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Problems for *Physik der Materie III*

Due by April 24, 2019

Series 2: Crystal structure

2.1 Diamond lattice

The diamond lattice consists of two interpenetrating face-centered cubic (fcc) Bravais lattices, displaced along the body diagonal of the cubic cell by one quarter the length of the diagonal (Fig. 1). It can be regarded as a face-centered cubic lattice with a two-point basis: $(0,0,0)$ and $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$.

1) What is the angle α between any of the two bonds joining a site of the diamond lattice to its four nearest neighbors ? How many atoms make up the *primitive unit cell* ?

2) The *conventional unit cell* of the diamond lattice is cubic (Fig. 1). How many atoms make up the conventional unit cell ? Give examples of elements that crystallize in the diamond (dia) structure.

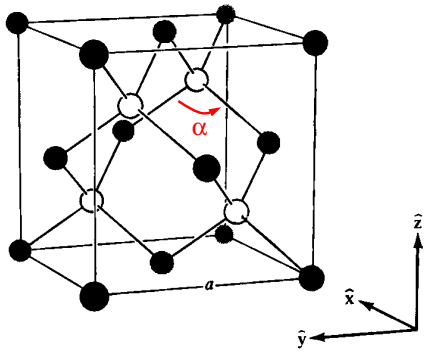

Figure 1: Conventional cubic unit cell of the diamond lattice. For clarity, sites corresponding to one of the two interpenetrating fcc lattices are represented by open circles.

2.2 Close Packing

A close-packing arrangement is defined by placing identical solid spheres on the sites of a given lattice, with the spheres on neighboring sites just touching without overlapping (*hard sphere model*). The close-packing arrangement for the face-centered cubic lattice is presented in Fig. 2.

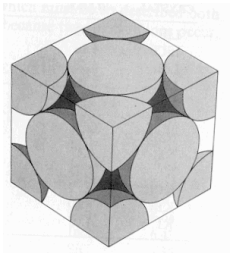

Figure 2: Hard sphere model of the fcc lattice.

1) Calculate the fraction of space ("packing fraction") filled by closely packed spheres arranged in the four following structures:

face-centered cubic (fcc):	0.74
body-centered cubic (bcc):	0.68
simple cubic (sc):	0.52
diamond (dia):	0.34

2) Prove that the ideal c/a ratio for the hexagonal close-packed structure is $\sqrt{8/3} = 1.633$.

3) What are the *coordination numbers*, i. e. the numbers of nearest neighbors, in the fcc, bcc, sc and dia lattices? Discuss the relation between coordination numbers and packing fractions.

2.3 Planar atomic density

The planar atomic density ρ of a crystal lattice plane is defined as

$$\rho = \frac{\textit{Number of atoms centered on a plane}}{\textit{Area of the plane}}$$

For the three cubic Bravais lattices, ρ can be given in units of $1/\mathrm{a}^2$, where a is the cubic lattice constant.

1) Show that the atomic densities of the (100), (110), and (111) planes of the fcc lattice are $\rho_{fcc}^{100} = 2/\mathrm{a}^2$, $\rho_{fcc}^{110}=\sqrt{2}/\mathrm{a}^2$, and $\rho_{fcc}^{111}=4/\sqrt{3}\mathrm{a}^2$, respectively.

2) Determine the corresponding planar atomic densities of the (100), (110), and (111) planes of the bcc lattice.

3) Which of the six planes is the most dense, and which is the least dense ?

4) Ni and Fe crystallize in the fcc and bcc structure, respectively (lattice constants $\mathrm{a}_{Ni}=3.52 \cdot 10^{-10}\mathrm{m}$ and $\mathrm{a}_{Fe}=2.87 \cdot 10^{-10}\mathrm{m}$). Calculate the planar atomic densities of the (100), (110), and (111) planes in units of $1/\mathrm{cm}^2$.