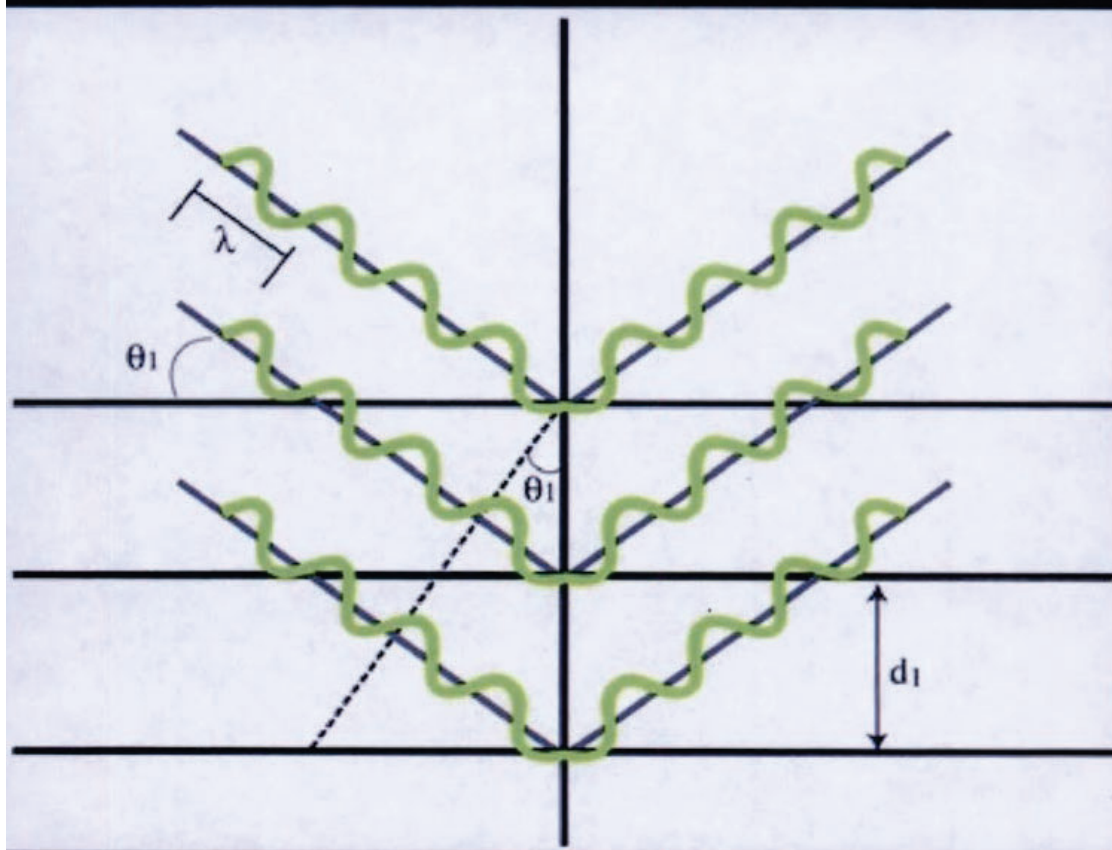


X-Ray Diffraction

A Practical Approach



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Close-Packed Structures

A close-packed structure is one that has the maximum volume of the unit cell occupied by atoms. The fraction of the unit cell occupied by atoms can be determined by calculating the atomic packing factor (APF) from the following equation:

$$\text{APF} = \frac{\text{number of atoms per cell} \times \text{volume of one atom}}{\text{volume of unit cell}} \quad (10)$$

We will go through the calculation of the APF for the fcc structure; you may calculate for the other cubic structures as an exercise.

Look back at the fcc structure in Fig. 20:

- The number of atoms per cell is 4.
- The volume of each atom is $(4/3)\pi r^3$ (we assume in these calculations that the atoms are rigid spheres with a radius r).
- The unit-cell volume is a^3 .

We can rewrite the lattice parameter a in terms of r (Fig. 21), where the figure shows that the atoms touch across the face diagonal of the cell. Therefore, $\sqrt{2}a = 4r$, or $a = 2\sqrt{2}r$. Using Eq. (10) we obtain

$$\text{APF} = \frac{4 \left(\frac{4}{3} \pi r^3 \right)}{(2\sqrt{2}r)^3} = 0.74$$

For the fcc structure, the atomic packing factor is 0.74. This is the *maximum* possible value for packing spheres of the same size. Crystal structures with an APF of 0.74 are called close-packed structures. Of the three cubic structures only the fcc structure is close-packed.

2.4.2. Two Atoms of the Same Kind per Lattice Point

The Hexagonal Close-Packed Structure

Many metals have the hexagonal close-packed (hcp) structure, including magnesium (Mg), titanium (Ti), zinc (Zn), and cadmium (Cd). The hcp structure is built on the hexagonal Bravais lattice with a basis consisting of two identical atoms associated with each lattice point. Using the relationship in Eq. (9), we have

Hexagonal P lattice + two atoms $\rightarrow$ Hexagonal close-packed (hcp) structure

Figure 22a shows the arrangement of atoms in the hcp structure. There are two atoms per unit cell, located at $0,0,0$ and $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$. However, in the