Physical Metallurgy Principles and Design 1st edition Haidemenopoulos Solutions Manual

SKU: 9781138627680-SOLUTIONS

Chapter 2

Problem 2.1 In FCC the relation between the lattice parameter and the atomic radius is $\alpha = \frac{4R}{\sqrt{2}}$, then α=4.95 Angstroms. On the cube phase (100) correspond 2 atoms (4x1/4+1). Then the density of the (100) plane is

$$_{(100)} = \frac{2}{4.95x10^{7}} = 8.2x10^{12} \text{ atoms/mm}^2$$

In the (111) plane there are 3/6+3/2=2 atoms. The base of the triangle is 4R and the height $2\sqrt{3}R$

After some math we get ρ(111)=9.5x10^{12} atoms/mm^2. We see that the (111) plane has higher density than the (100) plane, it is a close-packed plane.

Problem 2.2 The (100)-type plane closer to the origin is the (002) plane which cuts the z axis at ½. This has

$$d_{(002)} = \frac{a}{\sqrt{0+0+2^2}} = \frac{a}{2} = \frac{2R}{\sqrt{2}}$$

Setting R=1.749 Angstroms we get d(002)=2.745 Angstroms.

In the same way

$$d_{(111)} = \frac{a}{\sqrt{1+1+1}} = \frac{a}{\sqrt{3}} = \frac{4R}{\sqrt{6}}$$

and d(111)=2.85 Angstroms. We see that the close-packed planes have a larger interplanar spacing.

Problem 2.3. The structure of vanadium is BCC. In this structure, the close-packed direction is [111], which corresponds to the diagonal of the cubic unit cell where there is a consecutive contact of spheres (in the model of hard spheres). Furthermore, the number of atoms per unit cell for the BCC structure is 2. The first step is to find the lattice parameter α. The density is

$$\rho = \frac{2\frac{AB}{N_A}}{\alpha^3}$$

Where N_A is the Avogadro's number. Therefore the lattice parameter is

$$\alpha^3 = \frac{2\times 50.94}{5.8\times 6.023\times 10^{23}} \Rightarrow a = 3.08\times 10^{-8} cm = 3.08\times 10^{-10} m$$

Physical Metallurgy Principles and Design 1st edition Haidemenopoulos Solutions Manual

The length of the diagonal at the [111] close-packed direction is $a\sqrt{3}$, which corresponds to 2 atoms. Hence the atomic density of the close-packed direction of vanadium (V) is

$$\rho_{[111]} = \frac{2}{\alpha\sqrt{3}} = \frac{2}{3.08\times10^{-10}\sqrt{3}} = 3.75\times10^{9}\ atoms/m$$

The aforementioned atomic density result translates to 3750 atoms/μm or 3.75 atoms/nm.

Problem 2.4. The lattice parameter for the FCC structure is $\alpha = \frac{4R}{\sqrt{2}}$. The (100) plane is the face of the unit cell. The face comprises ¼ of atoms at each corner plus 1 atom at the center of the face. Hence the face consists of $4\times(1/4)+1=2$ atoms. The atomic density of the (100) plane is

$$\rho_{(100)} = \frac{2}{a^2} = \frac{2}{\left(\frac{4R}{\sqrt{2}}\right)^2} = \frac{1}{4R^2}$$

The (111) plane corresponds to the diagonal equilateral triangle of the unit cell. The base of this triangle is $4R$. Using the Pythagorean Theorem, we can calculate the height of the triangle which is $2\sqrt{3}R$. Thus the area of the triangle is $(base\times height/2) = 4\sqrt{3}R^2$. The equilateral triangle comprises 6 of the atoms at each corner and ½ of the atoms at the middle of each side. Thus the equilateral triangle consists of $3\times(1/6)+3\times(1/2)=2$ atoms. The atomic density of the (111) plane is

$$\rho_{(111)} = \frac{2}{4\sqrt{3}R^2} = \frac{1}{2\sqrt{3}R^2}$$

The ratio of the atomic densities is

$$\frac{\rho_{(111)}}{\rho_{(100)}} = \frac{2}{\sqrt{3}} = 1.154 > 1$$

Therefore $\rho_{(111)} > \rho_{(100)}$ and specifically the (111) plane has 15% higher atomic density than the (100) plane. This is important since the plastic deformation of metals (Al, Cu, Ni, γ-Fe, etc.) is accomplished with dislocation glide on the close-packed planes.

Problem 2.5. The ideal c/a ratio in HCP structure results when the atoms of this structure have an arrangement as dense as the atoms of the FCC structure. The distance between the (0001) bases of the HCP structure is c. Using the fact that the (0001) planes of HCP structure correspond to the (111) planes of the FCC structure, we get

$$c = 2\left[d_{(111)}\right]_{FCC}$$

Where $d_{(111)}$ is the distance between the (111) close-packed planes. We find that

Physical Metallurgy Principles and Design 1st edition Haidemenopoulos Solutions Manual

$$\left.\begin{array}{c} d_{(111)} = \dfrac{a}{\sqrt{h^2+k^2+l^2}} = \dfrac{a}{\sqrt{1^2+1^2+1^2}} = \dfrac{a}{\sqrt{3}} \\ a = \dfrac{4R}{\sqrt{2}} \end{array}\right\} \Rightarrow \left[d_{(111)}\right]_{FCC} = \frac{4R}{\sqrt{6}}$$

Thus,

$$\left.\begin{array}{c} c = \dfrac{8R}{\sqrt{6}} \\ HCP:\ a = 2R \end{array}\right\} \Rightarrow \frac{c}{a} = \frac{4}{\sqrt{6}} = 1.63$$

