

## Problem Set #2

1.a) Derive simple expressions for  $FF^*$  for Diamond, where  $F$  is the structure factor and  $F^*$  its complex conjugate, and hence determine the rules governing observed reflections.

Diamond is cubic with atoms in the following positions:

(I)  $0,0,0$ ;  $1/2,1/2,0$ ;  $1/2,0,1/2$ ;  $0,1/2,1/2$ .

(II)  $1/4,1/4,1/4$ ;  $3/4,3/4,1/4$ ;  $3/4,1/4,3/4$ ;  $1/4,3/4,3/4$ .

b) Zinc Blende (ZnS) has the same structure as Diamond except Zn atoms occupy (I) positions and S atoms occupy (II) positions. Derive simplified expressions for  $FF^*$  and hence determine simple rules governing observed reflections.

2. Measurement of the relative intensities of superlattice lines in x-ray Debye-Scherrer patterns is a common way to detect the degree of order in an ordered alloy (See B.D. Cullity and S.R. Stock, "Elements of X-ray Diffraction", Third Edition, page 315-326).

a) In what circumstances is it difficult to detect superlattice lines in an ordered alloy even when the alloy is fully ordered?

b) Calculate the relative intensities of the first seven lines on a Debye-Scherrer powder pattern of stoichiometric NiAl (lattice parameter = 0.288 nm) made using Cu  $K_{\alpha 1}$  radiation. NiAl is a strongly ordered (assume  $S = 1$ ) intermetallic compound. The crystal structure is B2, in which Ni atoms occupy  $0,0,0$  positions and Al atoms occupy  $1/2,1/2,1/2$  positions in a simple cubic unit cell. You may neglect the absorption and temperature factors.

3. When sufficient boron (>0.75 at.%) is added to  $Ni_3Al$  ( $Cu_3Au$  structure, simple cubic Bravais lattice) the  $\{331\}$  Cu  $K_{\alpha 1}$  lines on a Debye-Scherrer powder pattern become broadened. Assuming this broadening is due to a tetragonal distortion (expansion) of the unit cell, by how much would the lattice have to become tetragonal (i.e., the value of  $c$ ) before separate  $\{331\}$  and  $\{313\}$  lines were resolved. The lattice parameter for unalloyed  $Ni_3Al$  is 3.56 Å. Assume that the camera has a diameter of 57.3 mm and that lines have to be separated by 0.6 mm to be resolvable. (See B.D. Cullity and S.R. Stock, "Elements of X-ray Diffraction", Third Edition, page 113-118).

4. Metals A and B form a (cubic) terminal solid solution  $\square$ . The variation of lattice parameter,  $a$ , of  $\square$  with composition, determined by quenching single-phase alloys from an elevated temperature is found to be linear,  $a$  varying from 0.36060nm for pure A to 0.36140nm in  $\square$  - 4 wt.% B. The

solvus is to be determined by quenching a two-phase alloy containing 5 wt.% B from a series of temperatures and measuring the value of  $a$  for the contained  $\square$ .

- a) How precisely must  $a$  be measured if the solvus curve is to be located within  $\pm 0.1$  wt.% B?
- b) After being quenched from a series of temperatures the 5 wt.%  $\square$  alloy had the  $a$  values shown below. Plot the solvus curve over this temperature range.

Temperature ( $^{\circ}\text{C}$ )	Lattice Parameter (nm)
100	0.36082
200	0.36086
300	0.36091
400	0.36098
500	0.36106
600	0.36118

- c) What is the solubility of B in A at  $440^{\circ}\text{C}$ ?

5. The table below shows full-width, half-maximum values for five x-ray peaks taken from two diffractometer runs using  $\text{Cu K}\alpha$  radiation, one from powders of mechanically-milled FeCo, the other from powders of large-grained well-annealed FeCo. Calculate the grain size and lattice strain in the milled powders taking into account instrument broadening. You may assume that the lattice strain in the well-annealed powders is zero and that they produce negligible grain size size broadening of the x-ray peaks.

Table. Full-Width, Half-Maximum values for x-ray peaks from FeCo powders.

Position, $2\theta$ (degrees)	Well annealed sample (degrees)	Milled sample (degrees)
44.90	0.14	1.07
65.32	0.15	1.19
82.77	0.16	1.61
99.48	0.20	1.77
117.49	0.26	1.80