

3-32 Determine the planar density and packing fraction for FCC nickel in (100), (110), and (111) planes. Which, if any, of these planes is close packed?

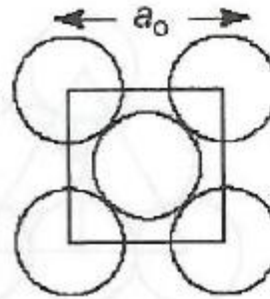
Solution:

$$a_0 = 3.5167 \text{ \AA}$$

For (100):

$$\text{planar density} = \frac{2}{(3.5167 \times 10^{-8} \text{ cm})^2} = 0.1617 \times 10^{16} \text{ points/cm}^2$$

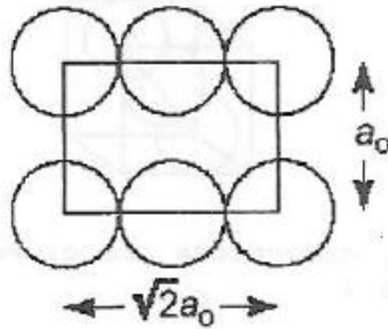
$$\text{packing fraction} = \frac{2(\pi r^2)}{(4r/\sqrt{2})^2} = 0.7854$$



For (110):

$$\begin{aligned} \text{planar density} &= \frac{2 \text{ points}}{(3.5167 \times 10^{-8} \text{ cm})(\sqrt{2})(3.5167 \times 10^{-8} \text{ cm})} \\ &= 0.1144 \times 10^{16} \text{ points/cm}^2 \end{aligned}$$

$$\text{packing fraction} = \frac{2(\pi r^2)}{\sqrt{2}(4r/\sqrt{2})^2} = 0.555$$



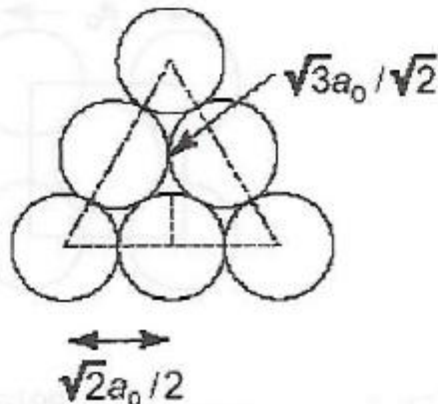
For (111):

From the sketch, we can determine that the area of the (111) plane is $(\sqrt{2}a_0/2)(\sqrt{3}a_0/\sqrt{2}) = 0.866a_0^2$. There are $(3)(1/2) + (3)(1/6) = 2$ atoms in this area.

$$\begin{aligned} \text{planar density} &= \frac{2 \text{ points}}{0.866(3.5167 \times 10^{-8} \text{ cm})^2} \\ &= 0.1867 \times 10^{16} \text{ points/cm}^2 \end{aligned}$$

$$\text{packing fraction} = \frac{2\pi(\sqrt{2}a_0/4)^2}{0.866a_0^2} = 0.907$$

The (111) is close packed.



3.49

Show that the theoretical density for ZnSe should be 5.2 g/cm³ when the lattice const. is 0.567 nm and the crystal structure is that of zinc blende.

$$a_0 = 0.567 \text{ nm}$$

coordinate # of ZnSe = 4

$$\rho = \frac{(\# \text{ of Zn})(\text{AW of Zn}) + (\# \text{ of Se})(\text{AW of Se})}{(\text{Volume of unit cell})(N_A)}$$

$$\rho = \frac{(4)(63.38 \text{ g/mol}) + (4)(78.96 \text{ g/mol})}{(0.567 \text{ nm})^3 (6.02 \times 10^{23} \text{ atoms/mol})}$$

$$\rho = 1.122 \times 10^{-20} \frac{\text{g}}{\text{nm}^3} = 5.26 \frac{\text{g}}{\text{cm}^3}$$

Q.E.D.

3.53 A sample of cubic SiC was analyzed using XRD. It was found that the (111) peak was located at 2θ of 16° . The wavelength (λ) of the X-ray radiation used in this experiment was 0.6975 \AA . Show that the lattice const. a_0 of this form of SiC is 4.0867 \AA .

Given. $\lambda = 0.6975 \text{ \AA}$

$$(hkl) = (111)$$

$$2\theta = 16^\circ \Rightarrow \theta = 8^\circ$$

$$\sin \theta = \frac{\lambda}{2d} \quad d_{hkl} = \frac{a_0}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{111} = \frac{\lambda}{\sin \theta} = \frac{0.6975 \text{ \AA}}{\sin 8^\circ} = 5.0117 \text{ \AA}$$

Also,

$$d_{111} = \frac{a_0}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{a_0}{\sqrt{3}}$$

$$\Rightarrow \frac{a_0}{\sqrt{3}} =$$

$$\Rightarrow a_0 = 4.0867$$

- 4-14 What are the Miller indices of the slip directions
- on the (111) plane in an FCC unit cell
 - on the (011) plane in a BCC unit cell?

Solution: $[\bar{0}\bar{1}1]$, $[0\bar{1}\bar{1}]$
 $[\bar{1}\bar{1}0]$, $[\bar{1}\bar{1}0]$
 $[\bar{1}0\bar{1}]$, $[10\bar{1}]$
 $[\bar{1}\bar{1}\bar{1}]$, $[\bar{1}\bar{1}\bar{1}]$
 $[\bar{1}\bar{1}\bar{1}]$, $[\bar{1}\bar{1}\bar{1}]$

