Physics 617 Problem 7   Due Monday, Oct. 29

(1) (a) For the simple cubic lattice of cube edge a, show that the lattice planes indexed by Miller indices (h, k, l) are separated by,

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}.$$

(b) For the orthorhombic lattice, with perpendicular cell edges a, b, and c, find the corresponding relationship for d in terms of the Miller indices.
[The rule for direction cosines of a 3d vector may be helpful: the sum of the three squares is equal to 1.]

(2) In the handout from Oct. 17, on the last page the nonzero x-ray reflection lines are shown for the simple cubic, BCC, and FCC lattices. The highest-order lines illustrated are (311) for simple cubic, (332) for BCC, and (440) for FCC. In each case find the next nonzero reflection line.

(3) X-ray scattering for GaAs: As described in class, the GaAs structure is similar to the diamond structure, except that the basis consists of two different atoms. Consider the atomic form factors for Ga and As to be f_{Ga} and f_{As}, respectively. Show that the structure factor has four different values, depending upon the reciprocal lattice vector, G. Find expressions for the structure factor in terms of f_{Ga} and f_{As}.

Note: there would be <u>three</u> different values if f_{Ga} and f_{As} were both real. The form factors include non-zero imaginary parts since the scattering has a phase shift that is slightly different for each atom. These phase shifts are particularly noticeable when the x-ray energy is near a resonant excitation for one of the constituent atoms, but in general the imaginary parts are small, and sometimes they are neglected.

(4) At low enough temperatures, the discreteness of lattice modes becomes important, and the behavior can deviate from the large-sample limit which we have been assuming. This is significant for very small samples.
(a) Assume a cubic sample, edge L, and modes determined by periodic boundary conditions. Using the Debye approximation with speed of sound c, at what temperature will the thermal energy equal the energy required to add one phonon in the lowest-frequency mode?
(b) If c = 3000 m/s, calculate the temperature from part (a) for L = 1 μm, and for L = 1 nm.
(c) For temperatures much smaller than calculated above, we can safely include only the lowest-energy mode (plus any possible degeneracy for this mode) in calculating average energies. Determine the specific heat in this case, showing that it decays exponentially rather than the usual T^3 behavior of the Debye model.