Assignment 4 Solutions

1. Calculate the equilibrium number of vacancies in 1 g of fcc Cu at 1200_C, given that the energy for formation of a vacancy is 0.9 eV/atom. The atomic weight of Cu is 63.546 g/mol and the Boltzmann constant can be expressed kB = 8.62×10−5 eV/K.

$$N_v = N \exp\left(-\frac{Q_v}{k_B T}\right)$$

$N_v = ((1 / 63.5460) * 6.02 \times 10^{23}) \exp (- 0.9 / (8.62 \times 10^{-5} * 1473))$
$N_v = 7.91 \times 10^{18}$

2. (a) Which is more likely to form a Frenkel defect and why: NaI or NaCl ? (b) Which is more likely to form a Schottky defect and why: MgO or NaCl ?

a.) NaI, The difference in ionic radii is greater in NaI than in NaCl, so Na ions are more easily able to slide into interstitials

b.) NaCl – Both are the rock salt structure so that is not the deciding factor, but because Mg and O both form ions by gaining/losing 2 electrons, removing one of them from the lattice will be harder than removing an Na^+ or Cl^-.

3. Sketch the following: (a) A line dislocation in a crystal showing the Burgers circuit and the Burgers vector. (b) A screw dislocation in a crystal showing the Burgers circuit and the Burgers vector.

Both of these are found in the book, and hand out of chapter 8 supplied in class. Fig 8.17 has all the important information.

4. Stacking faults in fcc Co are common, but not in NaCl (even though NaCl also has atoms on fcc lattices). Why ?

In fcc Co all atoms are of identical size and are neutral atoms. This leads to little preference of whether a B or C layer is placed down on top of an A layer, hence the common stacking faults. In NaCl however the presence of charged species leads to a highly preferred ordering to achieve the lowest free energy. Cation –cation and anion – anion repulsions will essential eliminate the possibility of stacking faults.

5. What is a grain boundary? Sketch a schematic of a low angle, and of a high angle grain boundary.

A grain boundary is the site where crystallographic orientation, dimensions or composition changes between two crystallites. Low angle grain boundaries have minimal

mismatch in orientation between crystallites. High angle grain boundaries have a much more pronounced mismatch in orientation.

6. When a cubic crystal converts to a tetragonal crystal (during some structural phase transition), why are a lot of planar defects created?

Phase transformations from cubic to tetragonal involve an elongation of the c axis, however in the cubic cell all axes are identical so any one of them can be elongated. This possibility leads to mismatch of which axes have elongated and the formation of many defects is the result.