Department of Physics, University of Maryland, College Park, MD 20742-4111

Physics 731 HOMEWORK ASSIGNMENT # 2 Due: Sept. 18, 2007 (Deadline: Sept. 20)
Read Ashcroft & Mermin (A&M), chaps. 5-6; Feng & Jin, 1.4, 2.2.4, 2.2.5, 2.3.2

1. A&M 5-3
2. A&M 6-2

3a) Show as a corollary to problem 2 [A&M 6-2] that the {111} planes of a simple cubic crystal are triangular lattices. (So are the {111} planes of the bcc crystal.) What is the interplanar spacing? [Hint: problem 1, A&M 5-3, may be helpful.]
b) For an fcc crystal, viewed from the [111] direction as a sequence of stacked close-packed planes, write down a third primitive vector $\mathbf{a_3}$, given that the first two are in a close-packed plane [e.g. $\mathbf{a_1} = a_{NN}\,\mathbf{x}$; $\mathbf{a_2} = (a_{NN}/2)\,(\mathbf{x} + \mathbf{y}\sqrt{3})$]. (I.e., find the components of $\mathbf{a_3}$ along $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$. Note that a_{NN} is the nearest-neighbor distance, so (1/2) times the conventional lattice constant. I often write a_{NN} as a_1, but in this case that might invite confusion.) Then show explicitly how the ABCABC stacking sequence is realized, i.e. that after 3 translations by $\mathbf{a_3}$ the lattice points coincide with those in the original plane, translated perpendicular to this plane by 3 times the interplanar spacing *d*.

4. A&M 6-3
5. A&M 6-5

6. Consider the reciprocal lattice of a two-dimensional (2D) or planar lattice (in a 3D space).
a) Write $\mathbf{k} = \mathbf{k}_{\parallel} + k_Z\mathbf{e}_Z$. Show that $\mathbf{K}_{3D} = \mathbf{K}_{2D} + K_Z\mathbf{e}_Z$, where K_Z is arbitrary, so that the reciprocal lattice can be represented by a net of rods. For elastic scattering, $|\mathbf{k}| = |\mathbf{k}|'$, write the relation between $\mathbf{k}_{\parallel}$ and $\mathbf{k}_{\parallel}'$. (Hint: Consider a 2D lattice as the limit of a (3D) family of planes with interplanar spacing *d* going to infinity. Cf. class websites, category "Reciprocal Lattices," item: Ewald construction for a surface or 2D lattice.) What added constraint comes from energy conservation?
b) Generalize Fig. 6.7 to show the Ewald construction for diffraction from a 2D lattice. Note that one observes a diffraction pattern of electrons from a surface for all values and orientations of the incident wavevector **k** above a critical value.
c) Show that for electrons incident perpendicularly on a {100} surface of a copper crystal, the critical (i.e. minimum) *energy* at which the first diffracted beam appears (as incident energy is raised) is about 22 eV. (Use the handy relationship $\lambda(\text{Å}) \approx 12/[E(\text{eV})]^{1/2}$. Note that the periodic table inside the front cover of A&M provides lattice constants of the elements, as well as lots of other information; alternatively, if you have Marder's text, use his table 2.1.)

7. a) i) Using problems 4 & 6, describe the reciprocal lattice of a sheet of graphene (i.e. a planar honeycomb).
ii) What is the geometric structure factor of each rod?
b) Complete the exercise in class showing the equivalence of lattice planes and reciprocal lattice points for fcc and bcc lattices: Find the explicitly the area of the unit cell of each of the 3 densest

planes for both cases, and then multiply by the corresponding interplanar spacing d to show that the volume of the unit cell is the same for the 3 lattice-family decompositions.

Read and think about (but do not turn in) A&M 5-4, A&M 6-4, as well as what happens if [a piece of] the graphene sheet is rolled into a carbon nanotube.