1.7 van der Waals bonding

Below 24.5 K, Ne is a crystalline solid with an FCC structure. The interatomic interaction energy per atom can be written as

\[ E(r) = -2 \epsilon \left[ 14.45 \frac{\sigma}{r}^6 - 12.13 \frac{\sigma}{r}^{12} \right] \text{ (eV/atom)} \]

where \( \epsilon \) and \( \sigma \) are constants that depend on the polarizability, the mean dipole moment, and the extent of overlap of core electrons. For crystalline Ne, \( \epsilon = 3.121 \times 10^{-3} \) eV and \( \sigma = 0.274 \) nm.

a. Show that the equilibrium separation between the atoms in an inert gas crystal is given by \( r_0 = (1.090)\sigma \). What is the equilibrium interatomic separation in the Ne crystal?

b. Find the bonding energy per atom in solid Ne.

c. Calculate the density of solid Ne (atomic mass = 20.18 g/mol).

1.22 BCC and FCC Crystals

a. Molybdenum has the BCC crystal structure, has a density of 10.22 g cm\(^{-3}\) and an atomic mass of 95.94 g mol\(^{-1}\). What is the atomic concentration, lattice parameter \( a \), and atomic radius of molybdenum?

b. Gold has the FCC crystal structure, a density of 19.3 g cm\(^{-3}\) and an atomic mass of 196.97 g mol\(^{-1}\). What is the atomic concentration, lattice parameter \( a \), and atomic radius of gold?

1.24 Planar and surface concentrations

Niobium (Nb) has the BCC crystal with a lattice parameter \( a = 0.3294 \) nm. Find the planar concentrations as the number of atoms per nm\(^2\) of the (100), (110) and (111) planes. Which plane has the most concentration of atoms per unit area?

Sometimes the number of atoms per unit area \( n_{\text{surface}} \) on the surface of a crystal is estimated by using the relation \( n_{\text{surface}} = n_{\text{bulk}}^{2/3} \) where \( n_{\text{bulk}} \) is the concentration of atoms in the bulk. Compare \( n_{\text{surface}} \) values with the planar concentrations calculated above and comment on the difference. [Note: The BCC (111) plane does not cut through the center atom and the (111) has 1/6th of an atom at each corner]

For the BCC crystalline structure the planes (100), (110) and (111) are drawn below.

(100), (110), (111) planes in the BCC crystal

1.25 Diamond and zinc blende

Si has the diamond and GaAs has the zinc blende crystal structure. Given the lattice parameters of Si and GaAs, \( a = 0.543 \) nm and \( a = 0.565 \) nm, respectively, and the atomic masses of Si, Ga, and As as 28.08 g/mol, 69.73 g/mol, and 74.92 g/mol, respectively, calculate the density of Si and GaAs. What is the atomic concentration (atoms per unit volume) in each crystal?
1.28 Si and SiO₂

a. Given the Si lattice parameter $a = 0.543$ nm, calculate the number of Si atoms per unit volume, in nm$^{-3}$.

b. Calculate the number of atoms per m$^2$ and per nm$^2$ on the (100), (110) and (111) planes in the Si crystal as shown on Figure 1.75. Which plane has the most number of atoms per unit area?

c. The density of SiO₂ is 2.27 g cm$^{-3}$. Given that its structure is amorphous, calculate the number of molecules per unit volume, in nm$^{-3}$. Compare your result with (a) and comment on what happens when the surface of an Si crystal oxidizes. The atomic masses of Si and O are 28.09 g/mol and 16 g/mol, respectively.

![Figure 1.75](image-url) Diamond cubic crystal structure and planes. Determine what portion of a black-colored atom belongs to the plane that is hatched.
1.31 Pb-Sn solder

Consider the soldering of two copper components. When the solder melts, it wets both metal surfaces. If the surfaces are not clean or have an oxide layer, the molten solder cannot wet the surfaces and the soldering fails. Assume that soldering takes place at 250 °C, and consider the diffusion of Sn atoms into the copper (the Sn atom is smaller than the Pb atom and hence diffuses more easily).

a. The diffusion coefficient of Sn in Cu at two temperatures is \( D = 1.69 \times 10^{-9} \text{ cm}^2 \text{ hr}^{-1} \) at 400 °C and \( D = 2.48 \times 10^{-7} \text{ cm}^2 \text{ hr}^{-1} \) at 650 °C. Calculate the rms distance diffused by an Sn atom into the copper, assuming the cooling process takes 10 seconds.

b. What should be the composition of the solder if it is to begin freezing at 250 °C?

c. What are the components (phases) in this alloy at 200 °C? What are the compositions of the phases and their relative weights in the alloy?

d. What is the microstructure of this alloy at 25 °C? What are weight fractions of the \( \alpha \) and \( \beta \) phases assuming near equilibrium cooling?

The equilibrium phase diagram of the Pb-Sn alloy.