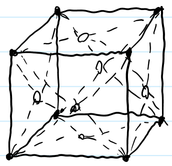
HW 1 Solutions

1.1: Determine the number of atoms/unit cell in

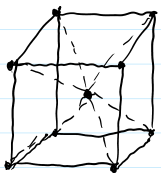
a) fcc;

$$\frac{\#}{\text{unit cell}} = \sum_i N_i V_i \quad : \text{corners + faces + contained}$$



$$\frac{\#}{\text{unit cell}} = \underbrace{8 \cdot \frac{1}{8}}_{\text{corner atoms}} + \underbrace{6 \cdot \frac{1}{2}}_{\text{face atoms}} = 4 \ \frac{\text{atoms}}{\text{unit cell}}$$

b) bcc:



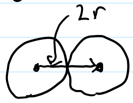
$$\frac{\#}{\text{unit cell}} = \underbrace{8 \cdot \frac{1}{8}}_{\text{corner atoms}} + \underbrace{1}_{\text{center atom}} = 2 \ \frac{\text{atoms}}{\text{unit cell}}$$

c) diamond: cf. Fig. 1.11

$$\underbrace{8 \cdot \frac{1}{8}}_{\text{corners}} + \underbrace{6 \cdot \frac{1}{2}}_{\text{faces}} + \underbrace{4}_{\text{enclosed}} = 8 \ \frac{\text{atoms}}{\text{unit cell}}$$

1.3: given $a_{Si} = 5.43$ Å, Calculate

a) distance from center of one Si atom to center of its nearest neighbor:
Si-Si bonds form a diamond lattice



There are 8 atoms/unit cell, each with radius r.
Along the body-diagonal of the lattice,

from corner to contained atom: $\frac{a}{4}(\bar{a} + \bar{b} + \bar{c}) = 2\vec{r}$

$$\Rightarrow (2r)^2 = \frac{a^2}{16}(\bar{a}\cdot\bar{a} + \bar{b}\cdot\bar{b} + \bar{c}\cdot\bar{c})$$

$$\Rightarrow 2r = \sqrt{\frac{3a^2}{16}} = \frac{\sqrt{3}\,a}{4} \quad \rightarrow \quad a = \frac{8r}{\sqrt{3}}$$

Therefore we find the distance from the center of one Si atom to its nearest neighbor to be

$$\boxed{2r = 2.35 \text{ Å}}$$

b) The number density of Si atoms ($\#/cm^3$)

We can use

$$\boxed{N = \frac{\sum_i N_i V_i}{a^3} = \frac{8}{a^3} = \frac{8}{(5.43\times10^{-8}\ cm)^3} = 5\times10^{22}\ \frac{\text{atoms}}{cm^3}}$$

c) mass density in g/cm^3

$$\rho = \frac{N \cdot M}{N_A}$$

M = atomic weight ; for Si, $M = 28.086\ u = 28.086\ \frac{g}{mole}$

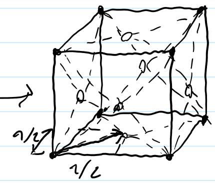
N_A = Avogadro's # = 6.022×10^{23}/mole

$$\Rightarrow \boxed{\rho = 2.33\ \frac{g}{cm^3}}$$

1.7: $r = 1.95\ \text{Å}$

a) simple cubic: $a = 2r = 3.9\ \text{Å}$

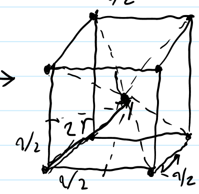
b) fcc : $a = \frac{4r}{\sqrt{2}} = 5.515\ \text{Å}$



$2\vec{r}_{fcc} = \sqrt{\left(\frac{a}{2}\right)^2 (2)} = \sqrt{\frac{a^2}{2}} = \frac{\sqrt{2}}{2} a$

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

c) bcc : $a = \frac{4r}{\sqrt{3}} = 4.503\ \text{Å}$



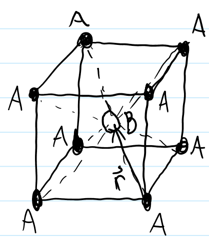
$2\vec{r} = \frac{a}{2}(\bar{a} + \bar{b} + \bar{c})$

$2r = \sqrt{\frac{a^2}{4}(3)} = \frac{\sqrt{3}\ a}{2}$

$\Rightarrow a = 4r/\sqrt{3}$

d) diamond: $a = \frac{8r}{\sqrt{3}} = 9.007\ \text{Å} \rightarrow$ (see 1.3a)

1.12: a)



