**Midterm Exam: Solid State Physics 476**
**Oct. 17, 2005**

Solution guide

1. Consider a simple cubic Bravais lattice.

   (a) What is the relationship between the lattice vectors (lengths and angles)? (2)

   **Answer:** $a = b = c$ or $a_1 = a_2 = a_3$ or $|\vec{a}_1| = |\vec{a}_2| = |\vec{a}_3|$. $\alpha = \beta = \gamma = 90^o$ or just say all angle are $90^o$.

   (b) Draw a sketch of the plane perpendicular to the 4-fold symmetry axes with the lattice points. Also sketch in the unit cell and indicate the positions of the 4-fold axes with a square. (4)

   **Answer:** This is just a square lattice. The conventional unit cell is just a square with lattice points at the corners. The 4-fold axes are at the lattice points and the cell centres.

   (c) What does it mean to add a "basis"? Give the basis if this is a body centred cubic system. (2)

   **Answer:** A basis is a spatial set of atoms (atom types and positions, often given in terms of the lattice units) that attaches to each lattice point. If this is a bcc then the basis that attaches to simple cubic is 000, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, both atoms the same.

   (d) What is one of the extra symmetry operations that a body-centred cubic lattice has as opposed to a simple cubic lattice? (You may have to consider elements that are not in the x-y plane and use results you know from 2-D as a guide. Specifically think of a symmetry operation that maps the basis atoms onto each other.) (2)

   **Answer:** This a bit tricky. The key location is at $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ (it is the point that is unchanged in the point group operations). From here you can have an inversion, a mirror plane perpendicular to [111], a two fold-axis that is perpendicular to [111] and passes through a cube edge, or (I think the one that really shows up but isn't a point group) a screw axis that is perpendicular to the cube faces but goes through a $\frac{1}{4}\frac{1}{4}$ position.

   (e) What is the benefit of using the non-primitive cubic unit cell? (2)

   **Answer:** It "looks" cubic so you can immediately see the 4-fold axis. The primitive cell may have a clearer 3-fold axis but the 4-folds are hard to see.

2. Consider a face-centred cubic crystal structure with a lattice constant of 5.5 Å.

   (a) Give the length of the reciprocal lattice vector associated with the (200) plane. (hint: $\vec{G} = h\vec{A} + k\vec{B} + l\vec{C}$) Feel free to take some shortcuts if you know the values for $\vec{A}$, $\vec{B}$, and $\vec{C}$. (2)

   **Answer:** You know that the reciprocal lattice vector for a cubic system are in the $x, y, z$ directions and each have length $\frac{2\pi}{a}$. Since $h = 2$ we have $|\vec{G}| = 4\pi/a = 2.28$ Å$^{-1}$.

   (b) What is the Laue condition for scattering? If the magnitude of the wavevector of the incident radiation is 4 Å$^{-1}$ draw the appropriate scattering diagram showing initial $\vec{k}_i$, final -$\vec{k}_f$ and $\vec{G}$. Calculate the scattering angle, what we usually call $2\theta$. (6).

   **Answer:** The Laue condition for scattering is $\Delta\vec{k} = \vec{G}$, $2\vec{k}_i \cdot \vec{G} = G^2$, or $\vec{k}_i \cdot \hat{G} = \frac{1}{2}G$. In 2006, I have tried to stay consistent with the book so that $\Delta\vec{k} = \vec{k}_f - \vec{k}_i$ so it would amke more sense to draw initial $-\vec{k}_i$, final $-\vec{k}_f$ along with $\vec{G}$. It is just an isosceles triangle with sides 4, 4, and 2.28. [if ($h00$) is depicted in the $x$ direction of reciprocal space then $\vec{G}$ would point this way and should terminate on a reciprocal lattice point. $2\theta$ is the angle at the apex of the triangle. Can get it from the law of cosines

$$2\theta = \cos^{-1}\left(\frac{16 + 16 - (2.28)^2}{(2)(4)(4)}\right) = 33.1^{\circ} \tag{1}$$

or simple construction since it is an isosceles triangle.

3. (a) What is the fundamental assumption concerning symmetry in a crystalline lattice? Give a mathematical statement. What are two instances in condensed matter physics studies where this would be violated? (Keywords please.) (5)

   **Answer:** The fundamental assumption is that of infinite translational symmetry. If $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ are three (linearly independent) vectors then all lattice points defined by

$$\vec{r} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3 \tag{2}$$

   with integer $u$ values are physically equivalent. I didn't cover the second part in 2006 but you could speak of glasses (amphorphous materials), surfaces, finite sized crystals, quasi-crystals, crystalline defects.

   (b) How are crystal structures classed? Is there an infinite numbers of possible crystal structures? (4)

   **Answer:** They are classed by their symmetry operations. For crystals (as opposed to just lattices) in 3-D there are 230 *space groups* that describe the possible unique sets of symmetry operations.

   (c) What are the three primary types of beams used for diffraction studies? Give two quick facts for each of the three types (such as type of source, expense, special features or limitations). (9)

   **Answer:**

   - X-rays: high energy, short wavelength photons, Cu tubes, synchrotron, interact with electrons, fairly inexpensive lab sources, not good at probing bulk or seeing hydrogen, high resoluiton possible
   - Neutrons: reactor sources, spallation sources, deBroglie waves, can scatter from nuclei, weak probe, senstive to bulk, expensive and only a few sources, sensitive to magnetism
   - Electrons: tens eV to thousands of eV, strongly interacts with sufaces, needs extremely clean surfaces, lots of electron guns, hard to use to determine bulk crystal structure, can use with focusing optics.

4. Bonus:Describe with a diagram a glide transformation. (4)

   **Answer:** see your notes, translation plus reflection, translation should either be half or a quarter of a unit cell dimension