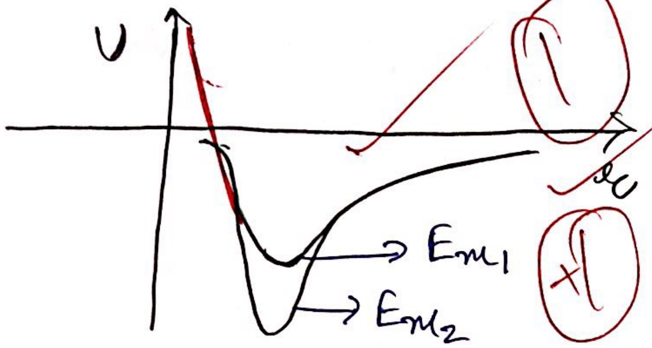
(a) Discuss various material properties that may be inferred by the nature of atomic bonding with the help of potential energy curves.

Ans(a)) 1) Elastic Modulus (E)



1

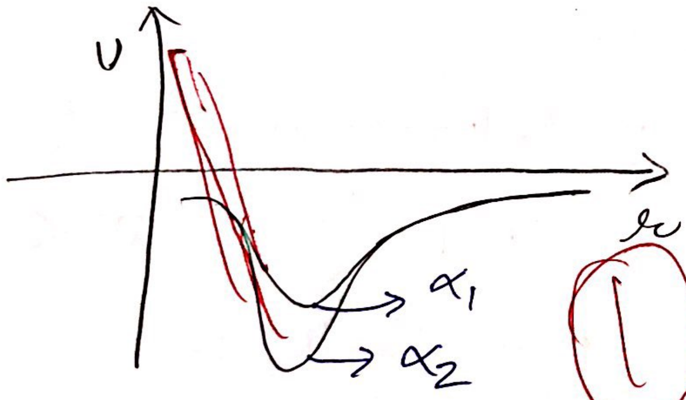
+1

$E_{m_2} > E_{m_1}$

1

because material with higher bond energy will have higher tendency to be stretched for given stress and retain its actual position.

2) Thermal Expansion Coefficient (α)

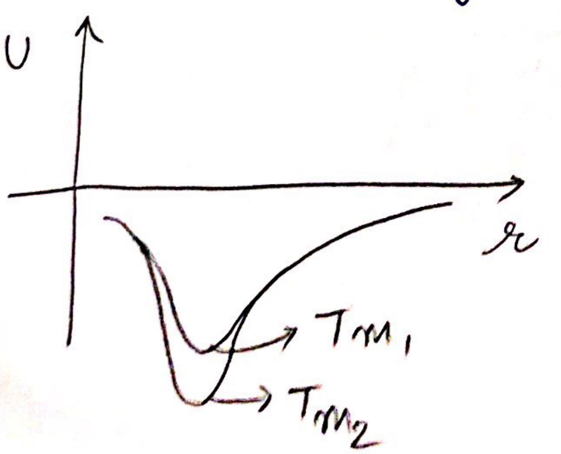


1

$\alpha_1 > \alpha_2$

Thermal expansion coefficient is higher for lower bond energy system because it will expand more for given ~~sa~~ energy due to less bond energy.

3) Melting point (T_m)



$T_{m_2} > T_{m_1}$

1

Higher bond energy leads to higher heat to break bond. So, Temp required will be higher. ~~[illegible]~~ i.e Melting point is higher.

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(b) Compute the number of ways of arranging 6 Ni atoms and 6 Cu atoms on 12 atomic sites. If we now have 7 Ni atoms and 5 Cu atoms on 12 atomic sites, would the configurational entropy increase?

Ans) $S = k \ln \omega$

ω = no. of possible configurations.

6 Ni atoms and 6 Cu atoms at 12 sites

12!

$$\omega_1 = \frac{12!}{6!6!} = 924$$

7 Ni atoms and 5 Cu atoms at 12 sites

$$\omega_2 = \frac{12!}{7!5!} = 792$$

$$\Delta S = k \ln \omega_2 - k \ln \omega_1$$

$$\Delta S = k \ln\left(\frac{792}{924}\right) = 1.3806 \times 10^{-23}$$

$$= -0.2128 \times 10^{-23} \text{ J/K}$$

Since the no. of configurations have decreased so, Entropy will be decreased as shown.

