

Assignment 1: Introduction to Solid State Physics

1) Given that the primitive basis vectors of a lattice are $\mathbf{a}=(a/2)(\mathbf{i}+\mathbf{j})$, $\mathbf{b}=(a/2)(\mathbf{j}+\mathbf{k})$, and $\mathbf{c}=(a/2)(\mathbf{k}+\mathbf{i})$, where \mathbf{i}, \mathbf{j} and \mathbf{k} are the usual three unit vectors along cartesian coordinates, what is the Bravais lattice?

2) In each of the following cases explain whether the structure is a Bravais lattice or not. If it is, give three primitive vectors; if it is not, describe it as a Bravais lattice with a basis.

i) Base-centered cubic (simple cubic with additional points in the centers of the horizontal faces of the cubic cell).

ii) Side-centered cubic (simple cubic with additional points in the centers of the vertical faces of the cubic cell).

3) The face-centered cubic (fcc), body-centered cubic (bcc), and diamond structure are the three most important crystal structures for materials typically used by physicists and engineers. The simple cubic structure is a bit rare. The face-centered cubic is the most dense and the simple cubic is the least dense of the three cubic Bravais lattices. The diamond structure is less dense than any of these. One measure of this is the coordination number (number of nearest neighbors). What is the coordination number for each of the following.

i) simple cubic ii) face-centered cubic

iii) body-centered cubic iv) diamond

4) For the following, let the side of the cubic unit cell have length 1. In terms of this measure, calculate a) the nearest neighbor distance r_1 and b) the next-nearest neighbor distance r_2 for each of the following lattices.

i) simple cubic ii) face-centered cubic

5) Suppose identical solid spheres are distributed through space in such a way that their centers lie on the points of each of the following structures, and spheres on neighboring points just touch, without overlapping. (Such an arrangement of spheres is called a close-packing arrangement). Assuming that the spheres have unit density, show that the density of a set of close-packed spheres on each of the four structures (the so-called packing fraction) is:

$$\text{fcc: } \sqrt{2}\pi/6 = 0.74 \qquad \text{bcc: } \sqrt{3}\pi/8 = 0.68$$

$$\text{sc: } \pi/6 = 0.52 \qquad \text{diamond: } \sqrt{3}\pi/16 = 0.34$$