Question Number V *(~~20~~ 15 Marks ~ 27 minutes)*

a) Iron atoms (M= 55.85 kg/kmol, molecular diameter = 2.5 Å) are arranged in a face-centered cubic lattice (FCC) above 1180 K, and a different structure below 1180 K (density below 1180K =7.71 g/cm^3).

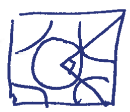
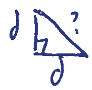
i. Calculate the density of iron above 1180 K. *(/2)*

FCC $\rho = \frac{\sqrt{2} m}{d^3}$ $m = \frac{M}{N_A} = \frac{55.85 \, kg/kmol}{6.023 \times 10^{26}/kmol} = 9.2727 \times 10^{-26} \, kg$

$\rho = \frac{\sqrt{2}(9.2727 \times 10^{-26} kg)}{(2.5 \times 10^{-10} m)^3}$

$\boxed{\rho = 8391 \, kg/m^3}$

ii. What is the length of a side of the unit cell above 1180 K? *(/1)*

FCC   $\rightarrow d^2 + d^2 = x^2$

$\boxed{x = \sqrt{2} d}$

iii. Determine the structure of iron below 1180 K. *(/2)*

$\rho = X \frac{m}{d^3}$ $m = 9.2727 \times 10^{-26} \, kg$

$d = 2.5 \times 10^{-10} \, m$

$7710 = X \frac{(9.27 \times 10^{-26})}{(2.5 \times 10^{-10} m)^3}$ $\rho = 7.71 \frac{g}{cm^3} \times \frac{1 kg}{1000 g} \times \left(\frac{100 \, cm}{1 m}\right)^3 = 7710 \frac{kg}{m^3}$

$X = 1.299 \rightarrow \boxed{BCC}$

iv. What would be the change in length for a cubic block of iron with a mass of 1000 kg transitioning from below 1180 to above 1180 K? *(/2)*

below $\rightarrow$ above

ρ 7710 $\rightarrow$ 8391

$\frac{1000 \, kg}{7710 \, kg/m^3} = 0.1297 \, m^3 = L_1^3 \rightarrow L = 0.50619 \, m$

$\frac{1000 \, kg}{8391 \, kg/m^3} = 0.1192 \, m^3 = L_2^3 \rightarrow L = 0.4921 \, m$

$\Delta L = -0.014 \, m$
$-1.4 \, cm$
(shorter)

Continued …

Question Number VI *(Continued)*

c) Nitrogen freezes at -210°C, and the Lennard Jones parameters for nitrogen are ε/k=96.3 K and b_o=0.0636 m^3/kmol.

i) Determine the separation distance where the potential energy between two nitrogen molecules will be a minimum. ***(/2)***

$\phi_{min} = -\epsilon$, $F = 0$ $r = r_o = 1.122\sigma$

$b_o = \frac{2\pi}{3}\sigma^3 N_A$

$$\boxed{r_o = 4.145 \times 10^{-10} m}$$

$0.0636 \frac{m^3}{kmol} = \frac{2\pi}{3}\sigma^3(6.023 \times 10^{26}/kmol) \rightarrow \sigma = 3.694 \times 10^{-10} m$

ii) What are the values of the potential energy and the force between 2 nitrogen molecules at the distance in i)? ***(/2)***

$$\boxed{F = 0}$$

$\epsilon/k = 96.3K = \epsilon/1.3805 \times 10^{-23} J/K$

$\phi_{min} = -\epsilon$

$\epsilon = 1.329 \times 10^{-21} J$

$$\boxed{\phi_{min} = -1.329 \times 10^{-21} J}$$

iii) What is the value of the force between two nitrogen molecules at a separation distance equal to 2.5x the minimum potential energy distance? ***(/4)***

$F = ?$ when $r = 2.5 r_o = 2.8\sigma$

$$\phi = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right]$$

$$F = \frac{d\phi}{dr} = 4\epsilon\left(-12\frac{\sigma^{12}}{r^{13}} + 6\frac{\sigma^6}{r^7}\right)$$

$$F = 4\epsilon\left[-12\frac{\sigma^{12}}{(2.8\sigma)^{13}} + 6\frac{\sigma^6}{(2.8\sigma)^7}\right] = \frac{4\epsilon}{\sigma}\left[\frac{-12}{(2.8)^{13}} + 6\frac{1}{(2.8)^7}\right]$$

$$F = \frac{4\epsilon}{\sigma}(4.428 \times 10^{-3})$$

$$\boxed{F = 6.373 \times 10^{-14} N}$$

Question Number V *(13 Marks ~ 23 minutes)*

Aluminum (M=26.98 kg/kmol, σ = 2.62 Å) is known to exist in an FCC structure at 25°C and 1 atm, has a Young's modulus 69 GPa, Poisson's ratio 0.33, coefficient of thermal expansion 22.68x10^{-6} K^{-1}, and thermal conductivity 190 W/mK.