7

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Question 2 [8+7]

(a) A reaction with activation energy equal to 100 kJ mol^{-1} takes 50 min for completion at 300 K. At what temperature will it complete in 5 min?

$$\text{rate} = A e^{-E_A/RT} \quad 2$$

$$1 \quad -\frac{dc}{dt} = A e^{-E_A/RT}$$

$$C = (A e^{-E_A/RT}) t.$$

Let $C = C_0$ i.e. const.

$$(e^{-E_A/RT}) t = \text{const}.$$

$$\Rightarrow (e^{-E_A/RT_1}) t_1 = (e^{-E_A/RT_2}) t_2$$

$$\Rightarrow \frac{t_2}{t_1} = e^{\frac{E_A}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}.$$

$$\Rightarrow \frac{E_A}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) = \ln\left(\frac{t_2}{t_1}\right). \quad 1$$

$$\Rightarrow \frac{100\ kJK}{8.314\ J}\left(\frac{1}{T_2} - \frac{1}{300}\right) = \ln\left(\frac{5}{50}\right)$$

$$\Rightarrow \frac{1}{T_2} = \frac{1}{300} + \frac{8.314}{100 \times 10^3} \ln\left(\frac{5}{50}\right). \quad 2$$

$$\Rightarrow \frac{1}{T_2} = 3.33 \times 10^{-3} - 1.91437 \times 10^{-4}$$

$$\Rightarrow \frac{1}{T_2} = 3.1419 \times 10^{-3} \Rightarrow T_2 = \frac{1000}{3.1419} K$$

$$2 \quad \Rightarrow T_2 = 318.2787 K$$

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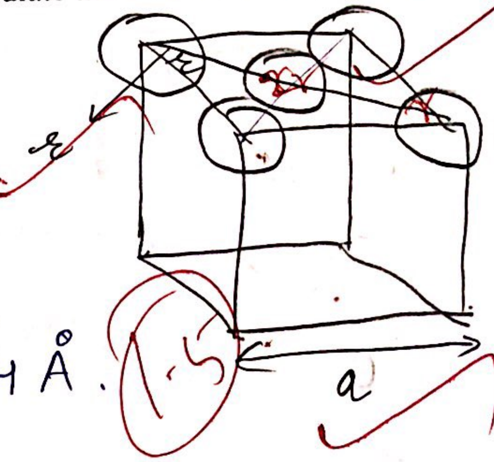
(b) If the atomic radius of aluminum is 0.143 nm, calculate the volume of its unit cell (CCP) in cubic meters.

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

$a = 2\sqrt{2}r$.

$a = (2\sqrt{2})(0.143)$ nm.

$a = 0.4044$ nm $= 4.04$ Å.



(1) Volume of cell $= a^3$

Volume of cell $= 66.167\,(\text{Å})^3$.

$\boxed{1\text{Å} = 10^{-10}\,m}$ (1)

So, Volume of cell $= 66.167 \times 10^{-30}\,m^3$.

(1)