$a_A = 2.2\ \text{Å}$

$a_B = 1.8\ \text{Å}$

$\vec{r} = \frac{a}{2}(\bar{a} + \bar{b} + \bar{c}) \Rightarrow r = \sqrt{\frac{a^2}{4}(3)} = \frac{\sqrt{3}\ a}{2}$

from corner A to center B (not 2r here since two different atoms compose the lattice)

so using $2r = a\sqrt{3} = 2(a_A + a_B) \Rightarrow \boxed{a = \frac{2}{\sqrt{3}}(a_A + a_B) = 4.62\ \text{Å}}$

and the volume density is

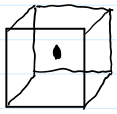
$$A: \frac{1}{2} \cdot \frac{2}{a^3} = \frac{1}{(4.62 \times 10^{-8}\ cm)} = 1.01 \times 10^{22}\ cm^{-3}$$

$$B: \frac{1}{2} \cdot \frac{2}{a^3} = \frac{1}{(4.62 \times 10^{-8}\ cm)} = 1.01 \times 10^{22}\ cm^{-3}$$

b) the answer is the same as a)

c) The materials are the same

1.14:



$\sum_i N_i V_i = 1$

a) $\boxed{N_v = \frac{1}{a_0^3}}$

$\boxed{N_s = \frac{1}{a_0^2 \sqrt{2}}}$

b) for simple cubic lattice

$N \cdot V = \frac{1}{8} \cdot 8 = 1$,

so the volume & surface densities are the same

1.17:

Take the ratios of the given lattice constant and lattice intercepts:

$$\left(\frac{4.83\ \text{Å}}{9.66\ \text{A}}, \frac{4.83\ \text{Å}}{19.32\ \text{Å}}, \frac{4.83\ \text{Å}}{14.49\ \text{Å}}\right) = \left(\frac{1}{2}, \frac{1}{4}, \frac{1}{3}\right)$$

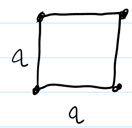
$$\left(\frac{4.83\text{Å}}{9.66\text{Å}}, \frac{4.83\text{Å}}{19.32\text{Å}}, \frac{4.83\text{Å}}{14.49\text{Å}}\right) = \left(\frac{1}{2}, \frac{1}{4}, \frac{1}{3}\right)$$

then multiply by the LCD (12) to obtain

$$\boxed{(6, 3, 4) \text{ Plane}}$$

1.19: a) simple cubic

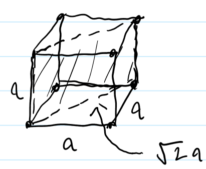
i) (100)



$\frac{1}{4} \cdot 4 = 1$

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

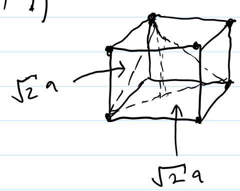
ii) (110)



$\frac{1}{4} \cdot 4 = 1$

$N_s = \frac{1}{\sqrt{2}\, a^2} = 3.16 \times 10^{14}\ cm^{-2}$

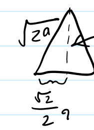
iii) (111)



$A_{111} = \frac{1}{2} b h$

$h^2 = 2a^2 + \frac{1}{2}a^2$

$\Rightarrow h = \frac{a\sqrt{6}}{2}$



$h^2 = 2a^2 + \frac{1}{2}a^2$

$= \frac{4}{2}a^2 + \frac{1}{2}a^2$

$= \frac{3}{2}a^2$

$\Rightarrow h = \sqrt{\frac{3}{2}}\, a = \frac{\sqrt{6}}{2} a$

so $A_{111} = \frac{1}{2}\left(\sqrt{2}\, a\right)\left(\frac{\sqrt{6}\, a}{2}\right) = \frac{a^2}{4}\sqrt{12}$

and there are $3 \times \frac{1}{6}$ atoms in the lattice plane, so

$N_s = \frac{2}{a^2\sqrt{12}} = 2.58 \times 10^{14}\ cm^{-2}$

b) bcc

i) (100) same as simple cubic case.

ii) (110) $\frac{1}{4} \cdot 4 + 1 = 2$ atoms in the lattice plane

$N_s = \frac{2}{a^2\sqrt{2}} = 6.32 \times 10^{14}\ cm^{-2}$

iii) (111) same as simple cubic case

c) fcc

i) (100) $4 \cdot \frac{1}{4} + 1 = 2$ atoms in the lattice plane

$N_s = \frac{2}{a^2} = 8.94 \times 10^{14}\ cm^{-2}$

ii) (110) same as bcc case

iii) (111) $3 \cdot \frac{1}{6} + 3 \cdot \frac{1}{2} = 2$ atoms in the lattice plane

$N_s = \frac{2}{A_{111}} = 1.03 \times 10^{15}\ cm^{-2}$