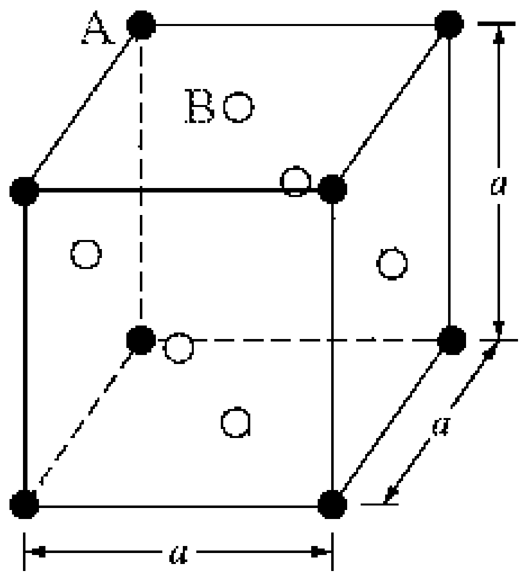
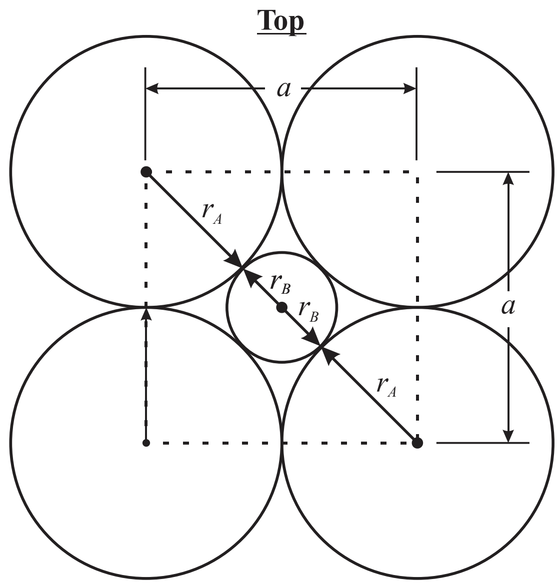
1.8 A crystal is composed of two elements, A and B. The basic crystal structure is a face-centered cubic with element A at each of the corners and element B in the center of each face. The effective radius of element A is $r_A = 1.035$ Å. Assume that the elements are hard spheres with the surface of each A-type atom in contact with the surface of its nearest A-type neighbor. Calculate (*a*) the maximum radius of the B-type element that will fit into this structure, (*b*) the lattice constant, and (*c*) the volume density (#/cm^3) of both the A-type atoms and the B-type atoms.





a) From the top view figure on the right above, the diagonal is

$$d = \sqrt{a^2 + a^2} = \sqrt{2}\,(a) = \sqrt{2}\,(2r_A) = r_A + r_B + r_B + r_A = 2r_A + 2r_B$$

$$\sqrt{2}(2)1.035 = (2)1.035 + 2r_B \quad \Rightarrow \quad r_B = \left(\sqrt{2}(2)1.035 - (2)1.035\right)/2$$

$\Rightarrow$ **r_B = 0.4287 Å**

b) From the top view picture on the right above, the lattice constant is

$a = 2\,(r_A) = 2\,(1.035)$ $\Rightarrow$ **a = 2.07 Å**

c) From figure on the left above, the atomic volume densities (*avd*) are

\# *A* atoms/unit cell = 8 corners (1/8 atoms/corner) = 1

$avd_A = 1$ atom$/a^3 = 1/(2.07\times10^{-10}\text{ m})^3 = 1.127\times10^{29}$ atoms/m^3

$\Rightarrow$ **$avd_A = 1.127\times10^{23}$ atoms/cm^3**

\# *B* atoms/unit cell = 6 faces (1/2 atoms/face) = 3

$Avd_B = 3$ atoms$/a^3 = 3/(2.07\times10^{-10}\text{ m})^3 = 3.382\times10^{29}$ atoms/m^3

$\Rightarrow$ **$avd_B = 3.382\times10^{23}$ atoms/cm^3**