a) For a solid sphere of metallic aluminum at 25°C and 1 atm with a volume of 10^{-3} cm^3, calculate values of the following quantities:

i. The specific volume of aluminum (m^3/kg) (/2)

FCC $\rho = \frac{\sqrt{2}m}{d^3}$ $\quad m = M/N_A = \frac{26.98\ kg/kmol}{6.023 \times 10^{26}} = 4.479 \times 10^{-26} kg$ 0.5

$d = 2.62 Å = 2.62 \times 10^{-10} m$ 0.5

$$\rho = \frac{\sqrt{2}(4.479 \times 10^{-26} kg)}{(2.62 \times 10^{-10} m)^3} = 3522\ kg/m^3$$

1

$$v = \frac{1}{\rho} = \boxed{2.84 \times 10^{-4}\ m^3/kg}$$

ii. The mass of the sphere. (/1)

$$v = \frac{V}{m} \rightarrow m = \frac{V}{v} = \frac{10^{-9} m^3}{2.84 \times 10^{-4} m^3/kg}$$

$V = 10^{-3} cm^3 \times \left(\frac{1 m}{100 cm}\right)^3$

$V = 10^{-9} m^3$

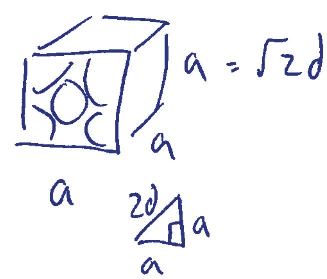
1

$$\boxed{m = 3.52 \times 10^{-6} kg}$$

iii. The total volume of void space in the sphere. (/2)

$$\text{void fraction} = \frac{\text{volume unit cell} - \text{volume molecules}}{\text{volume unit cell}}$$

0.5



$$= \frac{(\sqrt{2}d)^3 - 4 \times \frac{4}{3}\pi\left(\frac{d}{2}\right)^3}{(\sqrt{2}d)^3}$$

$$= \frac{(\sqrt{2})^3 - \frac{2\pi}{3}}{(\sqrt{2})^3} = 0.2595$$

1

$$\text{void volume} = 0.2595 \times 10^{-3} m^3 = \boxed{0.26 \times 10^{-3} m^3}$$

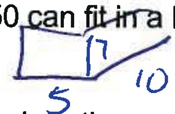
0.5

continued...

ABU

Question Number V *(15 Marks ~ 27 minutes)*

PART 1: You have been asked to design a system to pack oranges into boxes. Each orange can be thought of as a rigid 8 cm diameter sphere with density 900 kg/m^3. If the oranges are packed with a simple cubic pattern, then 350 can fit in a box (5 wide, 10 deep, and 7 high). That's a lot of oranges.



a) Calculate the fraction of empty space in the box when the oranges are packed in a simple cubic arrangement. Show your work. (/2)

Volume of box = $(5\times 8cm)(10\times 8cm)(7\times 8cm) = 179200\ cm^3$

Volume of orange = $\frac{4}{3}\pi\left(\frac{8cm}{2}\right)^3 = 268.08 cm^3$

Volume of oranges = $350 \times 268.08 = 93828\ cm^3$

frac void space = $\frac{\text{box} - \text{oranges}}{\text{box}} = \frac{179200 - 93828}{179200} = \boxed{0.476}$

47.6 %

b) Determine the mass of oranges in a box when the oranges are packed in a simple cubic arrangement. (/1)

vol = $93828\ cm^3 \times \left(\frac{m}{100\ cm}\right)^3 = 0.0938\ m^3$

$\rho = \frac{m}{V} \rightarrow m = \rho V = 900\frac{kg}{m^3} \times 0.0938\ m^3 = \boxed{84.44\ kg}$

c) Determine the effective density of the orange-filled box. The empty box weighs 2 kg. (/2)

$\rho = \frac{m}{V} = \frac{84.44\ kg + 2\ kg}{.1792\ m^3}$ $V = 179200\ cm^3 = 0.1792\ m^3$

$\boxed{\rho = 482.4\ kg/m^3}$

d) Using the limit of an infinitely large box, what percentage more oranges can fit in a box if the arrangement is face-centered cubic packing compared to simple cubic packing? (/2)

