489 Spring 2004 Homework 3

Due Wednesday, Feb. 11, 2004

1. A&M problem 5.1.

2. A&M problem 5.3.

3. In this problem you are asked to derive the structure factors for BCC, FCC and diamond using the conventional unit cell, i.e., each crystal is considered as simple cubic with translations $\mathbf{R} = a(n_1\hat{\mathbf{x}} + n_2\hat{\mathbf{y}} + n_3\hat{\mathbf{z}})$ and more than one atom in the basis. You may start from the general expression for the scattering amplitude of a crystal

$$F(\mathbf{q}) = \sum_{j=1}^{N_{atom}} f_j(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r_j}} \tag{1}$$

   (a) For BCC and FCC the form factors $f_j(\mathbf{q})$ are rigorously the same for each atom j in the conventional cell. Then $F(\mathbf{q}) \equiv f(\mathbf{q})S(\mathbf{q})$, where $S(\mathbf{q})$ is the geometrical structure factor. For each case:

      i. Write down the coordinates of the atoms in the conventional unit cell.

      ii. Write down the expression for $S(\mathbf{q})$ as a complex function of the indices h, k, l in the definition, $\mathbf{q} = (2\pi/a)(h\hat{\mathbf{x}} + k\hat{\mathbf{y}} + l\hat{\mathbf{z}})$

      iii. Determine the pattern of indices for which $S(\mathbf{q}) = 0$. Show that the reciprocal lattice vectors $\mathbf{q}$ for which $S(\mathbf{q}) \neq 0$ are the same as one finds when BCC and FCC lattices are treated as Bravais lattices.

   (b) For the diamond lattice do the same exercise. Assume the form factors are isotopic and the same for all atoms, i.e., $f_j(\mathbf{q}) = f(|q|)$.

      i. Give the values of the structure factor $S(\mathbf{q})$ as a function of $\mathbf{q}$.

      ii. Which reflections are allowed in FCC but not diamond? What about the reverse statement?

      iii. In fact, the finding that some FCC scattering amplitudes have zero strength in the present analysis for diamond is an approximation. *Some* of the cases found here to have zero structure factor, even though they are allowed for FCC, are not rigorously zero for real diamond crystals. Can you think of a reason why the assumptions made here for diamond are not rigorously correct?

4. A&M problem 6.1.

5. A&M problem 6.5.

You do not need to turn in the following suggested problems:

1. Brillouin zone geometry for FCC. Cut out the model of a truncated octahedron on the attached sheet. Fold it up using tabs and slots provided (or scotch tape). Compare with figure 5.2(b), and satisfy yourself that such objects can fill space completely. Note the conventional names given to the high symmetry points. Save your model for reference later on in the semester.
   (courtesy of Kevin O'Donovan, former P489 student, and Prof. I. Robinson)

2. Problems 5.2(a) and 6.2 of A&M, problems 1.3 and 1.17 of Mihaly and Martin, and problems 2.1, 2.2, and 2.4 of Kittel.