

Physics 140A: Homework Problem Set 3

Assigned 1/20/05. Due 1/27/05.

1. Fourier Components. 10 points.

A simple 1D lattice problem: find the Fourier components of

$$f(x) = A\sin(2\pi x/a) + B\cos(4\pi x/a) + C\sin(10\pi x/a)\cos(12\pi x/a).$$

The lattice constant is denoted by a .

2. Structure Factor. 10 points.

Determine the structure factor for these three lattices: diamond, ZnS, NaCl. [The last two are known by these names: zincblende, rocksalt, respectively.]

3. Structure Factor for the HCP Lattice. 10 points.

The *hexagonal close-packed* (hcp) structure for an elemental material (Be, Zn, Gd are examples) consists of a hexagonal Bravais lattice (described in text) and a basis of two atoms in the primitive cell, at $(0, 0, 0)$ and at $\frac{2}{3}\vec{R}_1 + \frac{1}{3}\vec{R}_2 + \frac{1}{2}\vec{R}_3$.

(a) Calculate the fundamental reciprocal vectors $\vec{G}_1, \vec{G}_2, \vec{G}_3$; show work.

(b) For a general reciprocal lattice vector $\vec{G} = h\vec{G}_1 + k\vec{G}_2 + \ell\vec{G}_3$, calculate the structure factor and identify regularities, extinctions, etc. Interpret what you find,

4. Angle in X-ray Diffraction. 10 points.

Cu $K\alpha$ radiation, which is 8028 eV, is used to study the crystal structure of a simple cubic crystal that has a lattice constant of 5\AA .

(a) What is the wavelength of the radiation? Then what is the magnitude of the wavevector \vec{k} ?

(b) For the (111) reflection, what is the angle between \vec{k} and \vec{k}' ? This is an application of Bragg's law. {Experimentally, one would measure this angle, which is 2θ in terms of the angle we used for discussing diffraction ("take a 2θ scan") and thereby learn the distance between (111) planes, or equivalently, the length of the (111) reciprocal lattice vector.}