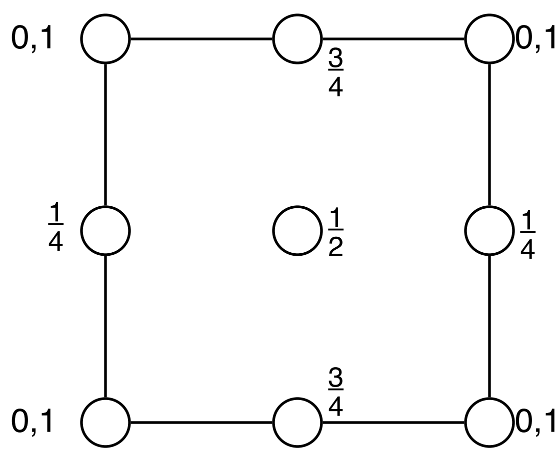
Problem Set #1

The problem set is meant as revision of basic crystallography. You may find it useful to read Chapter 1 of Microstructural Characterization of Materials by D. Brandon and W.D. Kaplan or Chapter 2 of 'Elements of X-Ray Diffraction' by B.D. Cullity and S.R. Stock before attempting the problems.

1) Tin exists as white tin at high temperatures and gray tin at low temperature. White tin which is tetragonal (a = 0.583nm; c = 0.318nm) is shown below in both a perspective view and as a plan (bird's eye) view along [001] (in the plan view the fractional coordinates along the z axis of atom positions are indicated). Gray tin is diamond cubic with a lattice parameter of 0.649 nm. The atomic weight of tin is 118.69.



a) How many atoms are there per unit cell?
b) What is the Bravais lattice?
c) What is the density of white tin?
d) How many (first) nearest-neighbors does each atom have?
e) What is the (first) nearest-neighbor distance?
f) What are the <u>specific</u> crystallographic directions to the nearest-neighbor atoms?
g) What is the second nearest-neighbor distance?
i) Determine the % change in volume (with respect to the volume of white tin) when white tin changes to gray tin.

2. For a cubic crystal:
a) Do the planes (301), (321) and (010) lie on the same zone?
b) Plot the planes in a) on a stereogram centered on (001) and measure the angles between them.
c) Include on your stereogram the zones which passes through
(i) (301) and (010) and (ii) (301) and (011)
d) Algebraically determine the poles which are at the points of intersection of the above two zones with the [110] zone?

3. In this question you will use graphical methods to locate the $(\bar{1}\bar{3}\,1)$ pole on a standard stereogram. <u>Show</u> all construction lines. Do <u>not</u> use a Wulff net. For a cubic crystal: plot the cube faces on a standard (001) stereogram of <u>20 cm</u> diameter and

a) Add the $(\bar{1}\bar{1}\,1)$ pole.
b) Calculate the angle between $(\bar{1}\bar{3}\,1)$ and (i) $(\bar{1}\bar{1}\,1)$ and (ii) $(0\bar{1}\,0)$.
c) By constructing a small circle whose radius is the answer to (i) about $(\bar{1}\bar{1}\,1)$ and another about $(0\bar{1}\,0)$ whose diameter is the answer to (ii), locate the $(\bar{1}\bar{3}\,1)$ pole.

4. Draw a standard (001) projection of white tin (tetragonal, c/a = 0.545), showing all {001}, {100}, {110}, {011}, {111} poles and all the important zone circles between them. Indicate the symmetry elements on your stereogram: for a diad axis, for a triad axis and for a tetrad axis. Compare your stereogram to Fig. 2-36(a) in "Elements of X-ray Diffraction" by Cullity.

5. Draw a standard {0001} projection of hexagonal beryllium (c/a = 1.57), showing all $\{2\bar{1}\bar{1}\,0\}$, $\{10\bar{1}\,0\}$, $\{2\bar{1}\bar{1}\,1\}$, $\{10\bar{1}\,1\}$ poles and the important zone circles between them. Compare your answer with Fig. 2.38 in "Elements of X-ray Diffraction" which is for zinc (c/a = 1.86).

6.a) Derive the relationships between the interplanar spacing, d_{hkl}, and the reciprocal lattice axes for the hexagonal system.
b) Derive the relationship between d_{hkl} and the (real space) crystal axes for the hexagonal system.
c) Derive the relationship between the interplanar angle and the reciprocal lattice axes for the orthorhombic system.
d) Derive the relationship between the interplanar angle and the (real space) crystal axes for the orthorhombic system.