Therefore, the ideal ratio c/a for close packing in HCP structure is equal to 1.63. The c/a ratio for zinc (Zn) is 1.86 while for titanium (Ti) is 1.59 (see Table 7.1, Book). This means that the distance between the (0001) planes is longer in Zn than in Ti. This fact affects the plastic deformation in these metals, since the slip on (0001) planes is easier in Zn than in Ti. Indeed the critical shear stress of Zn is only 0.18 MPa, while of Ti is 110 MPa. Due to this, the plastic deformation in Ti is performed on $(10\bar{1}0)$ plane, where the critical shear stress is approximately 49 MPa. Thus in Ti the slip is not performed on the close-packed planes of the crystal structure. For more details look at the 7.3 paragraph of the book (plastic deformation of single crystals with slip).

Problem 2.6. The cell volume of HCP structure is the product of the base area (hexagon) multiplied by the height c. The base of hexagon is $A = 6R^2\sqrt{3}$ and the height is $c = \dfrac{8R}{\sqrt{6}}$. As a result, the cell volume is

$$V = 24\sqrt{2}\,R^3$$

The number of atoms per unit cell for the HCP structure is 6, thus the atomic packing factor is

$$APF_{HCP} = \frac{6\,\frac{4}{3}\pi R^3}{24\sqrt{2}\,R^3} = \frac{\pi}{3\sqrt{2}} = 0.74$$

Regarding the BCC structure, the number of atoms per unit cell is 2 and the cell volume is a^3, where $a = \dfrac{4R}{\sqrt{3}}$. Therefore the atomic packing factor of BCC structure is

$$APF_{BCC} = \frac{2\,\frac{4}{3}\pi R^3}{\left(\frac{4R}{\sqrt{3}}\right)^3} = \frac{\pi\sqrt{3}}{8} = 0.68$$

Physical Metallurgy Principles and Design 1st edition Haidemenopoulos Solutions Manual

Since the atomic packing density of BCC is less than that of the HCP, the diffusion in BCC (movement of atoms inside the lattice) is faster.

Problem 2.7 The density is

$$\rho = \frac{mass\ of\ cell\ atoms}{cell\ volume}$$

The structure of copper (Cu) is FCC and the number of atoms per unit cell is 4. The atomic mass is $\frac{\mathrm{AB}}{N_A}$, where AB is the atomic weight and N_A is the Avogadro's number. The cell volume is $a^3 = \left(\frac{4R}{\sqrt{2}}\right)^3$, thus the density is

$$\rho = \frac{4\left(\frac{63.57}{6.023\times10^{23}}\right)}{\left(\frac{4\times1.276\times10^{-8}}{\sqrt{2}}\right)^3} \cong 9\,gr/cm^3$$

Problem 2.8 Notice that the atomic volume is not $\frac{4}{3}\pi R^3$! It is the corresponding volume of every atom of the structure plus the empty surrounding space inside the cell. Due to the fact that the structure of gold (Au) is FCC, the number of atoms per unit cell is 4. Therefore the atomic volume is

$$\Omega = \frac{\alpha^3}{4}$$

For the FCC structure we get that $\alpha = \frac{4R}{\sqrt{2}}$, hence

$$\Omega = \frac{\left(\frac{4R}{\sqrt{2}}\right)^3}{4}$$

After replacing the value of the atomic radius of gold R, we find that $\Omega = 1.7\times10^{-29}\,m^3$. Since $1\,\mathring{\mathrm{A}} = 10^{-10}\,m$, the atomic volume of gold is

$$\Omega = 17\,(\mathring{\mathrm{A}})^3$$

Physical Metallurgy Principles and Design 1st edition Haidemenopoulos Solutions Manual

The molar volume V_m is the volume corresponding to one mole of gold and is obtained by multiplying the atomic volume by the Avogadro's number. Thus the molar volume is

$$V_m = \Omega N_A = 1.02 \times 10^{-5}\ m^3 / mol$$

Problem 2.9

For the atomic radius of the iron atom, R_{FCC}=1.270 and R_{BCC}=1.241 Angtroms (A)

FCC has 4 atmos/cell while BCC has 2 atoms/cell.

In FCC $a = 4R\sqrt{2} = 3.591A, V_{FCC} = a^3 = 46.34A^3$

In BCC $a = 4R\sqrt{3} = 2.865A, V_{BCC} = 23.51A^3$

Taking 4 atoms as a reference, this corresponds to 1 FCC cell and 2 BCC cells, then

$$\frac{V}{V} = \frac{2V_{BCC} \quad V_{FCC}}{2V_{BCC}} = 0.0144$$

or 1.44% volume increase.

Assume that the initial volume is V and the final volume is V_t. Hence the volume change is

$$\frac{\Delta V}{V} = \frac{V_t - V}{V} = \frac{V_t}{V} - 1 \Rightarrow \frac{V_t}{V} = 1 + \frac{\Delta V}{V}$$

$$\frac{V_t}{V} = \frac{(L + \Delta L)^3}{L^3} = (1 + \frac{\Delta L}{L})^3$$

Using the two previous relations, we get that the respective length change is

$$(1 + \quad L / L)^3 = 1 + \quad V / V \Rightarrow \quad L / L = \sqrt[3]{1 + \quad V / V} \quad 1 = 0.00477$$

Therefore there is a 0.477% increase in length.

Physical Metallurgy Principles and Design 1st edition Haidemenopoulos Solutions Manual