Session #15: Homework Solutions

Problem #1

Iron ($\rho = 7.86\ g/cm^3$) crystallizes in a BCC unit cell at room temperature. Calculate the radius of an iron atom in this crystal. At temperatures above 910ºC iron prefers to be FCC. If we neglect the temperature dependence of the radius of the iron atom on the grounds that it is negligible, we can calculate the density of FCC iron. Use this to determine whether iron expands or contracts when it undergoes transformation from the BCC to the FCC structure.

Solution

In BCC there are 2 atoms per unit cell, so $\frac{2}{a^3} = \frac{N_A}{V_{molar}}$, where $V_{molar} = A/\rho$; A is the atomic mass of iron.

$$\frac{2}{a^3} = \frac{N_A \times \rho}{A}$$

$$\therefore\ a = \left(\frac{2A}{N_A \times \rho}\right)^{\frac{1}{3}} = \frac{4}{\sqrt{3}} r$$

$$\therefore\ r = 1.24 \times 10^{-8}\ cm$$

If we assume that change of phase does not change the radius of the iron atom, then we can repeat the calculation in the context of an FCC crystal structure, i.e., 4 atoms per unit cell and $a = 2\sqrt{2}r$.

$$\rho = \frac{4A}{N_A (2\sqrt{2}r)^3} = 8.60\ g/cm^3$$

FCC iron is more closely packed than BCC suggesting that iron contracts upon changing from BCC to FCC. This is consistent with the packing density calculations reported in lecture that give FCC as being 74% dense and BCC 68% dense. The ratio of the densities calculated here is precisely the same:

$$\frac{7.86}{8.60} = \frac{0.68}{0.74}$$

Problem #2

Determine the total void volume (cm^3/mole) for gold (Au) at 27°C; make the hard-sphere approximation in your calculation, and use data provided in the periodic table.

Solution

First determine the packing density for Au, which is FCC; then relate it to the molar volume given in the periodic table.

$$\text{packing density} = \frac{\text{volume of atoms/unit cell}}{\text{volume of unit cell}} = \frac{\frac{16\pi r^3}{3}}{a^3} = \frac{16\pi r^3}{3a^3}$$

$$\text{packing density} = \frac{16\pi r^3}{3 \times 16\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}} = 0.74 = 74\%$$

void volume = 1 − packing density = 26%

From the packing density (74%) we recognize the void volume to be 26%. Given the molar volume as 10.3 cm^3/mole, the void volume is:

$$0.26 \times 10.3\ cm^3 / \text{mole} = 2.68\ cm^3 / \text{mole}$$

Problem #3

Determine the atomic (metallic) radius of Mo. Do not give the value listed in the periodic table; calculate it from other data given.

Solution

Mo: atomic weight = 95.94 g/mole

ρ = 10.2 g/cm^3

BCC, so n = 2 atoms/unit cell

$$a^3 = \frac{(95.94\ \text{g/mole})(2\ \text{atoms/unit cell})}{(10.2\ g / cm^3)(6.023 \times 10^{23}\ \text{atoms/mole})} \times 10^{-6}\ \frac{m^3}{cm^3}$$

$$= 3.12 \times 10^{-29}\ m^3$$

$$a = 3.22 \times 10^{-10}\ m$$

For BCC, $a\sqrt{3} = 4r$, so $r = 1.39 \times 10^{-10}$ m

Problem #4

A metal is found to have BCC structure, a lattice constant of 3.31 Å, and a density of 16.6 g/cm^3. Determine the atomic weight of this element.

Solution

BCC structure, so n = 2

a = 3.31 Å = 3.31 x 10^{-10} m

ρ = 16.6 g/cm^3

$$\frac{\text{atomic weight}}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$\text{atomic weight} = \frac{(6.023 \times 10^{23}\ \text{atoms/mole})\ (3.31 \times 10^{-10}\ \text{m})^3}{(2\ \text{atoms/unit cell})(10^{-6}\ \text{m}^3/\text{cm}^3)} \times 16.6\ \text{g/cm}^3$$

$$= 181.3\ \text{g/mole}$$

Problem #5

At 100°C copper (Cu) has a lattice constant of 3.655 Å. What is its density at this temperature?

Solution

Cu is FCC, so n = 4

$a = 3.655$ Å $= 3.655 \times 10^{-10}$ m

atomic weight = 63.55 g/mole

$$\frac{\text{atomic weight}}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$\rho = \frac{(63.55\ \text{g/mole})(4\ \text{atoms/unit cell})}{(6.023 \times 10^{23}\ \text{atoms/mole})(3.655 \times 10^{-10}\ \text{m}^3)} = 8.64\ \text{g/cm}^3$$

Problem #6

Determine the second-nearest neighbor distance for nickel (Ni) (in pm) at 100° C if its density at that temperature is 8.83 g/cm^3.

Solution

Ni: n = 4

atomic weight = 58.70 g/mole

$\rho = 8.83\ \text{g/cm}^3$

For a face−centered cubic structure, the second nearest neighbor distance equals "a" (see LN4−11).

$$\frac{\text{atomic weight}}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$a^3 = \frac{(58.70\ \text{g/mole})(10^{-6}\ \text{m}^3/\text{cm}^3)(4\ \text{atoms /unit cell})}{(6.023 \times 10^{23}\ \text{atoms / mole})(8.83\ \text{g / cm}^3)}$$

$$= 4.41 \times 10^{-29}\ \text{m}^3$$

$$a = 3.61 \times 10^{-10}\ \text{m} \times \frac{10^{12}\ \text{pm}}{\text{m}} = 3.61 \times 10^2\ \text{pm}$$

Problem #7

Determine the highest linear density of atoms (atoms/m) encountered in vanadium (V).

Solution

V: atomic weight = 50.94 g/mole

$\rho = 5.8\ \text{g/cm}^3$

BCC, so n = 2

The highest density would be found in the [111] direction. To find "a":

$$\frac{\text{atomic weight}}{\rho} = a^3 \frac{N_A}{n} \rightarrow a^3 = \frac{50.94 \times 2}{5.8 \times 6.023 \times 10^{23}}$$

$$a = 3.08 \times 10^{-8}\ \text{cm} = 3.08 \times 10^{-10}\ \text{m}$$

The length in the [111] direction is $a\sqrt{3}$, so there are:

$$2\ \text{atoms} / a\sqrt{3} = 2\ \text{atoms}/(3.08 \times 10^{-10}\ \text{m} \times \sqrt{3})$$

$$= 3.75 \times 10^{9}\ \text{atoms/m}$$