

Exercises for Physics 460

Problem Set 4; Due Wednesday, February 27

1) **Hcp structure.** Show that the c/a ratio for an ideal hexagonal close-packed structure is $\sqrt{8/3} = 1.633$. If c/a is significantly larger than this value, the crystal structure may be thought of as composed of planes of closely packed atoms, the planes being loosely stacked.

2) Calculate the fraction of space which can be filled by hard spheres arranged in:
a) a simple cubic lattice; b) a body-centered cubic lattice; c) a face-centered cubic lattice.

3) **Interplanar separation.** Consider a plane hkl in a crystal lattice. (a) Prove that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to this plane. (b) Prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = 2\pi/|\mathbf{G}|$. (c) Show for a simple cubic lattice that $d^2 = a^2/(h^2 + k^2 + l^2)$.

4) **Hexagonal space lattice.** The primitive translation vectors of the hexagonal space lattice may be taken as

$$\mathbf{a}_1 = (\sqrt{3}a/2)\hat{x} + (a/2)\hat{y}; \quad \mathbf{a}_2 = -(\sqrt{3}a/2)\hat{x} + (a/2)\hat{y}; \quad \mathbf{a}_3 = c\hat{z}.$$

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

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

$$\mathbf{b}_1 = (2\pi/\sqrt{3}a)\hat{x} + (2\pi/a)\hat{y}; \quad \mathbf{b}_2 = -(2\pi/\sqrt{3}a)\hat{x} + (2\pi/a)\hat{y}; \quad \mathbf{b}_3 = (2\pi/c)\hat{z},$$

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

(c) Describe and sketch the first Brillouin zone of the hexagonal space lattice.

5) **Volume of 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: the volume of a Brillouin zone is equal to the volume of the primitive parallelepiped in Fourier space. Recall the vector identity $(\mathbf{c} \times \mathbf{a}) \times (\mathbf{a} \times \mathbf{b}) = (\mathbf{c} \cdot \mathbf{a} \times \mathbf{b})\mathbf{a}$.

6) **Diatomic line.** Consider a line of atoms $ABAB \dots AB$, with an $A-B$ bond length of $a/2$. The form factors are f_A, f_B for atoms A, B , respectively. The incident beam of x-rays is perpendicular to the line of atoms. (a) Show that the interference condition is $n\lambda = a \cos \theta$, where θ is the angle between the diffracted beam and the line of atoms. (b) Show that the intensity of the diffracted beam is proportional to $|f_A - f_B|^2$ for n odd, and to $|f_A + f_B|^2$ for n even. (c) Explain what happens if $f_A = f_B$.