22.14: Nuclear Materials, Spring 2015

Problem Set 4
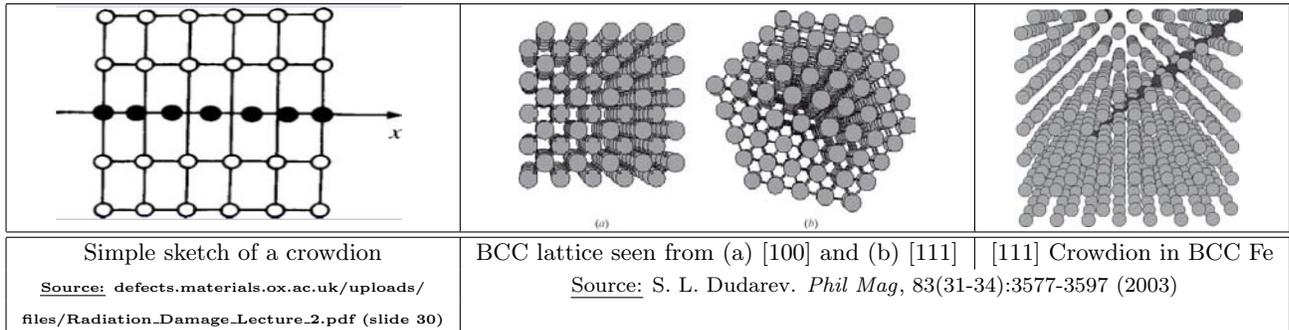
Topic: Radiation Damage

Purpose

An understanding of the damage left behind by radiation is the key to understanding how it affects material properties. In addition to simple vacancies and interstitials, a complex zoo of defect clusters can be left behind by a radiation damage cascade. In this problem set, you will explore the predicted effects of accounting for a third type of defect, besides vacancies and interstitials.

Assignment

We will consider the formation of a *crowdion*, or a one-dimensional defect made of self-interstitial atoms (SIAs). We will specifically consider the formation of crowdions in iron below its phase transformation temperature (BCC Fe) on the [111] directions. Some images to help explain what a crowdion is, along with a view of the BCC lattice from two angles, are shown below:

Simple sketch of a crowdion	BCC lattice seen from (a) [100] and (b) [111]	[111] Crowdion in BCC Fe
Source: defects.materials.ox.ac.uk/uploads/ files/Radiation_Damage_Lecture_2.pdf (slide 30)	Source: S. L. Dudarev. *Phil Mag*, 83(31-34):3577-3597 (2003)	

Courtesy of Steve Fitzgerald. Used with permission.

These crowdions can diffuse very quickly (low migration energy) in one dimension. The formation of crowdions, being interstitial in nature, must compete with the formation of single SIAs.

1 (30 points) New Point Defect Equations

1. (10 points) Assuming that $D_{\text{vacancy}} < D_{\text{interstitial}} \ll D_{\text{crowdion}}$ at all temperatures, develop a new set of point defect balance equations based on those from the reading (Was, "Fundamentals of Radiation Materials Science," p. 192) by introducing a fraction f_c of interstitial defects that become crowdions. Estimate the relative strength of any new rate constants to those that exist in the standard vacancy-interstitial point defect balance equations.

2. (20 points) Using your new balance equations, draw new *qualitative* curves showing the time evolution of the three types of defects as functions of temperature and sink density (four cases in total), as in the reading (Was, pp. 194-200).

2 (40 points) Improving the Kinchin-Pease Model with Stopping Powers

Let's assume that the Kinchin-Pease model is too simplistic (it really is simple, isn't it?). We would like to develop a more comprehensive model, which accounts for the continuously changing interplay between nuclear and electronic stopping power.

1. (20 points) Develop a new expression for $v(T)$, removing the assumption of a linear increase in displacements with any cutoff value. Start by looking at how much energy is lost by a PKA to nuclear displacing collisions, compared to the total amount of energy lost by the PKA over its whole recoil energy range. Use the Ziegler-Biersack-Littmark (ZBL) universal nuclear stopping power correlation in Was' book, equations 1.149-1.151 for the nuclear stopping power, and equations 1.182-1.183 for the electronic stopping power. Read Was, G. S. Chapters 1.3 in *Fundamentals of Radiation Materials Science: Metals and Alloys*. Springer, 2007, pp. 44–59. ISBN: 9783540494713, and assume self-ion irradiation.

2. (10 points) In many atomistic simulations (such as DFT, MD, etc.), a "cutoff energy" and/or "cutoff radius" is often employed, whereby very small variations in calculations over large values of distance or small values of energy are neglected to save time. Here, a maximum energy cutoff value is in order. Devise an expression for this cutoff energy in your expression in (2.1), assuming that some fraction of displacements is enough to model the total number of displacements caused by a PKA. What is this cutoff energy value for aluminum (Al) and lead (Pb)?

3. (10 points) Graph your expression for $v(T)$ on top of that for the Kinchin-Pease model for aluminum. How does your model improve upon the K-P model, and why? What shortcomings does your new model still have?

3 (30 points) Crowdions to the Rescue

1. The presence of crowdions has recently been suggested as *the* reason that nuclear structural materials can even exist. Here, you will read through a recent paper concerning crowdion energetics, and try to understand why crowdion stability can lead to decreased swelling.

   Read through the attached paper by Golubov et al., and explain in no more than one page why you think that crowdions are responsible for the far smaller observed void swelling compared to predicted levels. You may want to consider the following in your response:

   (a) What is the major issue being addressed, and why was this study necessary?

   (b) What assumptions were made in performing the simulations in this study?

   (c) What do the authors mean by "interaction energy landscapes?"

   (d) Why does the fact that crowdions can move in 1-D (as opposed to 3-D) help them escape the "pull" of dislocations?

   (e) Void swelling is typically caused by the coalescence of vacancies formed from radiation. Why would surviving crowdions help reduce void swelling?

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