PHYS 353 SOLID STATE PHYSICS STUDY GUIDE FOR PART 1

Crystal Structure

OUTLINE:

A. Basis

B. Lattice
   1. lattice vectors
   2. symmetries
   3. primitive lattice cell
   4. rotations, reflections, inversions
   5. Bravais lattices

C. Crystal directions and planes
   1. Miller indices
   2. body centered
   3. face centered
   4. NaCl, CsCl, diamond
   5. bonding

D. Fourier Series

E. Diffraction
   1. review
   2. Bragg's Law
   3. reciprocal lattice
   4. Brillouin zones
   5. amplitude factor, structure factor, atomic form factor
   6. temperature dependence

F. Crystal Binding
   1. Ionic
   2. Covalent
   3. Metal
   4. VandeWaal forces

STUDY QUESTIONS: (for 1st test - not for collected homework assignment)

1. Distinguish between basis, lattice, and crystal structure.

2. For a 2-D lattice, draw the 5 types of lattices and give the special symmetry operations that distinguish each from the rest.

3. Distinguish the NaCl from the CsCl structure. Give the basis and lattice type of each. Also distinguish the hcp from the fcc lattice.

4. Show the expansion of a periodic function in terms of a Fourier Series, and show how to determine the coefficients.

5. What is the Bragg Law for diffraction? How can it be explained by the wave theory?

6. Define the reciprocal lattice vector (**G**). Expand n(**r**) in a Fourier series and then show that n(**r**+**T**) = n(**r**) where **T** is a lattice translation vector, **r** is any position in the lattice, and n is the electron density.

7. Define the Brillouin zone and indicate how it relates to the Bragg Diffraction condition.

8. Define the scattering amplitude and relate the structure factor to it. Relate the form factor to the structure factor.

COLLECTED HOMEWORK ASSIGNMENTS:

1. Draw **five** different types of 2-D lattices, identify each type, and tell what distinguishes each type from the others.

2. In an sc lattice:
   a) where do the atoms touch?
   b) what is the side length, s, in terms of the radius of the atoms, r ?
   c) what is the hole size (diameter of sphere that would fit there) in terms of the side length?
   d) what is the hole size in terms of the radius of the atoms?

3. Answer the questions posed in problem 2 for an fcc lattice.

4. Answer the questions posed in problem 2 for a bcc lattice.

5. What is the packing fraction for: a) an sc type lattice? b) an fcc lattice? c) a bcc lattice?

6. Based on your answers to problems 2, 3 and 4, and based on the sizes of Na, Cs, and Cl ions given here: the Cl has a radius of 1.81 Angstroms; the Na 0.97 Angstroms, and the Cs 1.67 Angstroms; which lattice type would you expect for NaCl and which for CsCl - and WHY?

7. Demonstrate by means of a drawing that shows areas above and below the axis for two cases (i.e., chose different values for n and m values for each case) that:

$$\int_0^{2\pi} \sin(n\theta)\cos(\mathrm{m}\theta)\mathrm{d}\theta = 0$$

8. For a bcc lattice where $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are the primitive space lattice vectors, a is the side of the cube, and n,m,p are integers:

a) show that $n\mathbf{a}_1 + m\mathbf{a}_2 + p\mathbf{a}_3$ can reach all of the following lattice points: (a,0,0), (0,a,0), (0,0,a), (a,a,0), (½a,½a,½a);

b) show $\mathbf{a}_1$ is not perpendicular to $\mathbf{a}_2$ [Hint: recall what a dot product is];

c) show that $\mathbf{a}_1' = a\boldsymbol{x}$, $\mathbf{a}_2' = a\boldsymbol{y}$, $\mathbf{a}_3' = a\boldsymbol{z}$ do **not** form a set of primitive axis vectors (i.e., show that an integer combination of these do not reach all lattice points);

d) find the volume of the primitive lattice cell;

e) find $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ for the primitive lattice where $\mathbf{b}_i$ are the reciprocal lattice vectors.