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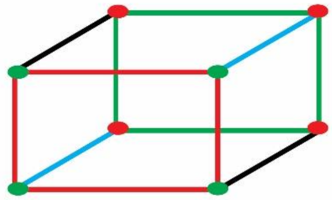

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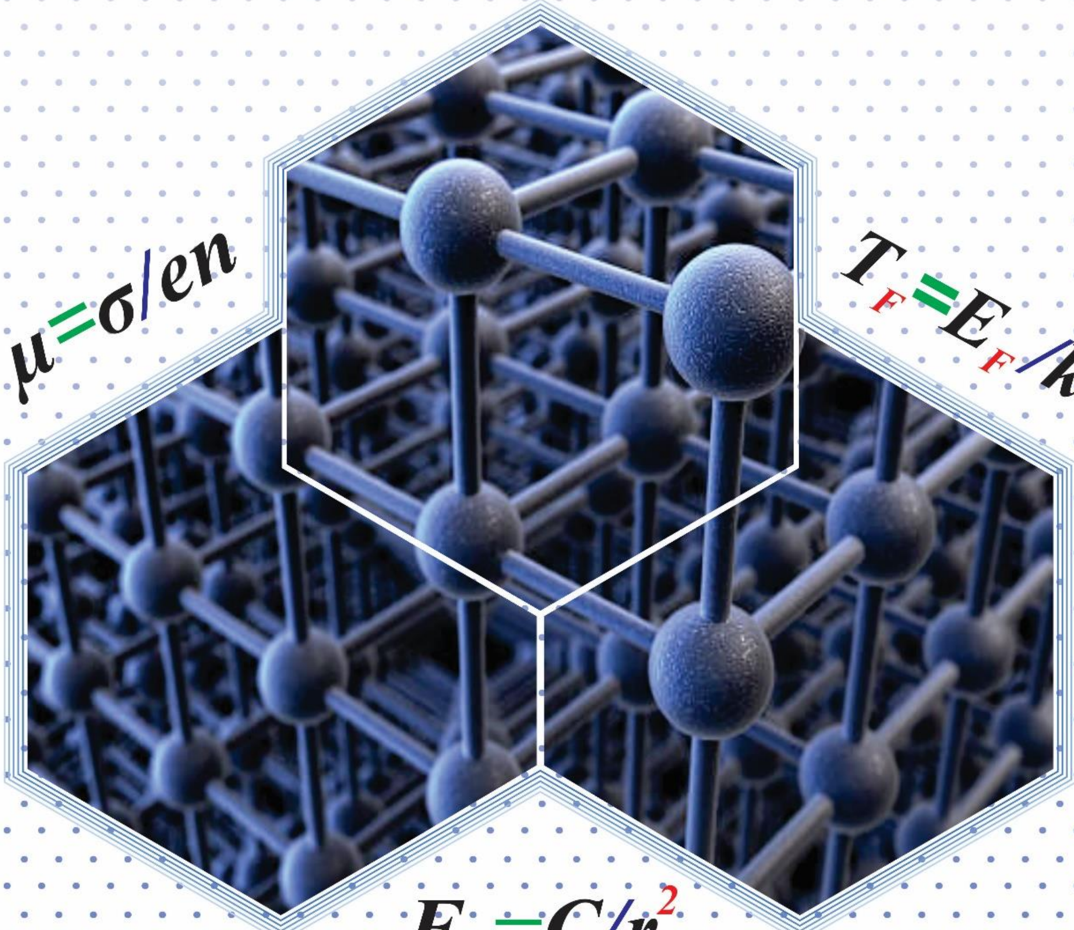
TEACH YOURSELF

SOLID STATE PHYSICS - I

For BS/M.Sc Physics Programme

$\mu=\sigma/en$

$T_F=E_F/k$



$E_B=C/r^2$

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TEACH YOURSELF

SOLID STATE PHYSICS - I

1st Edition

For **BS/M.Sc Physics** students of all Pakistani Universities/Colleges

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Contents

Chapter 1

Crystal Structure

SOLVED PROBLEMS

Problem: 1.1- A FCC crystal has an atomic radius of 1.246 $A°$. What are d_{200}, d_{220} and d_{111} spacings?

