

Physics 481: Condensed Matter Physics - Homework 3

due date: Friday, Feb 4, 2011

Problem 1: Hcp extinctions (Marder, problem 3.2, 20 points)

- a) The hexagonal Bravais lattice can be defined by the primitive vectors $(a, 0, 0)$, $(a/2, a\sqrt{3}/2, 0)$ and $(0, 0, c)$. Prove that the reciprocal lattice is another hexagonal lattice rotated by 30° with respect to the original one and find primitive vectors for the reciprocal lattice.
- b) The hcp lattice is built upon the hexagonal Bravais lattice with basis $(0, 0, 0)$ and $(a/2, a/(2\sqrt{3}), c/2)$. Show that the modulation factor induced by the basis is

$$F_{\vec{q}} = \left| 1 + e^{i(\pi/3)[2(n_1+n_2)+3n_3]} \right|^2$$

where n_1, n_2, n_3 are the coefficients of the momentum transfer in terms of the reciprocal primitive vectors.

- c) Find all Bragg peaks of the hexagonal lattice for which scattering from the hcp lattice vanishes by extinction.

Problem 2: Debye-Waller factor (20 points)

In the early days of X-ray structure determination, people posed the following objection: Due to the thermal motion, the atoms will not be exactly at their lattice positions but rather oscillate around them. Shouldn't this destroy the sharp Bragg peaks?

To explore this question, assume that the displacement of each atom from its lattice position \mathbf{R}_l is a random vector \mathbf{u}_l with a Gaussian distribution

$$P(\mathbf{u}_l) = \left(\frac{1}{2\pi\Delta^2} \right)^{3/2} e^{-\mathbf{u}_l^2/(2\Delta^2)} .$$

Average the structure factor

$$S(\mathbf{q}) = \frac{1}{N} \left| \sum_l e^{i\mathbf{q}\cdot(\mathbf{R}_l+\mathbf{u}_l)} \right|^2 .$$

Do you still find sharp Bragg peaks? What happens to the amplitude of the peaks?