MSEG 302 Spring 2018 HW #4 Answer Key

1) A certain metal is found to have a vacancy concentration Nv/N of 1.8 x 10-4 at a temperature of 400 C. If the vacancy concentration at room temperature (25 C) is 3.5 x 10-9, what is the energy required for the formation of a vacancy, in eV/atom?

Nv/N = exp[-Q/kT]

T=400 C = 673 K

k = 8.617 10^-5 eV/K

ln[Nv/N]=-Q/kT so Q= -kT ln[Nv/N] = 0.5 eV

Note that in this case the Nv/N ratio itself was sufficient to solve for Q, so the second part of the question was not needed.

2) Calculate the composition, in weight percent, of an alloy that contains 105 kg of Fe, 0.2 kg of C, and 1.0 kg of Cr.

wt% = m1/(m1+m2+m3) x 100

wt% = 98.9 wt% Fe, 0.19 wt% C, 0.94 wt% Cr.

3) Calculate the composition, in atomic percent, of an alloy that contains 105 kg of Fe, 0.2 kg of C, and 1.0 kg of Cr.

at% = n1/(n1+n2+n3) x 100

n1 = m1/m0

AFe = 55.845 amu, AC=12.0107, ACr=51.9961 amu. This gives:

at% = 98.1 at% Fe, 0.87 at% C, 1.00 wt% Cr.

4) For a BCC iron alloy that contains 0.1 wt% C, calculate the fraction of unit cells that would contain carbon atoms if the carbon was evenly distributed and the BCC structure was retained.

Say sample is 100 gms total. This means would be 0.1 gms C, 99.9 gms/iron. nFe = 99.9/AFe, nC=0.1/12. So nFE = 1.78888 moles, and nC = 0.00833 moles. This means there is one carbon for every 214 Fe atoms. Since there are 2 atoms of Fe in every BCC unit cell, that means one carbon for every 107 unit cells of Fe, or 0.93%.

Note that the actual solubility of carbon in BCC iron is actually only 0.022 wt% (at 727 C), and at room temperature it is even lower.

5) A sample of single crystalline silicon (a semiconductor) has been doped with phosphorous to create a locally conductive region. This process is called n-doping. If the silicon has been doped such that there are now 6 x 1021 atoms / m3 of phosphorous present, calculate the phosphorous concentration in a) weight percent and b) atom percent.

6 x 1021 atoms of phosphorous x AP (30.9737 g/mol) / Nav = 0.3087 gms in 1 m3.

Assume negligible change in density of silicon. Density of silicon = 2.3296 g/cm3. In 1 m3, mSi = 2.3296 g/cm3 \* (100 cm/m)3 = 2,329,600 g. So weight fraction = 0.3087/2329600.3087 = 1.325 10-7, weight percent = 1.325 10-5 wt%. This is quite small, so constant density assumption should be fine. Atomic fraction: np = 0.3087/30.9737, nSi = 2329600/28.0855. So atomic fraction is 1.20 10-7, or 1.2 10-5 at%. Not much different since atomic masses of P and Si are quite similar.

6) Iron (Fe) and vanadium (V) both form BCC crystals, and V forms a substitutional solid solution in Fe for concentrations up to about 20 wt% V at room temperature. Estimate the density and unit cell length for a 90 wt% Fe – 10 wt% V alloy.

Iron BCC density = 7.874 g/cm3 = 2 AFe/Nav/a3. AFe=55.845 g/mol, so aFe = 0.2867 nm

Vanadium density : 6.0 g/cm3 = 2 AV/Nav/a3. AV = 50.9415 g/mol. So lattice constant aV = 0.304 nm.

Assume that lattice parameter is directly proportional to molar concentration… So a (alloy) = fV (aV) + fFe (aFe), since each atom contributes to size per total number present. Need to calculate mole/atomic fraction from given weight fractions… if 100 gms alloy, 90 gms Fe, 10 gms V. So nFe = 1.6116 moles, nV = 0.196304 moles. So atomic f iron = nFe/(ntot) = 0.89, and aV = nV/(ntot) = 0.11. Mass and atomic Fractions actually not much different since atomic masses similar.

So estimated a (alloy) = 0.11 (0.304) + 0.89 (0.2867) = 0.289 nm

Mass of effective atom on each site is 0.89 (AFe) + 0.11(AV) = 0.89 (55.845)+0.11(50.9415) = 55.306 g/mol

So density = 2 (55.306)/Nav/(0.289 nm)3 = 7.61 g/cm3. This seems reasonable, since is less than but still close to the iron density.