Solution

For FCC crystal the interatomic distance is

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

But, given

$$r = 1.246 \text{ Å}$$

So,

$$a = 2\sqrt{2}r \times 1.246$$
$$a = 3.524 \text{ Å}$$

For a crystal,

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

Now,

$$
\begin{aligned}
d_{200} &= \frac{3.524}{\sqrt{2^2+0^2+0^2}} \\
d_{200} &= \frac{3.524}{\sqrt{4+0+0}} \\
d_{200} &= \frac{3.524}{2} \\
d_{200} &= 1.762 \text{ Å}
\end{aligned}
$$

also,

$$
\begin{aligned}
d_{220} &= \frac{3.524}{\sqrt{2^2+2^2+0^2}} \\
d_{220} &= \frac{3.524}{\sqrt{4+4+0}} \\
d_{220} &= \frac{3.524}{2\sqrt{2}} \\
d_{220} &= 1.245 \text{ Å}
\end{aligned}
$$

and,

$$
\begin{aligned}
d_{111} &= \frac{3.524}{\sqrt{1^2+1^2+1^2}} \\
d_{111} &= \frac{3.524}{\sqrt{1+1+1}} \\
d_{111} &= \frac{3.524}{\sqrt{3}} \\
d_{111} &= 2.034 \text{ Å}
\end{aligned}
$$

Problem: 1.2- Calculate the number of atoms per unit cell of metal having a lattice parameter of 2.9 Å and density 7.87 gram/cc. Atomic weight of the metal is 55.85 and Avogadro's constant is 6.023×10^{23}.

Solution

$$
\begin{aligned}
a &= 2.9\ A^\circ \\
a &= 2.9 \times 10^{-10}\ m\ =\ 2.9 \times 10^{-8}\ cm
\end{aligned}
$$

$$
\begin{aligned}
M &= 55.85 \\
N_A &= 6.023 \times 10^{23} \\
\rho &= 7.87 \text{ gm/cc} \\
n &= ?
\end{aligned}
$$

The density of the crystal is

$$
\begin{aligned}
\rho &= \frac{nM}{a^3 N_A} \\
n &= \frac{\rho a^3 N_A}{M} \\
n &= \frac{7.87 \times (2.9 \times 10^{-8})^3 \times 6.023 \times 10^{23}}{55.85} \\
n &= 2
\end{aligned}
$$

So, the number of atoms per unit cell are 2. And, hence, unit cell may be body centered cubic.

Problem: 1.3- Prove that:

1. The reciprocal lattice of FCC because BCC lattice.
2. The reciprocal lattice of BCC because FCC lattice.

Solution

Let the primitive translation vectors of a face centered cubic lattice are

$$
\begin{aligned}
\vec{a}' &= \frac{a}{2}\left(\hat{i} + \hat{j}\right) \\
\vec{b}' &= \frac{a}{2}\left(\hat{j} + \hat{k}\right) \\
\vec{c}' &= \frac{a}{2}\left(\hat{k} + \hat{i}\right)
\end{aligned}
$$

The primitive translation vectors of the reciprocal of face centered cubic lattice are given by

$$
\vec{A} = \frac{2\pi\left(\vec{b}' \times \vec{c}'\right)}{\vec{a}' \cdot \left(\vec{b}' \times \vec{c}'\right)}
$$

$$\vec{A} = 2\pi \left(\frac{\frac{a^2}{4}\left(\hat{i} + \hat{j} - \hat{k}\right)}{a^3/4} \right)$$
$$\vec{A} = \frac{2\pi}{a}\left(\hat{i} + \hat{j} - \hat{k}\right)$$

Similarly,

$$\vec{B} = \frac{2\pi\left(\vec{c}\,' \times \vec{a}\,'\right)}{\vec{b}\,' \cdot \left(\vec{c}\,' \times \vec{a}\,'\right)}$$
$$\vec{B} = 2\pi \left(\frac{\frac{a^2}{4}\left(-\hat{i} + \hat{j} + \hat{k}\right)}{a^3/4} \right)$$
$$\vec{B} = \frac{2\pi}{a}\left(-\hat{i} + \hat{j} + \hat{k}\right)$$

and,

$$\vec{C} = \frac{2\pi\left(\vec{a}\,' \times \vec{b}\,'\right)}{\vec{c}\,' \cdot \left(\vec{a}\,' \times \vec{b}\,'\right)}$$
$$\vec{C} = 2\pi \left(\frac{\frac{a^2}{4}\left(\hat{i} - \hat{j} + \hat{k}\right)}{a^3/4} \right)$$
$$\vec{C} = \frac{2\pi}{a}\left(\hat{i} - \hat{j} + \hat{k}\right)$$

