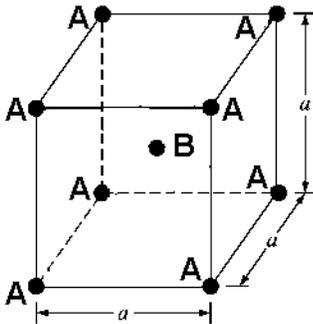


- 1.12** (a) A material is composed of two types of atoms. Atom A has an effective radius of 2.2 \AA and atom B has an effective radius of 1.8 \AA . The lattice is a bcc with atoms A at the corners and atom B in the center. Determine the lattice constant and the volume densities of A atoms and B atoms. (b) Repeat part (a) with atoms B at the corners and atom A in the center. (c) What comparison can be made of the materials in parts (a) and (b)?

a) bcc w/ atom B in the center



For this bcc lattice, the corner-to-corner diagonal is

$$d = r_A + 2r_B + r_A = 2r_A + 2r_B = \sqrt{a^2 + a^2 + a^2} = \sqrt{3}a.$$

Therefore, we get $a = (2r_A + 2r_B) / \sqrt{3} = [2(2.2) + 2(1.8)] / \sqrt{3}$

$$\Rightarrow \underline{a = 4.6188 \text{ \AA}}.$$

From the figure, the number of A atoms in the lattice is

$$8 \text{ corners } (1/8 \text{ atom/corner}) = 1 \text{ A atom.}$$

$$\text{A vol. \# density} = avd_A = 1 \text{ atom} / a^3 = 1 / (4.6188 \times 10^{-10} \text{ m})^3 = 1.0149 \times 10^{28} \text{ atoms/m}^3$$

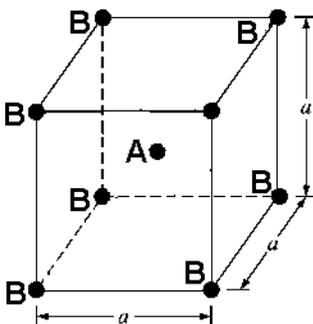
$$\Rightarrow \underline{avd_A = 1.0149 \times 10^{22} \text{ atoms/cm}^3}$$

From the figure, there is 1 B atom in the lattice at the center.

$$\text{B \# density} = avd_B = 1 \text{ atom} / a^3 = 1 / (4.6188 \times 10^{-10} \text{ m})^3 = 1.0149 \times 10^{28} \text{ atoms/m}^3$$

$$\Rightarrow \underline{avd_B = 1.0149 \times 10^{22} \text{ atoms/cm}^3}$$

a) bcc w/ atom A in the center



For this bcc lattice, the corner-to-corner diagonal is

$$d = r_B + 2r_A + r_B = 2r_A + 2r_B = \sqrt{a^2 + a^2 + a^2} = \sqrt{3}a.$$

Therefore, we get $a = (2r_A + 2r_B) / \sqrt{3} = [2(2.2) + 2(1.8)] / \sqrt{3}$

$$\Rightarrow \underline{a = 4.6188 \text{ \AA}}.$$

From the figure, there is 1 A atom in the lattice at the center.

$$\text{A \# density} = avd_A = 1 \text{ atom} / a^3 = 1 / (4.6188 \times 10^{-10} \text{ m})^3 = 1.0149 \times 10^{28} \text{ atoms/m}^3$$

$$\Rightarrow \underline{avd_A = 1.0149 \times 10^{22} \text{ atoms/cm}^3}$$

From the figure, the number of B atoms in the lattice is

$$\# B = 8 \text{ corners } (1/8 \text{ atom/corner}) = 1 \text{ B atom.}$$

$$\text{B vol. \# density} = avd_B = 1 \text{ atom} / a^3 = 1 / (4.6188 \times 10^{-10} \text{ m})^3 = 1.0149 \times 10^{28} \text{ atoms/m}^3$$

$$\Rightarrow \underline{avd_B = 1.0149 \times 10^{22} \text{ atoms/cm}^3}$$

c) The materials in parts a and b are the same!