Lesson 03: Lattice defects

Exercise 03.1: Interstitial sites

The number and size of interstitial sites are different for fcc and bcc lattices. Explore them by inspecting your sketches of lattice planes from exercise 02.2, the wanted posters from lecture 02 and using Unit Cell Visualizer or ChemTube3D.

- How large are the interstitial sites in relation to the size of the host atoms?
- How many interstitial sites are there in a unit cell of each lattice?
- Which lattice can host the largest foreign atoms on interstitial sites?

Interstitial sites in fcc lattice: 4 octahedral sites r_O=0.414 R, 8 tetrahedral sites r_T=0.230 R
Interstitial sites in bcc lattice: 6 octahedral sites r_O=0.150 R, 12 tetrahedral sites r_T=0.290 R
fcc lattices have the largest interstitial sites, despite being close-packed and highest density; while bcc has more interstitial sites per host atom! The fcc lattice can host larger foreign atoms.

These findings are relevant for interstitial solid solutions of smaller atoms in a metal, in particular for steel where carbon atoms dissolve in an iron lattice. Fe is bcc at room temperature (α-Fe), but fcc at elevated temperatures (γ-Fe), e.g. at 950 °C. The radius of a carbon atom is R_C = 0.077 nm and the radius of an iron atom R_{Fe} = 0.124 nm. Discuss the possibility of having carbon atoms in (a) a bcc Fe lattice and (b) an fcc Fe lattice. Which interstitial lattice sites will fit carbon atoms best?

Carbon atoms are too large for all of the interstitial sites (R_C/R_{Fe}=0.62) but the best possible fit are the octahedral sites in the fcc lattice. Therefore, it is expected that fcc Fe can dissolve much more carbon atoms than bcc Fe. The actual solubility of C in Fe is 2.14 wt.% for fcc Fe and 0.022 wt.% for bcc Fe.

Exercise 03.2: Point defects

- How to get an increased vacancy concentration?

  Increase temperature, hold to establish equilibrium and quench; plastically deform, motion of certain dislocations produce vacancies; irradiation

- Why are vacancies relevant?

  Atomic transport in the solid state! Thermal expansion

- How can foreign atoms get into the crystal lattice of an initially pure metal without melting that metal? (consider both substitutional and interstitial atoms)

  Interstitial foreign atoms can jump into empty interstitial sites by thermal activation, motion of substitutional foreign atoms require empty lattice, i.e. the presence of vacancies.

- What is the difference between a pure metal, a metal with impurities and an alloy?

  Pure metals consist of atoms of a single metallic element; an alloy is a mixture of at least two elements with mostly metallic bonding, a metal with impurities is a metal containing other elements, which might be in solid solution or as separate phases.

Exercise 03.3: Properties of lattice defects

Discuss whether lattice defects are beneficial or detrimental for materials properties; or can they be both? Consider various materials properties and explain your arguments.

Lattice defects may indeed be beneficial as well as detrimental for materials properties. For example, dislocations allow plastic deformation of crystals and provide ductility, but they also increase the strength and the brittleness if present in abundance.

Exercise 03.4: Dislocations

What is the total length of all dislocations in a rolled plate of size 100 x 20 x 1 mm^3 containing a dislocation density of $2 \cdot 10^{14}$ m^{-2}?

The total length can be calculated from the dislocation density and the volume $V = abc$

$$L = \rho V = \rho abc = 2 \cdot 10^{14} \text{ m}^{-2}\ 2000 \cdot 10^{-9} \text{ m}^3 = 4 \cdot 10^8 \text{ m}$$

i.e. slightly longer than the distance to the moon.

Exercise 03.5: Lattice defects

Classify each of the following defects as point, line, planar or volume defects

	Point defect	Line defect	Planar defect	Volume defect
Edge dislocation		X		
Grain boundary			X	
A single vacancy	X			
A cluster of about 50 vacancies				X
A local region of atoms with a bcc structure in an fcc matrix				X
The boundary between the bcc and fcc region above			X	
Some Ni-atoms in a Cu lattice	X			
A Fe-particle in copper				X

Relevant exercises from the Callister Rethwisch book (10th Global edition)

4.2, 4.4, 4.12, 4D1