Problem collection

 # 1-1) Given: Cu, fcc with $\rho = 8{,}93\ g/cm^3$

Wanted: a) Lattice parameter of conventional cell

b) Distance between nearest neighbors

c) Volume of the primitive unit cell

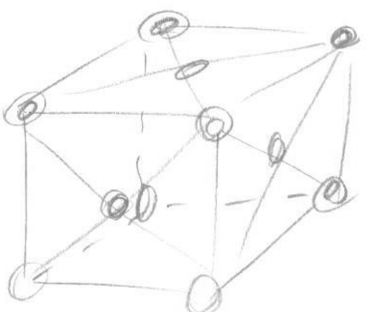
Solution

Cu has a mass number of 63.55 u

i.e. 63.55 g/mole

1 mole = $6.022 \cdot 10^{23}$ atoms

a)



a

The conventional cell contains

$8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$ atoms/cell

Density: $\rho = \dfrac{m}{V} =$

$$= \frac{4 \cdot M_{Cu}}{N_A \cdot a^3} \Rightarrow a = \left(\frac{4 \cdot M_{Cu}}{N_A \cdot \rho} \right)^{1/3}$$

$$a = \left(\frac{4 \cdot 63.55}{6.022 \cdot 10^{23} \cdot 8.93} \; \frac{\cancel{at} \cdot \cancel{g}/\cancel{mol}}{\frac{\cancel{at}}{\cancel{mol}} \; \cancel{g}/cm^3} \right)^{1/3} = 3.61 \cdot 10^{-8}\ cm =$$

$$= \underline{3.61\ \text{Å}}$$

b) Nearest neighbors: surface diagonal

$$\frac{1}{2}(\sqrt{2}a) = \frac{a}{\sqrt{2}} = \underline{2.56\ \text{Å}}$$

c) Volume of conventional cell $= a^3$

$\Rightarrow$ Volume of primitive cell $= \dfrac{a^3}{4} = \underline{\underline{11.8 \cdot 10^{-30}\ m^3}}$

#1-2

Given: Diamond, $a = 3{,}56$ Å

Wanted: Distance between a) nearest neighbors
b) second-nearest neighbors

Solution

Diamond: 2 fcc displaced by $\frac{1}{4}a(\hat{x}+\hat{y}+\hat{z})$

a) Nearest neighbors along diagonal

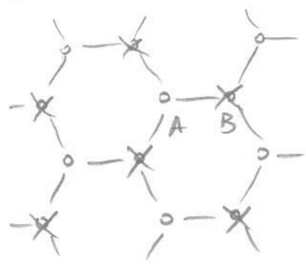
$$\Longrightarrow \frac{1}{4}\cdot\sqrt{3}\,a = \underline{\underline{1.54\ \text{Å}}}$$

b) second-nearest along surface diagonal

$$\Longrightarrow \frac{1}{2}\sqrt{2}\cdot a = 2.52\ \text{Å}$$

#1-3

Given:



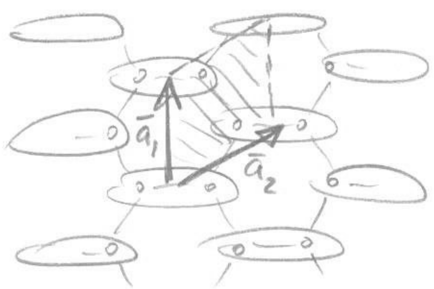
Wanted: a) Why not Bravaislattice?

Answer: atoms A and B do not see the same surrounding unless rotation

Wanted b) Primitive lattice vectors?
\# atoms in the basis?

Solution: We see 2 different kind of points.

