Phys 4050 Assignment 1

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

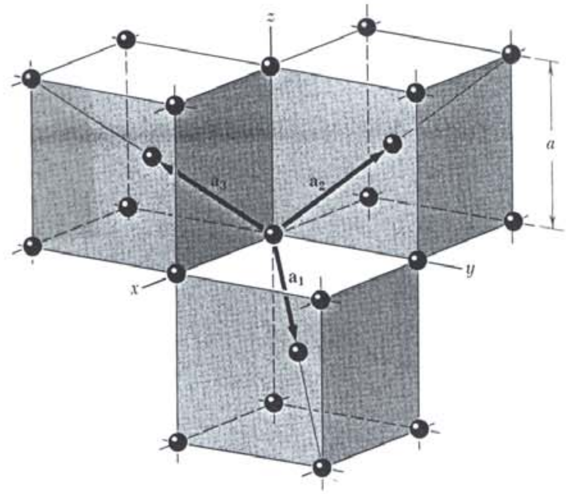

Figure 12 Primitive translation vectors of the body-centered cubic lattice; these vectors connect the lattice point at the origin to lattice points at the body centers. The primitive cell is obtained on completing the rhombohedron. In terms of the cube edge a the primitive translation vectors are

$$\mathbf{a}_1 = \tfrac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) ; \quad \mathbf{a}_2 = \tfrac{1}{2}a(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}) ;$$
$$\mathbf{a}_3 = \tfrac{1}{2}a(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}) .$$

2. Indices of planes. Consider the planes with indices (100) and (001); the lattice is fcc, and the indices refer to the conventional cubic cell. What are the indices of these planes when referred to the primitive axes of the figure shown below?

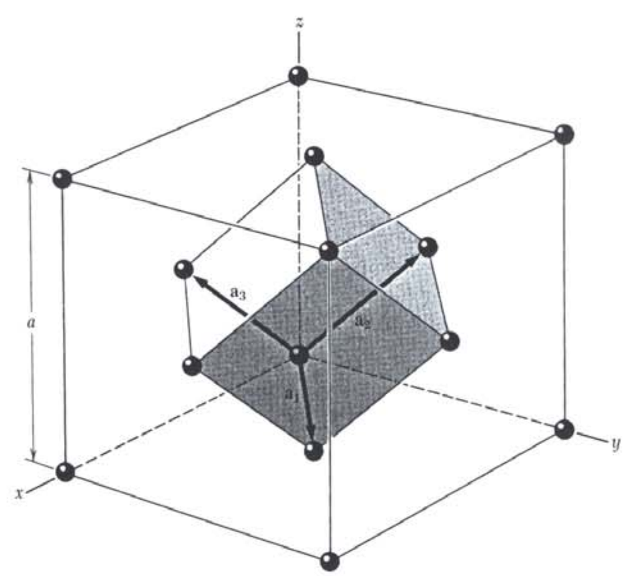

Figure 13 The rhombohedral primitive cell of the face-centered cubic crystal. The primitive translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ connect the lattice point at the origin with lattice points at the face centers. As drawn, the primitive vectors are:

$$\mathbf{a}_1 = \tfrac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}}) ; \quad \mathbf{a}_2 = \tfrac{1}{2}a(\hat{\mathbf{y}} + \hat{\mathbf{z}}) ; \quad \mathbf{a}_3 = \tfrac{1}{2}a(\hat{\mathbf{z}} + \hat{\mathbf{x}}) .$$

3. Hexagonal space lattice. The primitive translation vector of the hexagonal space lattice may be taken as

$$\vec{a}_1 = \frac{\sqrt{3}}{2} a\hat{x} + \frac{a}{2}\hat{y} \qquad \vec{a}_2 = -\frac{\sqrt{3}}{2} a\hat{x} + \frac{a}{2}\hat{y} \qquad \vec{a}_3 = c\hat{z}$$

a) Show that the volume of the primitive cell is $3^{1/2} a^2 c/2$.

b) Show that the primitive translations of the reciprocal lattice are

$$\vec{b}_1 = \frac{2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y} \qquad \vec{b}_2 = -\frac{2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y} \qquad \vec{b}_3 = \frac{2\pi}{c}\hat{z}$$

so that the lattice is its own reciprocal, but with a rotation of axes.

c) Find the volume of the first Brillouin zone.

4. Structure factor of diamond. The crystal structure of diamond is described by a basis consisting of eight atoms if the unit cell is taken as the conventional cube.

a) Find the structure factor S of this basis.

b) Find the zeros of S and show that the allowed reflections of the diamond structure satisfy h + k + l = 4n where all indices are even and n is any integer, or else all indices are odd.

5. Form factor of atomic hydrogen. For the hydrogen atom in its ground state, the number density is $n(r) = (\pi a_o^3)^{-1} \exp(-2r/a_o)$ where a_o is the Bohr radius. Show that the form factor is $f_G = 16\,(4 + G^2 a_o^2)^2$.