview

Work hardening (also called strain hardening) is the increase in strength of a material as it undergoes plastic deformation. In most materials, this is the combination of two factors: the increase in dislocation density as with plastic strain, and the increased stress necessary to move a dislocation as the dislocation density increases:

$$\frac{d\sigma}{d\varepsilon} = \frac{d\rho_\perp}{d\varepsilon} \cdot \frac{d\sigma}{d\rho_\perp}$$

The first term includes both dislocation production and annihilation terms, while the second term includes the interaction of dislocations with each other. While the chain rule expression is simple, developing accurate models for the two contributions for real materials is difficult, and experiments offer only limited quantitative information about individual mechanisms. In the past decades, discrete dislocation dynamics simulations began providing quantitative predictions about work-hardening, by explicitly simulating dislocations as discrete objects that interact with each other via their elastic fields. The kind of data that is now available can then be used in solid mechanics models of "crystal plasticity" by explicitly tracking changes in dislocation density.

Reading

For this topic, you'll want to review a paper on discrete dislocation dynamics (note: there are different simulation approaches in this area; we will consider one choice), a paper on dislocation density-based crystal plasticity that attempts to model mechanical behavior at a much larger scale, and finally a proposed mechanism for hydrogen embrittlement called "Hydrogen-Enhanced Localized Plasticity" (HELP) that relies on hydrogen changing how dislocations interact.

- Ryan B. Sills, William P. Kuykendall, Amin Aghaei, and Wei Cai, "Fundamentals of Dislocation Dynamics Simulations" in *Multiscale Materials Modeling for Nanomechanics* (Springer 2016), 53-87: doi:10.1007/978-3-319-33480-6_2
- P. Shanthraj, M.A. Zikry, "Dislocation density evolution and interactions in crystalline materials," *Acta Mater.* **59** 7695-7702 (2011): doi:10.1016/j.actamat.2011.08.041
- H. K. Birnbaum, P. Sofronis, "Hydrogen-enhanced localized plasticity–a mechanism for hydrogen-related fracture," *Mater. Sci. Eng. A* **176**, 191-202 (1994): doi:10.1016/0921-5093(94)90975-X

Team assignment

The mechanism behind HELP relies on a change in the interaction of dislocations due to a solute, which suggests that chemistry could affect work hardening in other systems. Considering the two modeling examples from the reading, what changes would needed to be accounted for to predict work-hardening in a material with

1. a change in temperature, and
2. introduction of a solute?

Prelecture questions

1. One simple model to predict the change in strength with dislocation density is to consider two parallel straight edge dislocations that are on different parallel slip planes that are a distance y apart, and find the maximum interaction force per length between the two dislocations. This maximum interaction force then becomes the stress (from the Peach-Kohler force) to glide one dislocation freely on its slip plane due to elastic interactions. From this, work out an expression for the shear stress needed to move dislocations for a given dislocation density; make whatever approximations you feel necessary to do this.
2. Another model to predict the change in strength with dislocation density is to consider a single dislocation that sees a density of dislocations on a *different* slip plane. These other dislocation lines look like a "forest" of sites that pin our moving dislocation. Our dislocation can move ahead by bowing out between the pinning sites; this requires a shear stress of $\tau = Gb/L$ for shear modulus G, Burgers vector b, and distance L between two pinning sites. From this, work out an expression for the shear stress needed to move dislocations for a given dislocation density; make whatever approximations you feel necessary to do this.
3. Compare and contrast what answers you get from these two models; what conclusions can you draw about the importance of different dislocation interactions in work hardening?
4. *Bonus:* What is the total force (not force per length, but integrated force) between two right-hand infinitely long straight screw dislocations that have *perpendicular* Burgers vectors and a distance of closest approach r?

Suggested background

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

- Course webnotes:
  - 5.2.3 Stress field of a dislocation
  - 5.2.4 Forces on a dislocation
  - 5.2.5 Interactions between dislocations
- D. Hull and D. J. Bacon, *Introduction to Dislocations.* Fifth ed. (Elsevier, 2011): doi:10.1016/B978-0-08-096672-4.00004-9 Chapter 4.
- D. Hull and D. J. Bacon, *Introduction to Dislocations.* Fifth ed. (Elsevier, 2011): doi:10.1016/B978-0-08-096672-4.00008-6 Chapter 8.
- Ali Argon, *Strengthening Mechanisms in Crystal Plasticity* (Oxford, 2007). Chapter 7: doi:10.1093/acprof:oso/9780198516002.003.0007
- Slides (on Google Drive):
  - 14.dislocation
  - 19.pileups
  - 23.computational-disl / 23.computational-disl-examples

Discussion: Nov. 17-19, 2020