Hence, reciprocal of face centered cubic lattice is body centered cubic lattice.
Let the primitive translation vectors of a body centered cubic lattice are

$$\vec{a}\,' = \frac{a}{2}\left(\hat{i} + \hat{j} - \hat{k}\right)$$
$$\vec{b}\,' = \frac{a}{2}\left(-\hat{i} + \hat{j} + \hat{k}\right)$$

$$\vec{c}\,' = \frac{a}{2}\left(\hat{i} - \hat{j} + \hat{k}\right)$$

The primitive translation vectors of the reciprocal of body centered cubic lattice are given by

$$\vec{A} = \frac{2\pi\left(\vec{b}' \times \vec{c}'\right)}{\vec{a}' \cdot \left(\vec{b}' \times \vec{c}'\right)}$$

$$\vec{A} = 2\pi\left(\frac{\frac{a^2}{2}\left(\hat{i}+\hat{j}\right)}{a^3/2}\right)$$

$$\vec{A} = \frac{2\pi}{a}\left(\hat{i}+\hat{j}\right)$$

Similarly,

$$\vec{B} = \frac{2\pi\left(\vec{c}' \times \vec{a}'\right)}{\vec{b}' \cdot \left(\vec{c}' \times \vec{a}'\right)}$$

$$\vec{B} = 2\pi\left(\frac{\frac{a^2}{2}\left(\hat{j}+\hat{k}\right)}{a^3/2}\right)$$

$$\vec{B} = \frac{2\pi}{a}\left(\hat{j}+\hat{k}\right)$$

and

$$\vec{C} = \frac{2\pi\left(\vec{a}' \times \vec{b}'\right)}{\vec{c}' \cdot \left(\vec{a}' \times \vec{b}'\right)}$$

$$\vec{C} = 2\pi\left(\frac{\frac{a^2}{2}\left(\hat{k}+\hat{i}\right)}{a^3/2}\right)$$

$$\vec{C} = \frac{2\pi}{a}\left(\hat{k}+\hat{i}\right)$$

Hence, reciprocal of body centered cubic lattice is face face centered cubic lattice with side $\frac{2\pi}{a}$.

Problem: 1.4- In a unit cell of simple cubic structure, find the angle between the normals to pair of planes whose Miller indices are (i) (100) and (010), (ii) (121) and (111).

Solution

The direction of two normals are $[100], [010]$ and $[121], [111]$ respectively. The angle θ between two directions $[u_1v_1w_1]$ and $[u_2v_2w_2]$ is given by:

$$\cos\theta = \frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{(u_1^2 + v_1^2 + w_1^2)}\sqrt{(u_2^2 + v_2^2 + w_2^2)}}$$

Now, (i)

$$\cos\theta = \frac{1\times 0 + 0\times 1 + 0\times 0}{\sqrt{(1^2 + 0^2 + 0^2)}\sqrt{(0^2 + 1^2 + 0^2)}}$$

$$\begin{aligned}\cos\theta &= \frac{0}{1}\\ \cos\theta &= 0\\ \theta &= \cos^{-1}(0)\\ \theta &= 90^\circ\end{aligned}$$

and,
(ii)

$$\begin{aligned}\cos\theta &= \frac{1\times 1 + 2\times 1 + 1\times 1}{\sqrt{(1^2 + 2^2 + 1^2)}\sqrt{(1^2 + 1^2 + 1^2)}}\\ \cos\theta &= \frac{4}{\sqrt{18}}\\ \cos\theta &= 0.9428\\ \theta &= \cos^{-1}(0.9428)\\ \theta &= 19.47^\circ\end{aligned}$$

Problem: 1.5- Calculate the Miller indices of crystal planes which cut through the crystal axes at (i) $(2a, 3b, c)$, (ii) $(6a, 3b, 3c)$and (iii) $(2a, -3b, -3c)$.

Solution

Let us prepare the table as follows:

(i)

a	b	c	
2	3	1	intercepts
$\frac{1}{2}$	$\frac{1}{3}$	1	reciprocals
3	2	6	clear fractions

Hence, the Miller indices are (326).

(ii)

a	b	c	
6	3	3	intercepts
$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	reciprocals
1	2	2	clear fractions

Hence, the Miller indices are (122).

(iii)

a	b	c	
2	-3	-3	intercepts
$\frac{1}{2}$	-$\frac{1}{3}$	-$\frac{1}{3}$	reciprocals
3	-2	-2	clear fractions

Hence, the Miller indices are $(3\bar{2}\bar{2})$.

Chapter 2

Crystal Binding and Elastic Constants

SOLVED PROBLEMS

Problem: 2.1- The energy of two particles in the field of each other at a separation r is given by,

$$U = \frac{A}{r} + \frac{B}{r^8}$$

Where A and B are constant. At what separation they will form a stable compound?

