

1.2(a) Simple cubic lattice: $a = 2r$

Unit cell vol = $a^3 = (2r)^3 = 8r^3$

1 atom per cell, so atom vol

$$= (1) \left(\frac{4\pi r^3}{3} \right)$$

Then

$$\text{Ratio} = \frac{\left(\frac{4\pi r^3}{3} \right)}{8r^3} \times 100\% = 52.4\%$$

(b) Face-centered cubic lattice

$$d = 4r = a\sqrt{2} \Rightarrow a = \frac{d}{\sqrt{2}} = 2\sqrt{2} \cdot r$$

Unit cell vol

$$= a^3 = (2\sqrt{2} \cdot r)^3 = 16\sqrt{2} \cdot r^3$$

4 atoms per cell, so atom vol

$$= (4) \left(\frac{4\pi r^3}{3} \right)$$

Then

$$\text{Ratio} = \frac{(4) \left(\frac{4\pi r^3}{3} \right)}{16\sqrt{2} \cdot r^3} \times 100\% = 74\%$$

(c) Body-centered cubic lattice

$$d = 4r = a\sqrt{3} \Rightarrow a = \frac{4}{\sqrt{3}} \cdot r$$

$$\text{Unit cell vol} = a^3 = \left(\frac{4}{\sqrt{3}} \cdot r \right)^3$$

2 atoms per cell, so atom vol

$$= (2) \left(\frac{4\pi r^3}{3} \right)$$

Then

$$\text{Ratio} = \frac{(2) \left(\frac{4\pi r^3}{3} \right)}{\left(\frac{4r}{\sqrt{3}} \right)^3} \times 100\% = 68\%$$

(d) Diamond lattice

Body diagonal

$$= d = 8r = a\sqrt{3} \Rightarrow a = \frac{8}{\sqrt{3}} \cdot r$$

$$\text{Unit cell vol} = a^3 = \left(\frac{8r}{\sqrt{3}} \right)^3$$

8 atoms per cell, so atom vol

$$= (8) \left(\frac{4\pi r^3}{3} \right)$$

Then

$$\text{Ratio} = \frac{(8) \left(\frac{4\pi r^3}{3} \right)}{\left(\frac{8r}{\sqrt{3}} \right)^3} \times 100\% = 34\%$$

1.7(a) Simple cubic: $a = 2r = 3.9 \text{ \AA}$ (b) fcc: $a = \frac{4r}{\sqrt{2}} = 5.515 \text{ \AA}$ (c) bcc: $a = \frac{4r}{\sqrt{3}} = 4.503 \text{ \AA}$ (d) diamond: $a = \frac{2(4r)}{\sqrt{3}} = 9.007 \text{ \AA}$ **1.9**(a) $a = 2r = 4.5 \text{ \AA}$

$$\# \text{ of atoms} = 8 \times \frac{1}{8} = 1$$

$$\begin{aligned} \text{Number density} &= \frac{1}{(4.5 \times 10^{-8})^3} \\ &= 1.097 \times 10^{22} \text{ cm}^{-3} \end{aligned}$$

$$\begin{aligned} \text{Mass density} = \rho &= \frac{N(\text{At.Wt.})}{N_A} \\ &= \frac{(1.0974 \times 10^{22})(12.5)}{6.02 \times 10^{23}} \\ &= 0.228 \text{ gm/cm}^3 \end{aligned}$$

(b) $a = \frac{4r}{\sqrt{3}} = 5.196 \text{ \AA}$

$$\# \text{ of atoms} = 8 \times \frac{1}{8} + 1 = 2$$

$$\begin{aligned} \text{Number density} &= \frac{2}{(5.196 \times 10^{-8})^3} \\ &= 1.4257 \times 10^{22} \text{ cm}^{-3} \end{aligned}$$

Mass density

$$= \rho = \frac{(1.4257 \times 10^{22})(12.5)}{6.02 \times 10^{23}} = 0.296 \text{ gm/cm}^3$$

