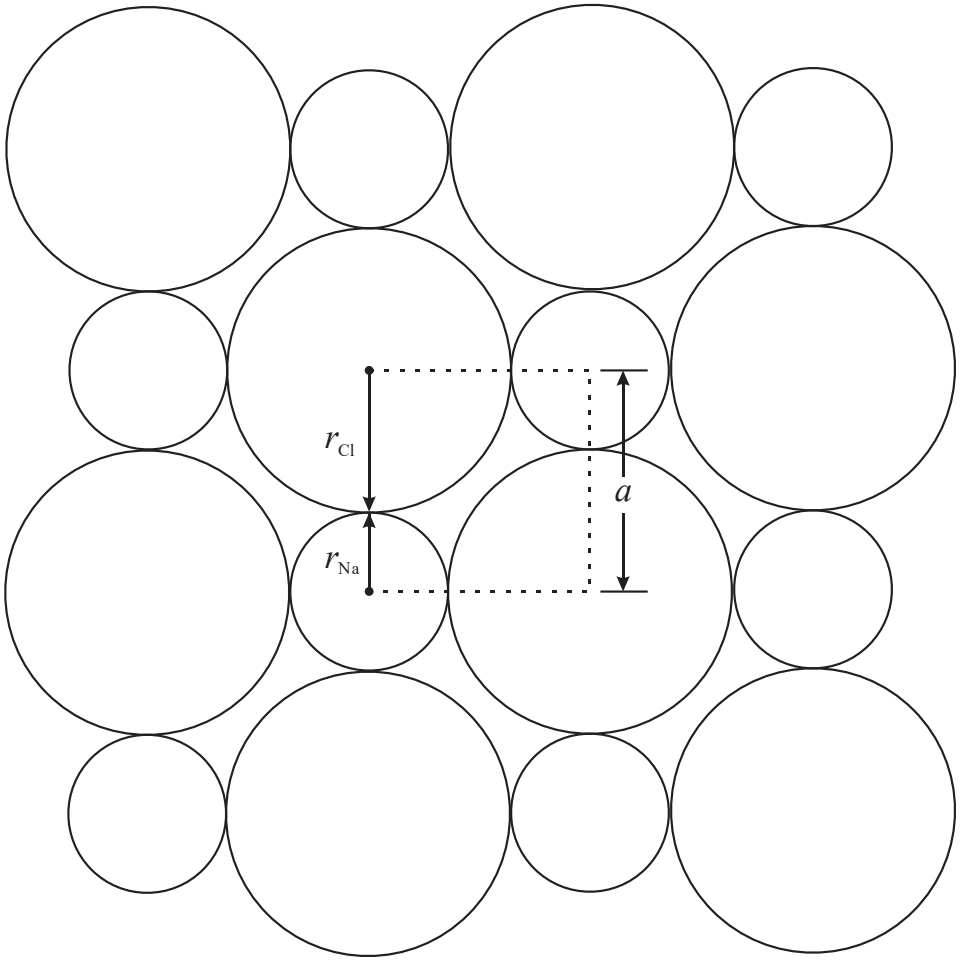
1.11 The crystal structure of sodium chloride (NaCl) is a simple cubic with the Na and Cl atoms alternating positions. Each Na atom is then surrounded by six Cl atoms and likewise each Cl atom is surrounded by six Na atoms. (*a*) Sketch the atoms in a (100) plane. (*b*) Assume the atoms are hard spheres with nearest neighbors touching. The effective radius of Na is 1.0 Å and the effective radius of Cl is 1.8 Å. Determine the lattice constant. (*c*) Calculate the volume density of Na and Cl atoms. (*d*) Calculate the mass density of NaCl.

a) Using CorelDraw-



b) From drawings of part a), the lattice constant is

$$a = r_{Cl} + r_{Na} = 1.8 + 1$$

$$a = 2.8\,\text{Å}$$

c) There are 8 corners to the cubic lattice, 4 Na atoms and 4 Cl atoms. Therefore, the atomic volume density is the same

$$N_{Na} = N_{Cl} = \frac{4\,\text{corners}\left(\frac{1}{8}\frac{\text{atom}}{\text{corner}}\right)}{a^3} = \frac{0.5\,\text{atom}}{(2.8\times10^{-10}\,m)^3}$$

$$N_{Na} = N_{Cl} = 2.2777\times10^{28}\,\frac{\text{atoms}}{m^3}$$

$$= 2.2777\times10^{22}\,\frac{\text{atoms}}{cm^3}$$

d) $$\text{Mass density} = \frac{(\text{At. wt. Na})N_{Na} + (\text{At. wt Cl})N_{Cl}}{\text{Avogadro's \#}}$$

From Appendix C, At. wt Na = 22.99

At. wt Cl = 35.45

$$\text{Mass density}_{NaCl} = \frac{22.99(2.2777\times10^{28}) + 35.45(2.2777\times10^{28})}{6.022\times10^{23}\,\text{atom/g}}$$

$$\text{Mass density}_{NaCl} = 2{,}210{,}375.1\,g/m^3 = 2.21\,g/cm^3$$