1.2 Atomic mass and molar fractions

a. Consider a multicomponent alloy containing $N$ elements. If $w_1, w_2, \ldots, w_N$ are the weight fractions of components 1, 2, ..., $N$ in the alloy and $M_1, M_2, \ldots, M_N$ are the respective atomic masses of the elements, show that the atomic fraction of the $i$-th component is given by

$$n_i = \frac{w_i / M_i}{w_1 / M_1 + w_2 / M_2 + \ldots + w_N / M_N}$$

Weight to atomic percentage

b. Suppose that a substance (compound or an alloy) is composed of $N$ elements, $A, B, C, \ldots$ and that we know their atomic (or molar) fractions $n_A, n_B, n_C, \ldots$. Show that the weight fractions $w_A, w_B, w_C, \ldots$ are given by

$$w_A = \frac{n_A M_A}{n_A M_A + n_B M_B + n_C M_C + \ldots}$$

$$w_B = \frac{n_B M_B}{n_A M_A + n_B M_B + n_C M_C + \ldots}$$

Atomic to weight percentage

Solution

a. Suppose that $n_1, n_2, n_3, \ldots, n_i, \ldots, n_N$ are the atomic fractions of the elements in the alloy,

$$n_1 + n_2 + n_3 + \ldots + n_N = 1$$

Suppose that we have 1 mole of the alloy. Then it has $n_i$ moles of an atom with atomic mass $M_i$ (atomic fractions also represent molar fractions in the alloy). Suppose that we have 1 gram of the alloy. Since $w_i$ is the weight fraction of the $i$-th atom, $w_i$ is also the mass of $i$-th element in grams in the alloy. The number of moles in the alloy is then $w_i / M_i$. Thus,

$$\text{Number of moles of element } i = w_i / M_i$$

$$\text{Number of moles in the whole alloy} = w_1 / M_1 + w_2 / M_2 + \ldots + w_i / M_i + \ldots + w_N / M_N$$

Molar fraction or the atomic fraction of the $i$-th elements is therefore,

$$n_i = \frac{\text{Number of moles of element } i}{\text{Total number of moles in alloy}}$$

$$\therefore \quad n_i = \frac{w_i / M_i}{w_1 / M_1 + w_2 / M_2 + \ldots + w_N / M_N}$$

b. Suppose that we have the atomic fraction $n_i$ of an element with atomic mass $M_i$. The mass of the element in the alloy will be the product of the atomic mass with the atomic fraction, i.e. $n_i M_i$. Mass of the alloy is therefore

$$n_A M_A + n_B M_B + \ldots + n_N M_N = M_{\text{alloy}}$$

By definition, the weight fraction is, $w_i = \text{mass of the element } i / \text{Mass of alloy}$. Therefore,

$$w_A = \frac{n_A M_A}{n_A M_A + n_B M_B + n_C M_C + \ldots}$$

$$w_B = \frac{n_B M_B}{n_A M_A + n_B M_B + n_C M_C + \ldots}$$

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?
Solution

a. Since molybdenum has BCC crystal structure, there are 2 atoms in the unit cell. The density is

\[ \rho = \frac{\text{Mass of atoms in unit cell}}{\text{Volume of unit cell}} = \frac{\left(\text{Number of atoms in unit cell}\times\text{Mass of one atom}\right)}{\text{Volume of unit cell}} \]

that is,

\[ \rho = \frac{2 \left( \frac{M_{\text{at}}}{N_A} \right)}{a^3} \]

Solving for the lattice parameter \( a \) we receive

\[ a = \left( \frac{2M_{\text{at}}}{\rho N_A} \right)^{\frac{1}{3}} \]

\[ = \left( \frac{2 \left( 95.94 \times 10^{-3} \text{ kg mol}^{-1} \right)}{10.22 \times 10^3 \text{ kg m}^{-3} \left( 6.022 \times 10^{23} \text{ mol}^{-1} \right)} \right)^{\frac{1}{3}} = 3.147 \times 10^{-10} \text{ m} = 0.3147 \text{ nm} \]

The Atomic concentration is 2 atoms in a cube of volume \( a^3 \), i.e.

\[ n_{\text{at}} = \frac{2}{a^3} = \frac{2}{\left( 3.147 \times 10^{-10} \text{ m} \right)^3} = 6.415 \times 10^{22} \text{ cm}^{-3} = 6.415 \times 10^{28} \text{ m}^{-3} \]

For a BCC cell, the lattice parameter \( a \) and the radius of the atom \( R \) are in the following relation (listed in Table 1.3):

\[ R = \frac{a\sqrt{3}}{4} = \frac{\left( 3.147 \times 10^{-10} \text{ m} \right) \sqrt{3}}{4} = 1.363 \times 10^{-10} \text{ m} = 0.1363 \text{ nm} \]

1.26 Zinc blende, NaCl and CsCl

a. InAs is a III-V semiconductor that has the zinc blende structure with a lattice parameter of 0.606 nm. Given the atomic masses of In (114.82 g mol\(^{-1}\)) and As (74.92 g mol\(^{-1}\)), find the density.

Solution
For zinc blende structure there are 8 atoms per unit cell (as shown in Table 1.3).

<table>
<thead>
<tr>
<th>Crystal Structure</th>
<th>$a$ and $R$ (R is the Radius of the Atom)</th>
<th>Coordination Number (CN)</th>
<th>Number of Atoms per Unit Cell</th>
<th>Atomic Packing Factor</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple cubic</td>
<td>$a = 2R$</td>
<td>6</td>
<td>1</td>
<td>0.52</td>
<td>No metals (Except Po)</td>
</tr>
<tr>
<td>BCC</td>
<td>$a = \frac{4R}{\sqrt{3}}$</td>
<td>8</td>
<td>2</td>
<td>0.68</td>
<td>Many metals: α–Fe, Cr, Mo, W</td>
</tr>
<tr>
<td>FCC</td>
<td>$a = \frac{4R}{\sqrt{2}}$</td>
<td>12</td>
<td>4</td>
<td>0.74</td>
<td>Many metals: Ag, Au, Cu, Pt</td>
</tr>
<tr>
<td>HCP</td>
<td>$a = 2R$</td>
<td>12</td>
<td>2</td>
<td>0.74</td>
<td>Many metals: Co, Mg, Ti, Zn</td>
</tr>
<tr>
<td></td>
<td>$c = 1.633a$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Diamond</td>
<td>$a = \frac{8R}{\sqrt{3}}$</td>
<td>4</td>
<td>8</td>
<td>0.34</td>
<td>Covalent solids: Diamond, Ge, Si, α-Sn</td>
</tr>
<tr>
<td>Zinc blende</td>
<td></td>
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</tr>
<tr>
<td>NaCl</td>
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</tr>
<tr>
<td>CsCl</td>
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</tr>
</tbody>
</table>

In the case of InAs, it is apparent that there are 4 In and 4 As atoms in the unit cell. The density of InAs is then

$$
\rho_{\text{InAs}} = \frac{4}{a^3} \left( \frac{M_{\text{atln}}}{N_A} + 4 \left( \frac{M_{\text{atAs}}}{N_A} \right) \right) = \frac{4 \left( M_{\text{atln}} + M_{\text{atAs}} \right)}{N_A a^3} = \frac{4(114.82 + 74.92) \times \left( 10^{-3} \text{kg mol}^{-1} \right)}{(6.022 \times 10^{23} \text{mol}^{-1})(0.606 \times 10^{-9} \text{m}^3)} = 5.66 \times 10^3 \text{ kg m}^{-3} = 5.66 \text{ g cm}^{-3}
$$