1.16

(a)

$$\left(\frac{1}{1}, \frac{1}{3}, \frac{1}{1}\right) \Rightarrow (313)$$

(b)

$$\left(\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right) \Rightarrow (121)$$

1.19

(a) Simple cubic

(i) (100) plane:

Surface density

$$= \frac{1}{a^2} = \frac{1}{(4.73 \times 10^{-8})^2} = 4.47 \times 10^{14} \text{ cm}^{-2}$$

(ii) (110) plane:

Surface density = $\frac{1}{a^2 \sqrt{2}}$

$$= 3.16 \times 10^{14} \text{ cm}^{-2}$$

(iii) (111) plane:

Area of plane = $\frac{1}{2} bh$

where $b = a\sqrt{2} = 6.689 \text{ \AA}$

Now

$$h^2 = (a\sqrt{2})^2 - \left(\frac{a\sqrt{2}}{2}\right)^2 = \frac{3}{4}(a\sqrt{2})^2$$

So $h = \frac{\sqrt{6}}{2}(4.73) = 5.793 \text{ \AA}$

Area of plane

$$= \frac{1}{2}(6.68923 \times 10^{-8})(5.79304 \times 10^{-8}) = 19.3755 \times 10^{-16} \text{ cm}^2$$

Surface density = $\frac{3 \times \frac{1}{6}}{19.3755 \times 10^{-16}}$

$$= 2.58 \times 10^{14} \text{ cm}^{-2}$$

(b) bcc

(i) (100) plane:

Surface density = $\frac{1}{a^2} = 4.47 \times 10^{14} \text{ cm}^{-2}$

(ii) (110) plane:

Surface density = $\frac{2}{a^2 \sqrt{2}}$

$$= 6.32 \times 10^{14} \text{ cm}^{-2}$$

(iii) (111) plane:

Surface density = $\frac{3 \times \frac{1}{6}}{19.3755 \times 10^{-16}}$

$$= 2.58 \times 10^{14} \text{ cm}^{-2}$$

(c) fcc

(i) (100) plane:

Surface density = $\frac{2}{a^2} = 8.94 \times 10^{14} \text{ cm}^{-2}$

(ii) (110) plane:

Surface density = $\frac{2}{a^2 \sqrt{2}}$

$$= 6.32 \times 10^{14} \text{ cm}^{-2}$$

(iii) (111) plane:

Surface density = $\frac{3 \times \frac{1}{6} + 3 \times \frac{1}{2}}{19.3755 \times 10^{-16}}$

$$= 1.03 \times 10^{15} \text{ cm}^{-2}$$

1.20

(a) (100) plane: - similar to a fcc:

Surface density = $\frac{2}{(5.43 \times 10^{-8})^2}$

$$= 6.78 \times 10^{14} \text{ cm}^{-2}$$

(b) (110) plane:

Surface density = $\frac{4}{\sqrt{2}(5.43 \times 10^{-8})^2}$

$$= 9.59 \times 10^{14} \text{ cm}^{-2}$$

(c) (111) plane:

Surface density = $\frac{2}{(\sqrt{3}/2)(5.43 \times 10^{-8})^2}$

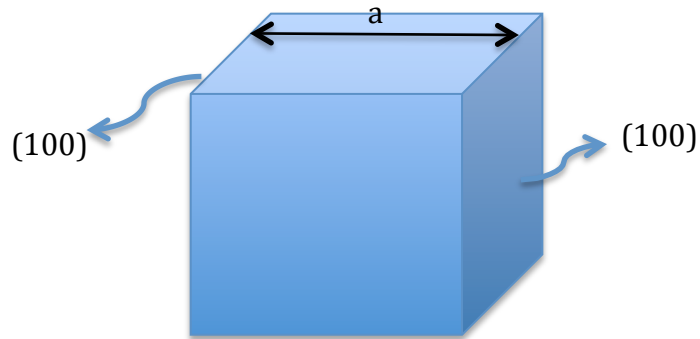
$$= 7.83 \times 10^{14} \text{ cm}^{-2}$$