$\Longrightarrow$ Form Bravaislattice between 1:st kind (*)
Form basis of <u>2 atoms</u>



$\bar{a}_1$ and $\bar{a}_2$ as in figure

$\Longrightarrow$ Contains $\frac{1}{4}\times 4 = 1$ base unit cell

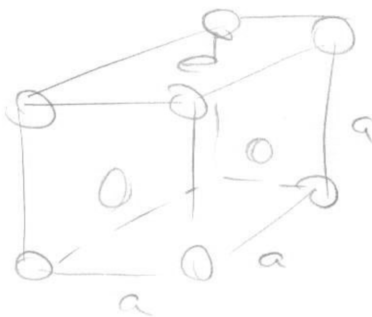
#1-4) Given: Al fcc $\rho = 2.70\ g/cm^3$

Wanted: a) Lattice parameter

b) Filling factor if hard spheres touching

Solution a) $M_{Al} = 26.98\ g/mol$

$N_A = 6.022 \cdot 10^{23}$ atoms/mol



fcc: 4 atoms/cell

cell volume a^3

$$\frac{4}{a^3} = \frac{\rho \cdot N_A}{M_{Al}}$$

$$\Longrightarrow a = \left(\frac{4 \cdot M_{Al}}{\rho N_A}\right)^{1/3} = \left(\frac{4\ at \cdot 26.98\ g/mol}{2.70\ g/cm^3 \cdot 6.022 \cdot 10^{23}\ at/mol}\right)^{1/3} =$$

$$= \underline{\underline{4.05\ \text{Å}}}$$

b) Spheres touching along surface diagonal

$$4r = \sqrt{2} \cdot a$$

$$f = \frac{4 \cdot \frac{4}{3}\pi r^3}{a^3} = \frac{4 \cdot \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} = \frac{\pi}{3\sqrt{2}} \approx 0.74 = \underline{\underline{74\%}}$$

1-5

Given: Co: hcp at R.T.
fcc at elevated temp.

Wanted: a) Volume for primitive cell in hcp, expressed in lattice param. a and c

b) Same density fcc, hcp $\Rightarrow$ fcc lattice param

$a_{hcp} = 2.51$ Å, $c = 4.07$ Å $\quad a_{fcc} = ?$

Solution

With primitive cell of hcp means the primitive cell of the underlying sh Bravaislattice, i.e, the hcp unit cell, which contains 2 atoms.

$\bar{a}_3$ perp. to $\bar{a}_1, \bar{a}_2$

$|\bar{a}_3| = c$

$$V_c = \bar{a}_3 \cdot (\bar{a}_1 \times \bar{a}_2) = c \cdot a^2 \cdot \sin 60° = \frac{\sqrt{3}}{2} a^2 c$$

b) fcc: 4 atoms/cell

$$\frac{4}{a_{fcc}^3} = \frac{2}{\frac{\sqrt{3}}{2} a^2 c} \Rightarrow a_{fcc} = \left(\sqrt{3}\, a^2 c\right)^{1/3} =$$

$$= \left(\sqrt{3} \cdot 2.51^2 \cdot 4.07\right)^{1/3} \text{Å} =$$

$$= 3.54 \text{ Å}$$

#1-6 <u>Given:</u> Si, $\rho = 2.33\ g/cm^3$

"Hard spheres"

<u>Wanted:</u> Rearrangement into close-packing $\Rightarrow$ density?

<u>Solution</u> Diamond structure $\Longleftrightarrow$ 2 fcc shifted $\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$

$\Rightarrow$ Spheres touching along diagonal

$$2r = \frac{1}{4}\cdot\sqrt{3}\cdot a \quad \Rightarrow \quad f = \frac{8\cdot\frac{4}{3}\pi r^3}{\left(\frac{4\cdot 2r}{\sqrt{3}}\right)^3} =$$

$$= \frac{\sqrt{3}\cdot 4}{64}\cdot\pi = \frac{\sqrt{3}}{16}\cdot\pi \approx \underline{\underline{0.34}}$$

filling factor

Close-packing: Filling factor as for fcc

$$4r = \sqrt{2}\cdot a \qquad f = \frac{4\cdot\frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} = \frac{\pi}{3\sqrt{2}} \approx \underline{\underline{0.74}}$$

$\Rightarrow$ the density would increase by a factor $\frac{0.74}{0.34} = 2.18$

$$\Longrightarrow \quad \rho_{\text{close packed}} = 2.18\cdot 2.33\ g/cm^3 = \underline{\underline{5.07\ g/cm^3}}$$

#5-1) **Given**: Free electron approximation

Wanted: Mean free path of conduction electrons in Ag at room temperature

Solution

$l = v_F \tau$ what do we need to obtain τ?

