Physics 375 **Fall (12) 2003**

Solid State Physics: Problem Set #3

Structural Determination via X-Ray Scattering

Due: Friday Jan. 31 by 6 pm

Reading assignment: for Monday, 3.2-3.3 (structure factors for different lattices)
for Wednesday, 3.4-3.7 (scattering methods)
for Friday, 4.1-4.3 (mechanical properties of crystals)

Problem assignment:

Chapter 3 Problems: *3.1 Debye-Scherrer analysis (identify the crystal structure) **[Robert]**
3.2 Lattice parameter from Debye-Scherrer data
3.11 Measuring thermal expansion with X-ray scattering

A1. The unit cell dimension of fcc copper is 0.36 nm. Calculate the longest wavelength of X-rays which will produce diffraction from the close packed planes. From what planes could X-rays with λ=0.50 nm be diffracted?

*A2. Single crystal diffraction: A cubic crystal with lattice spacing 0.4 nm is mounted with its [001] axis perpendicular to an incident X-ray beam of wavelength 0.1 nm. Initially the crystal is set so as to produce a diffracted beam associated with the (020) planes. Calculate the angle through which the crystal must be turned in order to produce a beam from the (*hkl*) planes where:

a) (*hkl*)=(030)
b) (*hkl*)=(130) **[Brian]**
c) Which of these diffracted beams would be forbidden if the crystal is: i) sc; ii) bcc; iii) fcc

A3. Structure factors for the fcc and diamond bases.

a) Construct the structure factor S_{hkl} for the fcc lattice and show that it vanishes unless *h*, *k*, and *l* are all even or all odd.

b) Construct the structure factor S_{hkl} for the diamond lattice and show that it vanishes unless *h*, *k*, and *l* are all odd or $h+k+l=4n$ where *n* is an integer. (Note: the diamond lattice is given by an fcc lattice with a two-point basis of (000),(1/4,1/4,1/4) at each fcc site, so there are 8 atoms per unit cell).

c) For the above two structures give all {*hkl*} combinations, with $h^2+k^2+l^2 \leq 20$, which give diffraction. (Hint: see Fig. 3.4)

A4. The following scattering angle data (2θ) were obtained from Debye-Scherrer diffraction experiments using Cu K_α radiation:

Sample A	Sample B	Sample C
42.2º	28.8º	42.8º
49.2º	41.0º	73.2º
72.0º	50.8º	89.0º
87.3º	59.6º	115.0º

a) Assuming the samples are monatomic cubic crystals, identify the structure in each case.
b) Determine the length of the side of the conventional unit cell for each sample.

*To be presented in class on Friday.