Physics 375 **Fall (12) 2003**

Solid State Physics: Problem Set #2
Crystal Structure and the Reciprocal Lattice

Due: Friday Jan. 24 by 5pm

Reading assignment: for Monday, No Class: MLK day
for Wednesday, 3.1-3.3 (theory of X-ray scattering)
for Friday, 3.4-3.7 (structural determination via scattering)

Problem assignment:

Chapter 2 Problems:
7 Inter-planar separation
*11 Reciprocal space bcc = "real space" fcc **[Peter]**
12 Miller indices depend on choice of primitive vectors

A1. Consider the (100) and (001) planes of an fcc lattice where the Miller indices refer to the conventional cell. What are the indices of these planes when referred to the primitive axes shown Fig. 2.5 (or more clearly in Kittel's Fig. 1.13).

*A2. Show that the angle θ between the two planes (h_1,k_1,l_1) and (h_2,k_2,l_2) in a cubic lattice is given by

$$\cos\theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{(h_1^2 + k_1^2 + l_1^2)^{1/2}(h_2^2 + k_2^2 + l_2^2)^{1/2}}$$

Verify this formula for the two pairs: (100) and (011) ; (100) and (110). Calculate the angle between the (111) and $(\bar{1}\,\bar{1}0)$ planes. **[Melissa]**

A3. Hexagonal lattice in reciprocal space: The primitive translation vectors of the hexagonal space lattice may be taken as

$$\vec{a} = (3^{1/2}a/2)\hat{x} + (a/2)\hat{y} \ ; \ \vec{b} = -(3^{1/2}a/2)\hat{x} + (a/2)\hat{y} \ ; \ \vec{c} = c\hat{z}$$

(a) Show that the volume of the primitive cell is $(3^{1/2}/2)a^2c$.
(b) Show that the primitive reciprocal lattice vectors are

$$\vec{A} = (2\pi/3^{1/2}a)\hat{x} + (2\pi/a)\hat{y} \ ; \ \vec{B} = -(2\pi/3^{1/2}a)\hat{x} + (2\pi/a)\hat{y} \ ; \ \vec{C} = (2\pi/c)\hat{z}$$

(Note that the hexagonal lattice is its own reciprocal, just rotated).

*To be presented in class on Friday.

Experiment #1: Crystallography at home.
Build a conventional unit cell of cubic zinc suflide as shown in Kittel's Fig. 1.26 (see also Myers' Fig. 2.12). Your crystal kit contains gold, black, and white spheres. The gold and black spheres represent zinc. For clarity, use gold for the corner sites and black for the face-centered sites. The white spheres represent sulfur. There are four sulfur atoms inside the unit cell. Use the large white spheres for these. Use the small while spheres as sulfur atoms outside the unit cell needed to provide connections to the four unconnected corner sites shown in Kittel's figure. Make a list of the coordinates of *every* sphere in your model following the system used by Kittel in describing the ZnS structure.