Solution

The energy of two particles in the field of each other at a separation r is given by,

$$U = \frac{A}{r} + \frac{B}{r^8}$$

They will form a stable compound at a separation r_o such that separation the energy U is a minimum. That is,

$$\left(\frac{dU}{dr}\right)_{r=r_o} = 0$$

$$-\frac{A}{r_o^2} - \frac{8B}{r_o^9} = 0$$
$$\frac{A}{r_o^2} + \frac{8B}{r_o^9} = 0$$

$$A = \frac{8B}{r_o^7}$$
$$r_o^7 = \frac{8B}{A}$$
$$r_o = \left(\frac{8B}{A}\right)^{\frac{1}{7}}$$

Problem: 2.2- Form date given below, determine whether a gaseous molecules A^+B^- will bw stable w.r.t the separated A and B gaseous atoms:

$$\text{First ionization energy of } A = 502\text{kj/mol}$$
$$\text{Electron affinity for } B \text{ atom} = 335\text{kj/mol}$$
$$\text{Inter-ionic } (A^+ - B^-) \text{ separation} = 3A^o$$

Solution

Potential energy is,

$$U = -\frac{e^2}{4\pi\epsilon_o r}$$
$$U = -\frac{9\times10^9 Nm^2C^{-2}(1.6\times10^{-19}C)^2}{3\times10^{-10}m}$$
$$U = -7.673\times10^{-19}\text{j/ion pair}$$

$$U = -7.673\times10^{-19}\times6.023\times10^{23}\text{kj/mol}$$
$$U = -463\text{kj/mol}$$
$$\text{Dissociation energy} = -463+502-335 = -296\text{kj/mol}$$

Negative sign shows that molecules A^+B^- is stable.

Problem: 2.3- Using

$$\begin{aligned}\lambda =& 0.34\times 10^{-8} erg\\ \alpha =& 1.638\\ z =& 4\\ \rho =& 0.326\times 10^{-8} A^o\end{aligned}$$

Find cohesive energy of KCl in cubic ZnS structure. Compare with value calculated for KCl in $NaCl$ structure.

Solution

For cubic crystals, at equilibrium separation, we have

$$\frac{r_o^2}{\rho^2}e^{-\frac{r_o}{\rho}} = -\frac{\alpha q^2}{z\lambda\rho}$$

Put $\frac{r_o}{\rho} = x$ to get

$$\begin{aligned}x^2 e^{-x} =& 8.53\times 10^{-3}\\ \frac{x}{\rho} =& 9.2\\ x =& 2A^o\end{aligned}$$

Cohesive energy is,

$$\begin{aligned}U =& -\frac{q\alpha^2}{r_o}\left(1-\frac{p}{r_o}\right)\\ \frac{U}{q^2} =& -0.489\end{aligned}$$

For actual KCl structure,

$$\frac{U}{q^2} = -0.495$$

This is 0.1% less than calculated value for ZnS structure.

Problem: 2.4- Calculate potential energy of a system of Na^+ and Cl^- ions when they are at a distance of $2A^o$.

Solution

Potential energy is,

$$
\begin{aligned}
U &= -\frac{e^2}{4\pi\epsilon_o r} \\
U &= -\frac{9\times 10^9 Nm^2C^{-2}(1.6\times 10^{-19}C)^2}{3\times 10^{-10}m} \\
U &= -\frac{9\times 10^9 Nm^2C^{-2}(1.6\times 10^{-19}C)^2}{3\times 10^{-10}m\times 1.6\times 10^{-19}\text{j/eV}} \\
U &= -7.2\text{eV}
\end{aligned}
$$

Problem: 2.5- The potential energy of a diatomic molecule in terms of inter-atomic separation r is given by

$$U = -\frac{A}{r^2} + \frac{B}{r^{10}}$$

Find values of constant A and B when equilibrium separation is 3Å and dissociation energy is 4 eV.

Solution

Dissociation energy is

$$
\begin{aligned}
E_d &= \frac{A}{r_\circ^2}\left(1-\frac{n}{m}\right) \\
&= \frac{A}{r_\circ^2}\left(1-\frac{2}{10}\right) = \frac{4A}{5r_\circ^2}
\end{aligned}
$$

$$A = \frac{5r_\circ^2 E_d}{4} = \frac{5\times(3\times 10^{10}m)^2\times 4\times 1.6\times 10^{-19}J}{4} = 7.2\times 10^{-38}\,\text{Jm}^2$$