Resistivity: $\sigma = \frac{n e^2 \tau}{m}$

$\left(\varrho = \frac{1}{\sigma} \right)$ *

$$v_F = \frac{\hbar k_F}{m}$$

$$k_F = (3\pi^2 n)^{1/3}$$

$$n = \frac{N}{V} = N_A \cdot \frac{Z \cdot \varrho_{Ag}}{M_{Ag}}$$

density

Z = valence = 1 for Ag ("conduction electron")

$\varrho_{Ag} = 10.5 \ g/cm^3$

$M_{Ag} = 107.9 \ g/mol$

$\varrho_* = 1.51 \ \mu\Omega cm$ from A.M. @ 273K

$$l = v_F \tau = \frac{\hbar k_F}{m} \cdot \frac{m}{n e^2 \varrho_*} = \frac{\hbar (3\pi^2)^{1/3}}{e^2 \varrho_*} \cdot \frac{1}{n^{2/3}} =$$

$$= \frac{\hbar (3\pi^2)^{1/3}}{e^2 \varrho_*} \cdot \left(\frac{M_{Ag}}{Z \cdot N_A \cdot \varrho_{Ag}} \right)^{2/3} = \left\{ \begin{array}{l} \hbar = 1.05 \cdot 10^{-34} \ J \cdot s \\ e = 1.602 \cdot 10^{-19} \ C \end{array} \right\}$$

$$\approx \underline{\underline{55 \ nm}}$$

#5-2) Given : CuZn alloy , $\frac{N_{at}}{V}$ equal to $\frac{N_{at}}{V}$ for Cu

Wanted : Fermi energy

Solution

$$\mathcal{E}_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3} \qquad \text{where} \quad n = \frac{N_{at}\cdot Z}{V}$$

Z: Cu 1 $\qquad \mathcal{E}_{F,Cu} = 7.0\ \text{eV}$ from A.M.

Zn 2

$$\Rightarrow \quad n_{CuZn} = n_{Cu}\cdot\frac{\frac{1+2}{2}}{1} = 1.5\cdot n_{Cu}$$

$$\Rightarrow \quad \mathcal{E}_{F,CuZn} = \mathcal{E}_{F,Cu}\cdot 1.5^{2/3} = \underline{\underline{9.2\ \text{eV}}}$$

$\mathcal{E}_{F,Cu}$ – Check

$$n = \frac{N_{at}\cdot 1}{V} = N_A\cdot\frac{\rho_{Cu}}{M_{Cu}} \qquad \text{at/mol}\ \frac{\text{g/cm}^3}{\text{g/mol}}$$

$$= 6.022\cdot 10^{23}\cdot\frac{8.96}{63.55}\ \text{cm}^{-3} = \underline{8.49\cdot 10^{22}\ \text{cm}^{-3}} = \underline{8.49\cdot 10^{28}\ \text{m}^{-3}}$$

$$\left.\begin{aligned}\hbar &= 1.054\cdot 10^{-34}\ \text{Js}\\ m_e &= 9.1\cdot 10^{-31}\ \text{kg}\end{aligned}\right\} \quad \mathcal{E}_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3} = 1.13\cdot 10^{-18}\ \text{J} =$$

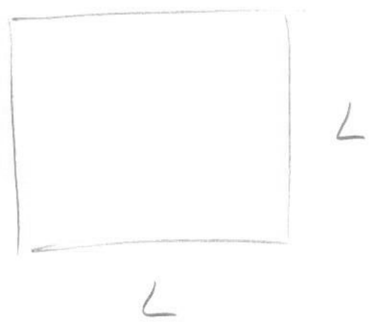
$$= \frac{1.13\cdot 10^{-18}}{1.602\cdot 10^{-19}}\ \text{eV} =$$

$$= \underline{\underline{7.04\ \text{eV}}}$$

#5-3) Given : 3D : $\mathcal{E}_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$

Wanted : 2D $\mathcal{E}_F(n)$ $n =$ number of el / area $= \frac{N}{A}$

Solution Consider electron gas contained in 2D



$A = L^2$

Schrödinger eq : $-\frac{\hbar^2}{2m}\nabla^2\psi = \mathcal{E}\psi$

Plane-wave solution $\psi_k(\bar{r}) = \frac{1}{C} e^{i\bar{k}\cdot\bar{r}}$

$$\mathcal{E}(\bar{k}) = \frac{\hbar^2 k^2}{2m}$$

Apply periodic boundary conditions

$$\psi(x+L) = \psi(x) \Rightarrow k_x = n_x \cdot \frac{2\pi}{L}$$

$$k_y = n_y \cdot \frac{2\pi}{L}$$

...

