Physics 601 **Homework Set 1** **Fall, 2007**

Due date: Monday Sept. 24.

Reading: Ziman Ch. 1; Kaxiras Ch. 1.1, 3.1-2, 3.6-8

1) (25 points.)
(In class, I presented an analysis of the following problem for the case of a bcc crystal, but now we do it for an fcc one.)
If a *conventional cubic* unit cell is used to describe an fcc crystal:
   a) What are the allowed values for the indices (n_1, n_2, n_3) and (m_1, m_2, m_3) of the real and reciprocal lattice vectors, respectively?
   b) Consider the (001) plane and the [001] row in the conventional notation. How would these be indexed using the primitive vectors?

2) (15 points.) Let $f(\mathbf{r})$ be a superposition of the localized, spherically-symmetric functions $v(r)$ at atomic sites:

$$f(\mathbf{r}) = \sum_{ij} v\left(|\mathbf{r} - \mathbf{R}_i - \boldsymbol{\tau}_j|\right)$$

where $\mathbf{R}_i$ are the lattice vectors and $\boldsymbol{\tau}_j$ are the basis vectors giving the positions of the atom within the unit cell.
   a) Show $f(\mathbf{G}) = S(\mathbf{G})V(G)$ where $G = |\mathbf{G}|$,

$$S(\mathbf{G}) = \sum_{j} e^{-i\mathbf{G}\cdot\boldsymbol{\tau}_j} \ ,$$

   and

$$V(q) = \frac{4\pi}{\Omega q} \int_0^\infty dr\ r\, v(r)\ \sin(qr) \ .$$

   $S(\mathbf{G})$ and $V(q)$ are called the structure factor and form factor, respectively.
   b) Show $S(\alpha\mathbf{G}) = e^{-i(\alpha\mathbf{G})\cdot\boldsymbol{\tau}} S(\mathbf{G})$ if $\{\alpha|\boldsymbol{\tau}\}$ is a symmetry of the crystal.

3) (20 points.)
The simple hexagonal crystal structure is a Bravais crystal with lattice vectors $\mathbf{a}_1 = \frac{a\sqrt{3}}{2}\hat{x} - \frac{a}{2}\hat{y}$, $\mathbf{a}_2 = \frac{a\sqrt{3}}{2}\hat{x} + \frac{a}{2}\hat{y}$, $\mathbf{a}_3 = c\hat{z}$.
   a) Find the primitive reciprocal lattice vectors, and show that the resulting reciprocal lattice to the hexagonal lattice is another hexagonal lattice rotated by 30° with respect to the real-space one.

b) The hcp lattice is built upon the hexagonal one, with a basis given by $\boldsymbol{\tau}_1 = 0$, $\boldsymbol{\tau}_2 = \frac{a}{\sqrt{3}}\hat{x} + \frac{c}{2}\hat{z}$. Show that the structure factor $S(\mathbf{G})$ (see previous problem) is given by

$$S(\mathbf{G}) = 1 + e^{2\pi i\left(\frac{1}{3}m_1 + \frac{1}{3}m_2 + \frac{1}{2}m_3\right)}$$

where $\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$.

c) Find the $\mathbf{G}$'s for which there are "missing spots" ("extinctions").

4) (25 points.) A two-dimensional crystal has a rectangular unit cell defined by $\mathbf{a}_1 = (a, 0)$ and $\mathbf{a}_2 = (0, b)$, and there are four identical atoms per cell at $\boldsymbol{\tau}_1 = (x_0, y_0)$, $\boldsymbol{\tau}_2 = (-x_0, y_0)$, $\boldsymbol{\tau}_3 = (\frac{a}{2} + x_0, -y_0)$, $\boldsymbol{\tau}_4 = (\frac{a}{2} - x_0, -y_0)$.

a) Sketch the crystal, showing several unit cells. So that all our sketches look similar, let's take $a > b$, $x_0 \simeq a/10$, and $y_0 \simeq b/6$.

b) Find the primitive reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$, and sketch the Brillouin zone.

c) List all of the symmetry operators in the point group. For those operations that are non-symmorphic (given the above choice of origin), give the associated translation vector. Is the crystal symmorphic?

d) Are there missing spots in the diffraction pattern associated with the non-symmorphic operations? Explain.

e) Suppose $y_0 = b/4$ exactly. Is the primitive unit cell area still the same? If not, give a new set of primitive real-space lattice vectors and report the area of the new unit cell.