Question 2

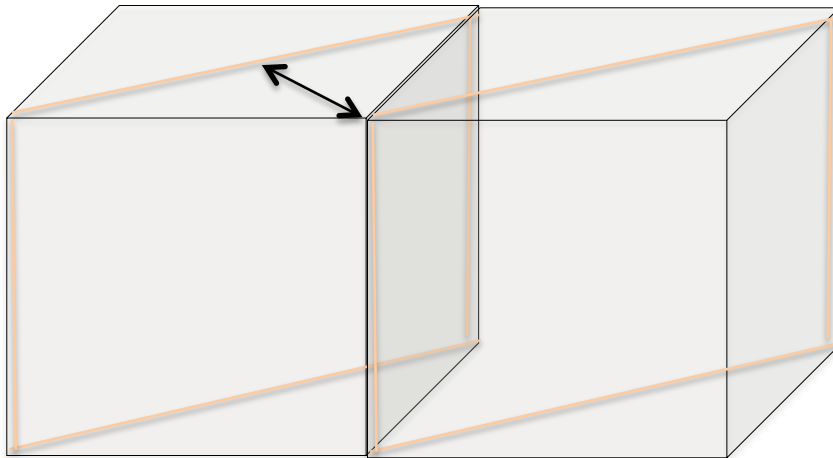
Calculate the surface density of silicon atoms in each plane as it is done in supplemental to module 1, then multiply each by 4 since each silicon atom has four valence electrons.

Question 3

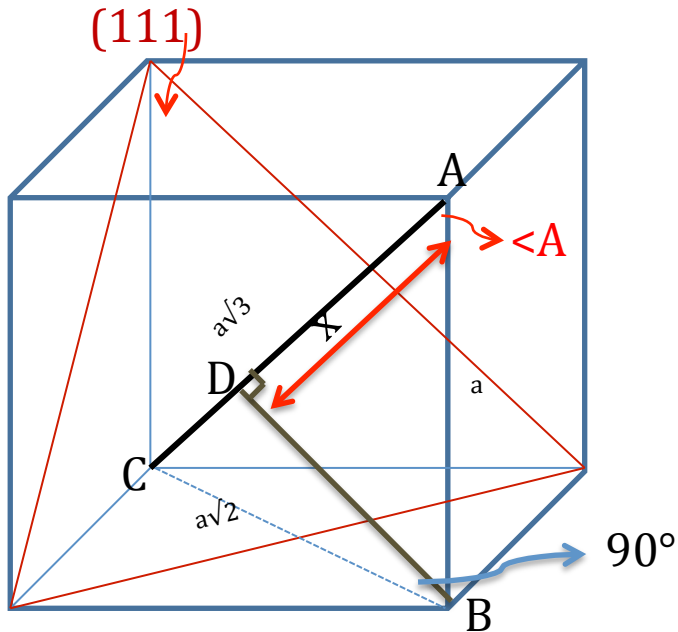
For {100} planes the distance between planes is a (lattice constant)



For {110} planes it is half of face diagonal (shown in the figure below)



For {111} planes it is 1/3 of body diagonal



In ABC triangle $\cos(\angle A) = a/(a\sqrt{3}) = 1/\sqrt{3}$
 In ABD triangle $\cos(\angle A) = 1/\sqrt{3} = x/a$ so: $x = a/\sqrt{3}$

Question 4

Number of atoms in 110 plane is $4 \times \frac{1}{2} = 2$ atoms

$$\text{Surface density in 110 plane} = \frac{\# \text{ atoms}}{\text{surface area of the plane}} = \frac{2}{(a)^2 \sqrt{2}} \text{ atoms/cm}^3$$