

**Exercise 6**

**a)** Determine the atomic diffusion coefficients  $D_a^v$  (for the vacancy mechanism) and  $D_a^i$  (for the self-interstitial mechanism) for bcc iron at 300°C, given the following defect formation and migration data:

Property	Vacancy	Self-interstitial
$E_f^x$	2.15 eV	4.10 eV
$S_f^x$	2.5 $k_B$	0.7 $k_B$
$E_m^x$	0.71 eV	0.31 eV
$S_m^x$	0	0

(x denotes either vacancy or self-interstitial)

The lattice parameter of iron is 2.86 Å and the Debye frequency is 15 THz.

**b)** Calculate also the defect diffusion coefficients,  $D^v$  for vacancies and  $D^i$  self-interstitials. Discuss differences wrt **a)**!

**Exercise 7**

We recently discussed the link between diffusion seen as a random walk process (microscopic picture), or as a process governed by the diffusion equation (macroscopic picture).

Microscopically, we found that the mean deviation  $\langle r^2 \rangle$  from a given starting point is  $\langle r^2 \rangle = \lambda^2 \Gamma t$ , where the  $\Gamma$  is the jump frequency,  $t$  is the time, and  $\lambda$  is the jump length. Macroscopically this situation is described by the diffusion equation in spherical coordinates,

$$\frac{dC}{dt} = D \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dC}{dr} \right)$$

Assuming that the diffusing object starts out at the origin at  $t = 0$ , the solution is

$$C(r, t) = N \frac{\exp(-r^2/4Dt)}{(4\pi Dt)^{3/2}}$$

where  $N$  is the number of diffusing atoms. Starting from this solution, calculate  $\langle r^2 \rangle$ .

Compare  $\langle r^2 \rangle$  obtained by the two expressions to show that

$$D = \frac{1}{6} \lambda^2 \Gamma$$

**Exercise 8**

The displacement threshold is often taken as a single value, e.g. 40 eV in Fe. However, this value is an average over all lattice directions and the minimum value is crystal structure dependent. It is easier to displace an atom in certain crystallographic directions than in other, as you have seen in the MD lab.

Estimate the displacement energy in Fe along the  $\langle 100 \rangle$ ,  $\langle 110 \rangle$  and  $\langle 111 \rangle$  directions. In order to do that, you can make the following assumptions:

1. Choose a simple potential  $V(r)$  to describe the atomic interactions.
2. Assume that the surrounding atoms do not relax.
3. Ignore thermal displacement of the atoms.
4. Any other assumptions you think are reasonable.

There is a model description of this in the book for fcc Cu. Consider how this works and how you would need to adapt it to work for bcc Fe.

**Exercise 9**

Calculate the net density of edge dislocations in a thin simple cubic crystal with lattice parameter  $a_0 = 3 \text{ \AA}$  if it is bent to have a radius of curvature of 10 cm. Note that the thickness of the crystal is no greater than 1 mm. These are so-called geometrically necessary dislocations.

**Exercise 10**

When point defects cluster in a matrix they do so in a particular way.

- a) Explain why defects cluster, generally speaking.
- b) Make clear drawings of how self-interstitials should collect into clusters of size two and three (di- and tri-interstitials) in the bcc lattice and in the fcc lattice. Motivate the configurations.
- c) Explain how vacancies are likely to cluster.