FCC

$a = \sqrt{2}d$ FCC

volume box = $(\sqrt{2}d)^3 = 2\sqrt{2}d^3$

$\frac{1}{2}\times 3 + \frac{1}{8}\times 8 = 4$ atoms

volume of atoms = $\frac{4}{3}\pi\left(\frac{d}{2}\right)^3 = \frac{\pi}{6}d^3$.

frac empty space = $\frac{2\sqrt{2}\cancel{d^3} - \frac{\pi}{6}\cancel{d^3}\times 4}{2\sqrt{2}\cancel{d^3}} = \frac{0.7336}{2.828}$ 0.26

continued...

percentage more oranges = $\frac{(1-0.476)-(1-0.26)}{(1-0.476)} = .454 \rightarrow$ $\boxed{45.4\%\text{ more oranges}}$

Question Number VI *(Continued)*

PART 2: Use the parameters below to answer the following questions:

	M, kg/kmol	ε/k, K	σ, Å
Oxygen	32	154	2.33
Nitrogen	28	78	2.94

a) Assuming ideal gas behavior, calculate the diffusivity of nitrogen gas at 50°C and 3 atm. ***(/2)***

$$D = \frac{RT}{PN_A\pi\sigma^2}\sqrt{\frac{RT}{\pi M}} \qquad T = 273.15 + 50 = 323.15\,K$$

$$D = \frac{8.314\,\frac{kPa\,m^3}{kmol\,K} \times 323.15\,K}{3\times 101.325\,kPa \times 6.023\times10^{26}/kmol \times \pi \times (2.94\times10^{-10}\,m)^2}\sqrt{\frac{8314\,\frac{Pa\,m^3}{kmol\,K} \times 323.15\,K}{\pi \times 28\,kg/kmol}}$$

$$\boxed{D = 9.44\times10^{-6}\ m^2/s}$$

b) Assuming ideal gas behavior, calculate the value of the Prandtl number ($C_p\mu/k$) for nitrogen at 50°C and 3 atm. ***(/2)***

$$Pr = \frac{C_p\mu}{k} = \frac{\dfrac{C_p M}{N_A\pi\sigma^2}\sqrt{\dfrac{RT}{\pi M}}}{\dfrac{C_v}{N_A\pi\sigma^2}\sqrt{\dfrac{RT}{\pi M}}} \times \frac{1}{M}$$

μ units = Pa.s

k units = $\frac{W}{mK} = \frac{Pa\,m^2}{K\,s}$

C_p units = $\frac{kJ}{kmol\,K}$

C_v units = $\frac{kJ}{kmol\,K}$

$$Pr = \frac{C_p}{C_v} = \frac{\frac{5}{2}R}{\frac{3}{2}R} = \boxed{\frac{5}{3} \text{ for ideal gas}}$$

continued…

Question Number VI *(Continued)*

c) Determine the net force between two molecules of oxygen separated by a distance of 3 times the minimum potential distance. ***(/2)***

$$F = \frac{d\phi}{dr} = \frac{d}{dr}\left(4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]\right)$$

ϕ_{min} @ $F=0$

@ $r = 1.122\sigma$

$$F = -48\epsilon\frac{\sigma^{12}}{r^{13}} + 24\epsilon\frac{\sigma^{6}}{r^{7}}$$

Let $r = 3 \times 1.122\sigma = 3.366\sigma$

$$F = -48\epsilon\frac{\sigma^{12}}{(3.366\sigma)^{13}} + 24\epsilon\frac{\sigma^{6}}{(3.366\sigma)^{7}}$$

$\frac{\epsilon}{k} = 154\ K$

$\epsilon = 2.126 \times 10^{-21} J$

$\sigma = 2.33\ Å$

$$F = -\frac{24\epsilon}{\sigma}\left(\frac{2}{(3.366)^{13}} - \frac{1}{(3.366)^{7}}\right)$$

$$F = -\frac{24(2.126 \times 10^{-21} J)}{2.33 \times 10^{-10} m}\left(-2.0398 \times 10^{-4}\right)$$

$$\boxed{F = 4.467 \times 10^{-14} N}$$

d) What is the minimum potential energy that occurs between two molecules of oxygen? ***(/2)***

$\min \phi = -\epsilon$

$$\boxed{\phi_{min} = -2.126 \times 10^{-21} J}$$

continued…

Question Number V *(15 Marks ~ 27 minutes)*

PART 1:

The density of silver (M = 107.88 g/mol) at 20°C is 10520 kg/m^3, and the closest interatomic distance is 2.888 Angstroms.

a) Determine the structure of silver at 20°C. (/2)

