

## Topic 5: what is the core structure of a dislocation?

### Overview

When considering a defect, the most fundamental question is: what is its structure? In the case of dislocations, this can be a difficult question to answer. The existence of dislocations was hypothesized 80 years ago, and the first experimental evidence goes back 60 years ago. Elasticity solutions for the strains from a dislocation were developed starting in the 1960s, and require only the Burgers vector and elastic constants; however, they fail to work near the center (the “core”) of the dislocation line. This has driven significant efforts in characterization down to the atomic scale and advanced computational methods to treat the large distortions at the core. For this week’s topic, we’ll consider what is required to explore the geometry at the center of a dislocation, and what can be done with modern tools.

### Reading

As this is our first foray into dislocations, you’ll want to catch up with more background reading (below). For this week’s topic, there’s a recent review article on computational simulation of dislocation cores, and a fairly new characterization of screw dislocations in a compound semiconductor.

- D. Rodney, L. Ventelon, E. Clouet, L. Pizzagalli, F. Willaime, “Ab initio modeling of dislocation core properties in metals and semiconductors.” *Acta Mater.* **124**, 633-659 (2017): doi:10.1016/j.actamat.2016.09.049
- H. Yang, J. G. Lozano, T. J. Pennycook, L. Jones, P. B. Hirsch, and P. D. Nellist, “Imaging screw dislocations at atomic resolution by aberration-corrected electron optical sectioning.” *Nature Comm.* **6**, 7266 (2015): doi:10.1038/ncomms8266

### Team assignment

Dislocation core structures are difficult to measure experimentally, and also difficult to determine computationally. However, microscopy is reaching smaller length scales, and predictive computational techniques are able to simulate more and more atoms. Your team is in charge of a grant decision: you can fund one effort below, but you’re going to have to get it past the other program managers! Select the topic that you think is most promising (highest impact and best chance of success), and prepare your arguments. But also be ready to point out possible problems in the other proposals.

1. Aberration-corrected annular dark field scanning transmission electron microscopy of dislocation cores in pure magnesium (a promising light-weight material).
2. Aberration-corrected annular dark field scanning transmission electron microscopy of dislocation cores in  $\text{Co}_3\text{Al}$  (a promising new superalloy intermetallic).
3. Density-functional theory calculations of dislocation cores in the BCC-base multi-principal element alloy TiZrNbHfTa (equal concentrations of each).
4. Density-functional theory calculations of dislocation cores in  $\text{Co}_3\text{Al}$ .

## Prelecture questions

1. Consider a screw dislocation in Al ( $b = 2.9\text{\AA}$ ,  $G = 28\text{ GPa}$ ).
  - a. Calculate the elastic contribution (i.e., no core energy) to the energy of a screw dislocation in Al; use  $5b$  and  $10^5b$  for the inner and outer radii.
  - b. Calculate the dislocation energy using the Peierls-Nabarro model; ignore separation into partials (i.e., use  $\gamma(u) = [Gb^2/(2\pi)^2a](1 - \cos(2\pi u/b))$  for the misfit energy where  $a$  is the distance between planes), and use  $10^5b$  for the outer radius.
  - c. How does this compare with the energy of a row of vacancies?
2. Estimate partial splitting in Cu for a screw and an edge dislocation.
3. Identify three properties that depend on dislocation core structure.

## Suggested background

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

- Course webnotes:
  - 5.1.1 Introduction to Dislocations
  - 5.1.2 Volterra construction
  - 5.2.1 Basic elasticity
  - 5.2.2 Stress field of a dislocation
  - 5.2.3 Energy of a dislocation
  - 5.4.1 Stacking-faults and close-packing
  - 5.4.2 Reactions involving partials
- D. Hull and D. J. Bacon, *Introduction to Dislocations*. Fifth ed. (Elsevier, 2011): doi:10.1016/B978-0-08-096672-4.00002-5 Chapter 2.
- D. Hull and D. J. Bacon, *Introduction to Dislocations*. Fifth ed. (Elsevier, 2011): doi:10.1016/B978-0-08-096672-4.00005-0 Chapter 5.
- Slides (on Google Drive):
  - Dislocation Introduction
  - Dislocation Stress
  - Dislocation Energy

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Discussion: Oct. 25-27, 2022