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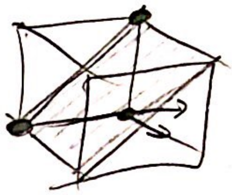
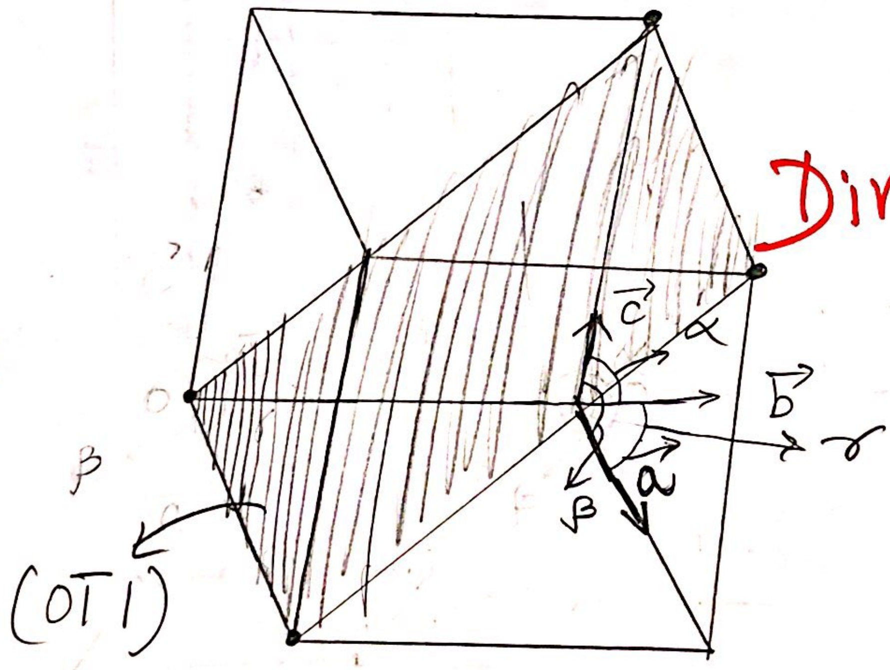
Question 3 **[7+8]**

(a) Sketch a monoclinic unit cell and show $[0\bar{1}1]$ direction. Axes and origin must be clearly shown.

$a = b \neq c$
$\alpha \neq \beta \neq \gamma$

$a = b \neq c$
$\alpha \neq \beta \neq \gamma.$





Direction.

-0-

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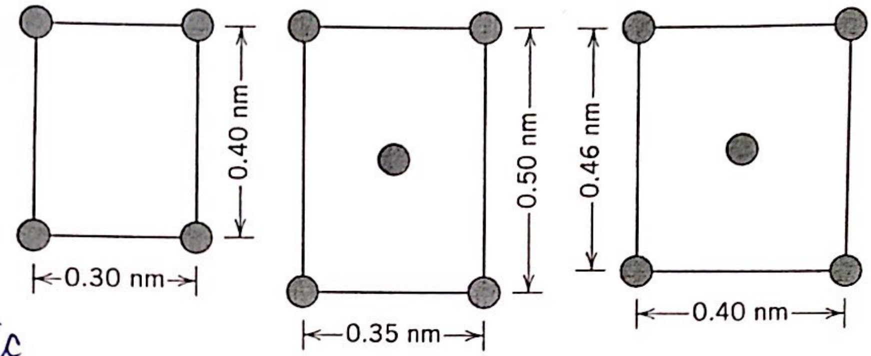
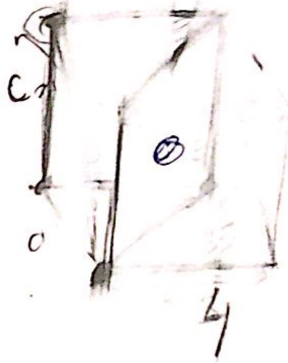
(b) The accompanying figure shows three different crystallographic planes for a unit cell of a hypothetical metal. The circles represent atoms.

(i) Draw the complete unit cell, clearly showing the axes and origin and indicate the atomic planes shown below.
(ii) To what crystal system does the unit cell belong?
(iii) What would this crystal structure be called?

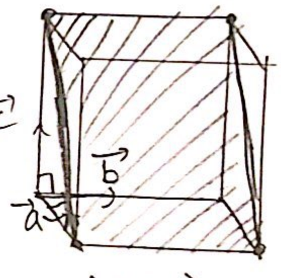
$a = 0.3$ nm
$b = 0.4$ nm
$C = \cancel{0.25}$ 0.35 nm
$\alpha = \beta = \gamma = 90^\circ$.
~~BCC~~
Orthorhombic



(001) (110) (101)



In all three
$\vec{a} = 0.3$ nm
$\vec{b} = 0.4$ nm
$\vec{c} = 0.35$ nm
$\alpha = \beta = \gamma = 90^\circ$.