2/2

$$\rho = X\frac{m}{d^3} \quad \tfrac{1}{2} \qquad m = \frac{M}{N_A} = \frac{107.88\ \text{kg/kmol}}{6.023\times10^{26}/\text{kmol}} = 1.7911\times10^{-25}\ \text{kg} \quad \tfrac{1}{2}$$

$$X = \frac{\rho d^3}{m} \qquad d = 2.888\times10^{-10}\ \text{m} \qquad \rho = 10520\ \text{kg/m}^3$$

$$X = \frac{(10520\ \text{kg/m}^3)(2.888\times10^{-10}\ \text{m})^3}{1.7911\times10^{-25}\ \text{kg}} = 1.4147 \quad \tfrac{1}{2} \quad \simeq \sqrt{2} = \boxed{FCC} \quad \tfrac{1}{2}$$

b) A 10 kg bar of silver is 4 cm wide by 4 cm high. Estimate the length of the bar at 20°C. (/3)

3/3

$$\rho = \frac{\text{mass}}{\text{volume}} \rightarrow \text{volume} = \frac{\text{mass}}{\rho} = \frac{10\ \text{kg}}{10520\ \text{kg/m}^3} = 9.506\times10^{-4}\ \text{m}^3 \quad 1$$

$$\text{volume} = L\times W\times H \quad 1$$

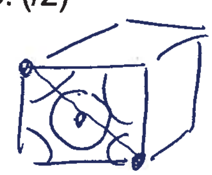
$$9.506\times10^{-4}\ \text{m}^3 = (4\times10^{-2}\ \text{m})(4\times10^{-2}\ \text{m})(L)$$

$$\boxed{L = 0.594\ \text{m}} \quad 1$$

c) Calculate the fraction of void space in the bar of silver at 20°C. (/2)

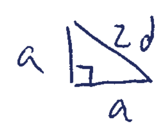
2/2

$$\text{FCC} \qquad n = 6\times\tfrac{1}{2} + 8\times\tfrac{1}{8} = 4$$



$$\text{Void fraction} = \frac{\text{unit cell} - \text{molecules}}{\text{unit cell}} \quad \tfrac{1}{2}$$

$$= \frac{(\sqrt{2}d)^3 - 4\left(\frac{\pi}{6}d^3\right)}{(\sqrt{2}d)^3} \quad \tfrac{1}{2}$$



$$\rightarrow a^2 + a^2 = (2d)^2$$
$$2a^2 = 4d^2$$
$$\tfrac{1}{2} \quad a = \sqrt{2}d$$

$$= \frac{2\sqrt{2} - \frac{2\pi}{3}}{2\sqrt{2}}$$

continued…

$$\boxed{= 0.259} \quad \tfrac{1}{2}$$

Question Number VI *(15 Marks ~ 36 minutes)*

PART 1:

The Lennard-Jones parameters for a substance (M=28) are: $\varepsilon=133\times10^{-23}$J, $b_o=0.064m^3/kmol$.

a) Calculate the separation distance at which the net force between two adjacent molecules is zero. (/2)

$F=0$, $r=r_o=1.122\sigma$

$b_o=\frac{2\pi}{3}\sigma^3 N_A$

$0.064\frac{m^3}{kmol}=\frac{2\pi}{3}\sigma^3\, 6.023\times10^{26}/kmol$

$\sigma=3.702\times10^{-10}m$ 1

$r_o=1.122\times3.702\times10^{-10}m$ 1

$\boxed{r_o=4.1536\times10^{-10}m}$

2

b) What is the potential energy between two adjacent molecules when the net force is zero? (/2)

$\phi=\phi_{min}=-\epsilon=\boxed{-133\times10^{-23}J}$ 1 1

**

2

c) Calculate the net force between two adjacent molecules when the separation distance is 3 times the molecular diameter. (/3)

$F=?$ $r=3\sigma$

$\phi=4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right]$

$F=\frac{d\phi}{dr}=4\epsilon\left[-12\left(\frac{\sigma^{12}}{r^{13}}\right)+6\left(\frac{\sigma^6}{r^7}\right)\right]$ 1

$F=4\epsilon\left[-12\frac{\sigma^{12}}{(3\sigma)^{13}}+6\frac{\sigma^6}{(3\sigma)^7}\right]$

$\rightarrow F=\frac{4\epsilon}{\sigma}\left[\frac{-12}{3^{13}}+\frac{6}{3^7}\right]$

$F=\frac{4\epsilon}{\sigma}(2.736\times10^{-3})$ 1

$F=\frac{4\times133\times10^{-23}}{3.702\times10^{-10}}(2.736\times10^{-3})$

$\boxed{F=3.931\times10^{-14}N}$ 1

3

continued…