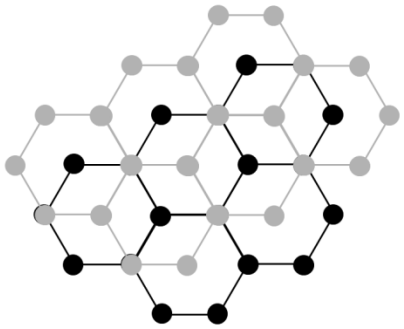
Phys 231, Fall 2007, Homework 1, due Oct 12

(4 points per each problem)

1. Problem 4.6 of A&M
2. Problem 5.3 of A&M
3. Problem 6.5 of A&M
4. The crystal structure of graphite is shown schematically (and only partially in each infinite honeycomb lattice plane) here, with each circle denoting a C atom. The two honeycomb lattices, black and gray, are separated by 3.36 Å, while the shortest C-C distance in the diagram is 1.42 Å. Various stacking sequences occur in graphite, but the most common one is the AB stacking (…-A-B-A-B-…), in which the two honeycomb lattices shown here are repeated indefinitely perpendicular to the paper. (a) What is the primitive Bravais lattice of this structure? Give the value of lattice parameters (a,b,c, and angles). What is the ratio of c/a and how does it compare with the hcp value? How many C atoms comprise the primitive basis? Give their coordinates in terms of a,c and standard unit vectors in the Cartesian coordinate. (b) If this structure is invariant under a translation operation whose z-component is 3.36 Å (the spacing of the honeycomb lattices), identify such operation(s). How about screw axis operation(s)? How about glide plane operation(s)? Is the space group of graphite symmorphic or non-symmorphic? [Non-symmorphic space group often has interesting unusual consequences in spectroscopy, as in high temperature superconductors.]



5. For a hexagonal Bravais lattice, let's define primitive vectors $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$ as $|\mathbf{a_1}|=|\mathbf{a_2}|=a$, $|\mathbf{a_3}|=c$, angle($\mathbf{a_1}$, $\mathbf{a_2}$)=120^o, and angle($\mathbf{a_1}$, $\mathbf{a_3}$)=angle($\mathbf{a_2}$, $\mathbf{a_3}$)=90^o. Consider a basis consisting of three identical atoms [or molecules] placed at origin, $(2\mathbf{a_1}+\mathbf{a_2}+\mathbf{a_3})/3$, and $-(2\mathbf{a_1}+\mathbf{a_2}+\mathbf{a_3})/3$. What is the primitive lattice of this structure, in the case of arbitrary values of a,c? [You may now understand why, for this particular primitive lattice, researchers almost always use the hexagonal lattice for defining the lattice system or the conventional unit cell.] What is the primitive lattice of this structure when c/a is the close-packing ratio $\sqrt{\frac{8}{3}}$ (this is not a trick question, but merely a reminder of what we covered in class)?