Area per k-point : $\left(\frac{2\pi}{L}\right)^2$ in k-space

Fermi circle : $\mathcal{E}_F = \frac{\hbar^2 k_F^2}{2m}$ contains $\frac{\pi k_F^2}{\left(\frac{2\pi}{L}\right)^2}$ points

N electrons fill up $\frac{N}{2}$ points (spin ↑↓)

$$\Rightarrow \frac{N}{2} = \frac{\pi k_F^2}{4\pi^2} \cdot V \Rightarrow \frac{N}{V} = \frac{1}{2\pi} k_F^2$$

$$k_F = (2\pi n)^{1/2}$$

$$\underline{\mathcal{E}_F = \frac{\hbar^2}{2m} \cdot (2\pi n)} = \left(\frac{\pi\hbar^2}{m} \cdot n\right)$$

5-4 Given a) $\mathcal{E}_{av} = \langle \mathcal{E} \rangle = \frac{3}{5} \mathcal{E}_F$ Show this!

Solution Free, degenerate electron gas

$$\mathcal{E} = \frac{\hbar^2 k^2}{2m}, \quad g(\mathcal{E}) = \frac{3}{2} \frac{n}{\mathcal{E}_F} \left(\frac{\mathcal{E}}{\mathcal{E}_F} \right)^{1/2} \sim \sqrt{\mathcal{E}}$$

$$\langle \mathcal{E} \rangle = \frac{\int_0^{\mathcal{E}_F} \mathcal{E} \cdot g(\mathcal{E})\, d\mathcal{E}}{\int_0^{\mathcal{E}_F} g(\mathcal{E})\, d\mathcal{E}} = \frac{\int_0^{\mathcal{E}_F} \mathcal{E} \cdot \sqrt{\mathcal{E}}\, d\mathcal{E}}{\int_0^{\mathcal{E}_F} \sqrt{\mathcal{E}}\, d\mathcal{E}} = \frac{\left[\frac{2}{5} \mathcal{E}^{5/2} \right]_0^{\mathcal{E}_F}}{\left[\frac{2}{3} \mathcal{E}^{3/2} \right]_0^{\mathcal{E}_F}} = \underline{\underline{\frac{3}{5} \mathcal{E}_F}}$$

Wanted: b) Cu, cube 1,00 cm side

Compress $\Rightarrow$ cube 0.99 cm side

Energy only for compressing el. gas

$\mathcal{E}_F = 7.0\,\text{eV}, \quad Z = 1$

Energy required?

Solution: $U = N \cdot \langle \mathcal{E} \rangle = \frac{3}{5} N \cdot \mathcal{E}_F$

N const. but $\mathcal{E}_F = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}$

$$n = \frac{N}{V} = \frac{N}{L^3} \Rightarrow n' = \frac{N}{V'} = \frac{N}{L'^3} = n \cdot \left(\frac{L}{L'} \right)^3$$

$$\mathcal{E}_F' = \mathcal{E}_F \cdot \left(\frac{n'}{n} \right)^{2/3} = \mathcal{E}_F \cdot \left(\frac{L}{L'} \right)^2$$

$$\Delta U = U' - U = \frac{3}{5} N (\mathcal{E}_F' - \mathcal{E}_F) = \frac{3}{5} N \mathcal{E}_F \left[\left(\frac{L}{L'} \right)^2 - 1 \right]$$

$$N = N_A \cdot \frac{\rho_{Cu}}{M_{Cu}} \cdot V = \left\{ \begin{array}{l} \#5\text{-}2 \quad n = 8.49 \cdot 10^{22}\,\text{cm}^{-3} \\ V = 1\,\text{cm}^3 \end{array} \right\} = 8.49 \cdot 10^{22}$$

$$\Rightarrow \Delta U = \frac{3}{5} \cdot 8.49 \cdot 10^{22} \cdot 7.0 \cdot \left[\left(\frac{1.00}{0.99} \right)^2 - 1 \right] \text{eV} = 7.24 \cdot 10^{21}\,\text{eV} = \underline{\underline{1160\,\text{J}}}$$

c) Kinetic energy, pot. energy or both?