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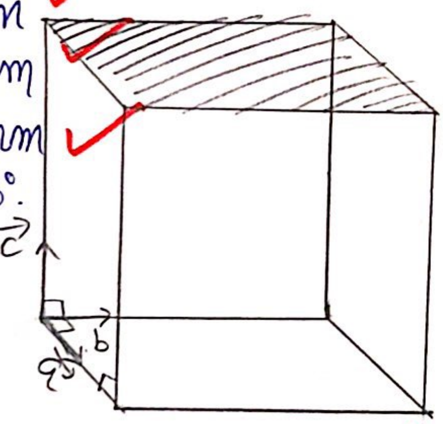

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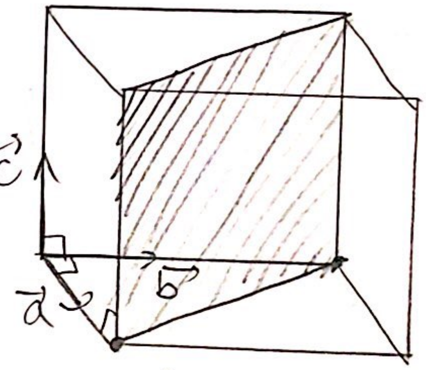

(110)

8

(b) The ~~Ca~~ Unit cell belongs to Body Centred Orthorhombic crystal system
i.e $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90^\circ$.

Body Centred Orthorhombic Crystal Structure

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(a) The metal rubidium has a BCC crystal structure. If the angle of diffraction (2θ) for the (321) set of planes occurs at 27.00 degree (first-order reflection) when monochromatic x-radiation having a wavelength of 0.0711 nm is used, compute the interplanar spacing for this set of planes and the lattice parameter.

$\lambda = 0.0711 nm$ $n = 1$ $2\theta = 27°$. $\theta = 13.5°$.

0.233445

$\lambda = 2 d_{hkl} \sin\theta$.

$$d_{hkl} = \frac{\lambda}{2\sin\theta} = 0.15228 \text{ nm}.$$

So, Interplanar spacing of this set of plane from parallel plane passing through origin is 0.15228 nm.

$\because$ $d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$

where a = lattice parameter

$\Rightarrow a = d_{hkl} \times \sqrt{h^2+k^2+l^2}$

$\Rightarrow a = 0.15228 \times \sqrt{9+4+1} = 0.569779$ nm

So, lattice parameter $= 0.569779$ nm.

9

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(b) Briefly discuss the key difference between thermoplast and thermoset polymers in terms of their internal structure and properties with simple sketches.

Thermoplast

1) They can be melted again and again to change the shape of material. ~~due to~~

2) High temp. melting occurs.

3) Can be sold in any form

6

4) Weak ~~intermolecu~~ forces of attraction b/w 2 chains like Van der Waal force or Hydrogen bonding which forms again on cooling

eg→ Butter, plastics

Thermoset

~~1) They are melted once~~

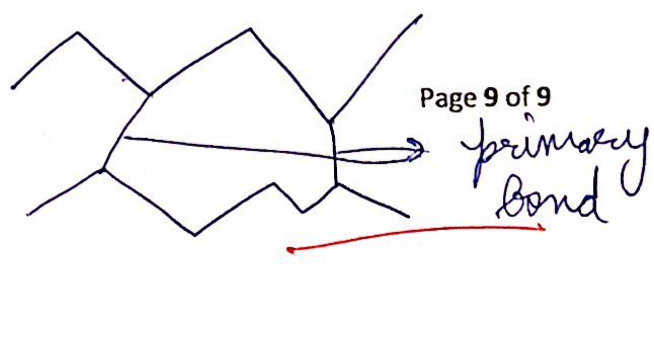
1) These become hard on heating to completion of bonding and can't be reshaped again.

2) High temp. deformation occurs with completion of bonding.

3) Sold in intermediate form so that can be used where necessary.

4) Primary bonding occurs after one heating followed by cooling making it brittle in nature

eg→ Bakelite.



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