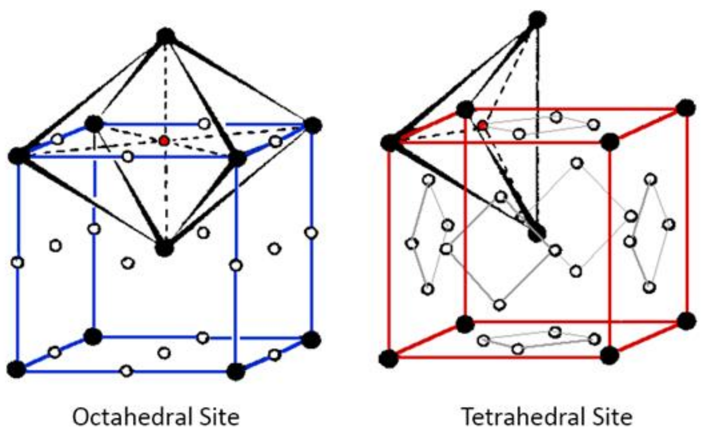
MATRL 100A: Structure and Properties I, Assignment 4

This assignment is due on Wednesday, November 8.

Chapter 4

1. The energy for vacancy formation in iron is 1.08 eV/atom. Calculate the concentration of vacancies in iron at room temperature (20°C) and at 700° C. The density and atomic weight for iron are 7.65 g/cm^3 and 55.85 g/mol respectively.

2. BCC packings have two main types of interstitial sites as shown in the figure below. Octahedral sites are found at the centers of each face and edge of the unit cell, while tetrahedral sites are found 4 on each face at the (1/2, 1/4, 0) positions. Calculate the maximum radius r of an interstitial impurity that can fit into each type of interstitial site without straining the crystal lattice. Put your answer in terms of R, the radius of the host atoms in the BCC packing.



3. Molybdenum forms a substitutional solid solution with Tungsten. Compute the number of Mo and W atoms per cubic centimeter for a 50 wt% Mo - 50 wt% W alloy given the relevant information below.

Element	Density (g/cm^3)	Atomic Mass (g/mol)
Mo	10.2	95.94
W	19.3	183.84

4. Aluminum-lithium alloys see frequent use in the aerospace industry due to their low density compared to other metals. Calculate the concentration of lithium that is required to achieve a density of 2.47 g/cm^3. Give your answer in both weight % and atom %. The relevant properties of Al and Li are tabulated below.

Element	Density (g/cm^3)	Atomic Mass (g/mol)
Al	2.70	26.982
Li	0.523	6.941

5. Silicon forms a substitutional solid with germanium that has the diamond crystal structure. Compute the average lattice constant of a 30 wt% Ge - 70 wt% Si alloy given the following information:

Element	Density (g/cm^3)	Atomic Mass (g/mol)	Lattice Constant (nm)
Si	2.328	28.09	0.5431
Ge	5.323	72.64	0.5658

Note: there are ways to solve this problem without calculating the a/r ratio for diamond. You will, however, need to know some information about the diamond unit cell such as the number of atoms per cell.

6. Consider a sample of AISI 6120 steel which has the following composition:

Element	Weight %
Fe	98.1
Mn	0.80
Cr	0.80
C	0.20
V	0.10
P, S, Si	Impurities from ore

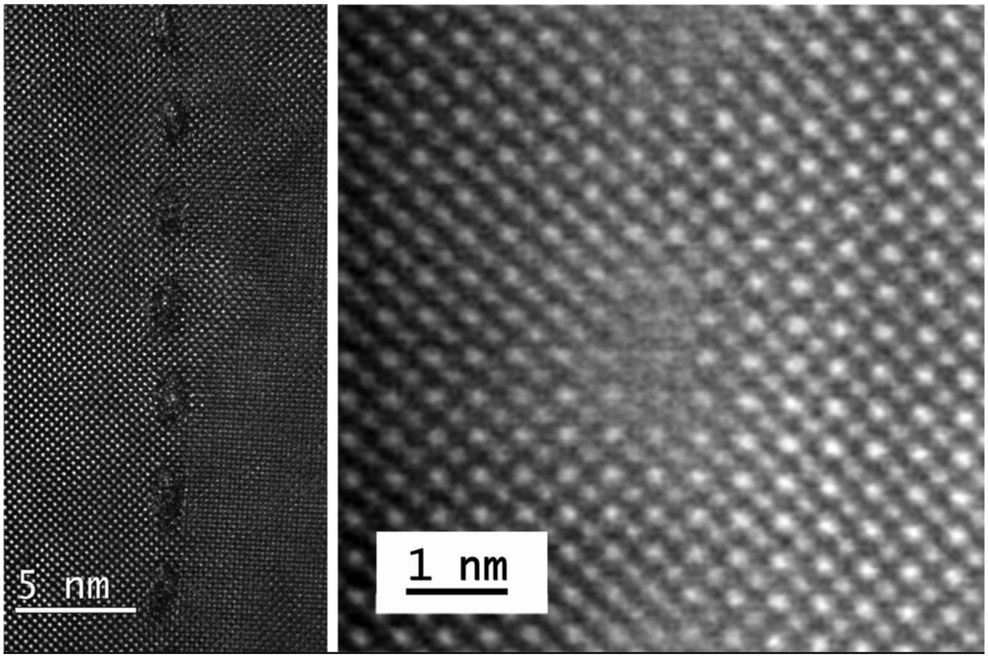
Ignoring the impurities and assuming that everything forms a single phase solid solution, answer the following questions:

(a) Determine whether atoms of each element will substitute iron atoms in the iron BCC lattice or if they will fill interstitial sites. Explain your reasoning.

(b) Convert the given composition in weight % to atom %

(c) Assuming the interstitial atoms only fill tetrahedral interstitial sites, calculate the fraction of tetrahedral interstitial sites that are full (the figure from problem 2 may prove useful).

7. Below is an scanning tunneling electron microscope (STEM) image of a low angle grain boundary in strontium titanate ($SrTiO_3$) viewed along the [001] direction. In this image, each bright spot corresponds to a column of atoms. Unfortunately, the image gets fuzzy around the dislocation cores that make up this grain boundary, and it is hard to tell what is going on. Additionally, it is hard to tell whether these are point defects, or dislocation lines viewed end on. Use a Burger's circuit and the resulting Burger's vector to classify the dislocation as either an edge, screw, or point dislocation (point dislocations have a burgers vector of 0).



Metlenko V., et. al. *Nanoscale*, 2014, **6**, 12868.

8. Rank the (100), (110), and (111) planes in order of increasing surface energy for FCC crystals. Justify your answer based on the relative planar densities of these planes.

9. For each of the following stacking sequences found in FCC metals, cite the type of planar defect that exists:

   (a) . . . A B C A B C B A C B A . . .

   (b) . . . A B C A C A B C A B C . . .

   Copy the stacking sequences and indicate the position(s) of planar defect(s) with a vertical dashed line.