#5-5 Assume × Maxwell-Bolzmann distribution

× Resistivity due to collisions with ions

× Mean free path $\ell = \text{const.} \approx a_0$

distance between ions.

× Scattering randomly

Show : Model gives $\rho \sim \sqrt{T}$

Solution

$$\rho = \frac{1}{\sigma} \qquad \sigma = \frac{ne^2\tau}{m} = \{ \ell = v_0 \tau \}$$

here average $\langle|v|\rangle$

Fermi-Dirac: v_F

$$\Rightarrow \rho = \frac{m \cdot v_0}{ne^2 \ell}$$

$$v_0 = \langle|v|\rangle \qquad \frac{mv_0^2}{2} = \frac{3}{2} k_B T \quad \text{for M.B.}$$

$$\Rightarrow v_0 \sim \sqrt{T} \Rightarrow \rho \sim \text{const} \cdot \sqrt{T}$$

b) How does this agree with experiments?

Solution v_0 is actually v_F which is constant (indep. of T)

However, (resistivity as a funct. of T) is obtained from changes in ℓ.

The regular ion lattice does not scatter the electrons.

Two main types of lattice imperfections contribute to ρ:

1) Thermal vibrations
2) Impurity atoms, point defects

Extreme conditions, low Temp. el-el scattering $\rho \sim T^2$

Lattice vibrations decrease with decreasing T

ideal crystal

$$\rho = \rho_{cr} + \rho_{imp} \quad ; \quad \rho_{cr} \approx T^5 \text{ at low } T \quad \sim T \text{ at high } T$$

$\rho_{imp} \sim$ const. but $\sim$ number of imp.

$$\frac{1}{\ell} = \frac{1}{\ell_{\text{thermal vib}}} + \frac{1}{\ell_{imp.}}$$

Matthiessen's law

#5-6 | Given: Cu at R.T.

Neutron irrad. $\Rightarrow$ increase defects $\Rightarrow$ double ρ

Wanted: Estimate l for scattering of el. against the defects.

Solution

$$\sigma = \frac{ne^2\tau}{m} \Rightarrow \rho = \frac{mv_F}{ne^2 l}$$

$\rho_{Cu}(273\,K) = 1.56\,\mu\Omega cm$

$$\frac{1}{l} = \frac{1}{l_{ideal}} + \frac{1}{l_{imp}}$$

$$\rho_{Cu} = \frac{mv_F}{ne^2 l_{ideal}}$$

$$2\rho_{Cu} = \frac{mv_F}{ne^2 l} = \underbrace{\frac{mv_F}{ne^2}\left(\frac{1}{l_{ideal}}\right.}_{\rho_{Cu}} + \left.\frac{1}{l_{imp}}\right)$$

$$2\rho_{Cu} - \rho_{Cu} = \rho_{Cu} = \frac{mv_F}{ne^2} \cdot \frac{1}{l_{imp}}$$

$$l_{imp} = \frac{mv_F}{ne^2} \cdot \frac{1}{\rho_{Cu}}$$

$\rho_{Cu} = 1.56 \cdot 10^{-8}\,\Omega m$

$m = m_e = 9.1 \cdot 10^{-31}\,kg$

$n = \{\#5\text{-}2\} = 8.49 \cdot 10^{28}\,m^{-3}$

$e = 1.602 \cdot 10^{-19}\,C$

$\Rightarrow l_{imp} = \underline{\underline{42\,nm}}$

$$\mathcal{E}_F = \frac{mv_F^2}{2} = 7.0\,eV = 7.0 \cdot 1.602 \cdot 10^{-19}\,J$$

$$\Rightarrow v_F = \sqrt{\frac{2\mathcal{E}_F}{m}} = 1.57 \cdot 10^6\,m/s$$