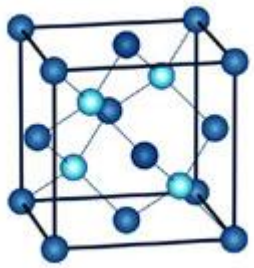
ESS 551Homework 2, Due October 12, 2006

1. The angles between the tetrahedral bonds of diamond are the same as the angles between the body diagonals of a cube. Use elementary geometry/vector analysis to find the value of the angle.



2. Volume of a Brillouin Zone. Show that the volume of the first Brillouin zone is $(2\pi)^3/V_c$, where V_c is the volume of a crystal primitive cell. Hint: Go back to the equations that define reciprocal lattice directions and work through this.

3. Show that the simple cubic lattice can be represented as a trigoanl lattice with primitive vectors $\mathbf{a}_i$ at 60° angles to one another with a two-point basis ±¼ ($\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$).

4. What structure results if the basis of the trigonal lattice in problem 3 is taken to be ±(1/8)

5. Below are some deflection angles of an xray experiment carried out to high pressures. The anode material was Mo (λ = 0.703 Å) and the material is MgO (the values below 6 GPa are taken from a real data set. You will find uncertainties typical in a simple experiment. You will need to average d values). The final goal is to determine the lattice constants at each pressure, plot V/V_0 versus pressure, and estimate a K_{T0} from this data.

At atmospheric pressure, the lattice constants of MgO are:

d/ A	I/I_o	hkl
2.431	10	111
2.106	100	200
1.489	52	220
1.270	4	311
1.216	12	222
1.0533	5	400
0.9665	2	331
0.9419	17	420
0.8600	15	422
0.8109	3	511

Questions for to be answered for the included excel file of values for MgO angles versus pressure.

a. Find the d values for each reflection
b. Find the reduced volume from the averaged value (where necessary).
c. Make a table of pressures versus V/V_0
d. Plot these values and calculate the initial bulk modulus for MgO.