For equilibrium separation

$$\left(\frac{dU}{dr}\right)_{r=r_\circ} = 0 - \frac{2A}{r_\circ^3} - \frac{10B}{r_\circ^{11}} = 0 \qquad \Rightarrow \qquad B = \frac{Ar_\circ^8}{5}$$

$$\Rightarrow \qquad B = \frac{7.2 \times 10^{-38}\ \mathrm{Jm}^2 \times (3 \times 10^{10} m)^8}{5} = 9.44 \times 10^{-115}\ \mathrm{Jm}^{10}$$

Chapter 3

Cohesive Energy

SOLVED PROBLEMS

Problem: 3.1- The mutual potential energy V of two particles depends on their spatial separation as follow:

$$V = \frac{a}{r^2} - \frac{b}{r};\ a > 0;\ b > 0$$

For what separation are the particles in static equilibrium?

Solution

$$V = \frac{a}{r^2} - \frac{b}{r};\ a > 0;\ b > 0$$

For equilibrium, we have

$$\begin{aligned} \left.\frac{dV}{dr}\right|_{r=r_e} &= 0 \\ \frac{d}{dr}\left(\frac{a}{r^2} - \frac{b}{r}\right)\Big|_{r=r_e} &= 0 \\ a\frac{d}{dr}\left(\frac{1}{r^2}\right)\Big|_{r=r_e} - b\frac{d}{dr}\left(\frac{1}{r}\right)\Big|_{r=r_e} &= 0 \\ a\frac{d}{dr}\left(r^{-2}\right)\Big|_{r=r_e} - b\frac{d}{dr}\left(r^{-1}\right)\Big|_{r=r_e} &= 0 \end{aligned}$$

$$a\left(-2r^{-3}\right)\Big|_{r=r_e} - b\left(-1r^{-2}\right)\Big|_{r=r_e} = 0 \qquad \because \frac{d}{dx}x^n = nx^{n-1}$$

$$a\left(\frac{-2}{r^{-3}}\right)\Big|_{r=r_e} - b\left(\frac{-1}{r^{-2}}\right)\Big|_{r=r_e} = 0$$

$$a\left(\frac{-2}{r_e^3}\right) - b\left(\frac{-1}{r_e^2}\right) = 0$$

$$-\frac{2a}{r_e^3} + \frac{b}{r_e^2} = 0$$

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

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

$$r_e = \frac{2a}{b}$$

Hence, the separation of particles in static equilibrium is $\frac{2a}{b}$.

Problem: 3.2- Calculate the cohesive energy per molecule if $\frac{1}{n}$ is $0.0948, r_\circ$ is $3.14 \times 10^{-10}\ m$ and the Madelung constant α is 1.75.

Solution

$$\frac{1}{n} = 0.0948$$

$$r_\circ = 3.14 \times 10^{-10}\ m$$

$$\alpha = 1.75$$

$$e = 1.6 \times 10^{-19}\ C$$

$$\frac{1}{4\pi\varepsilon_\circ} = 9 \times 10^9\ Nm^2C^{-2}$$

$$U = ?$$

The cohesive energy is defined as

$$U = -\alpha\frac{e^2}{4\pi\varepsilon_\circ r_\circ}\left(1 - \frac{1}{n}\right)$$

$$U = -1.75\frac{(1.6\times10^{-19})^2}{3.14\times10^{-10}}\times9\times10^9\,(1-0.0948)$$
$$U = -7.26\times1.6\times10^{-19}\ J/\text{ion-pair}$$
$$U = -7.26\ eV/\text{ion-pair}$$

Problem: 3.3- Using Lennard Jones potential, calculate the cohesive energy of neon in BCC structure. The lattice sum for BCC structure are:

$$\sum_{i\neq j} M_{ij}^{-12} = 9.11418 \quad \text{and} \quad \sum_{i\neq j} M_{ij}^{-6} = 12.2533$$

Solution

$$\sum_{i\neq j} M_{ij}^{-12} = 9.11418$$
$$\sum_{i\neq j} M_{ij}^{-6} = 12.2533$$
$$\frac{r}{\sigma} = 1.14 \quad \text{for Neon}$$
$$\frac{\sigma}{r} = 0.877$$
$$U(r) = ?$$

The Lennard-Jones potential is:

$$U(r) = 2\epsilon\sum_{i\neq j}\left(-M_{ij}^{-6}\left(\frac{\sigma}{r}\right)^6 + M_{ij}^{-12}\left(\frac{\sigma}{r}\right)^{12}\right)$$
$$U(r) = 2\epsilon\left(-12.253\,(0.877)^6 + 9.114\,(0.877)^{12}\right)$$
$$U(r) = 2\epsilon\,(-5.575+1.88)$$
$$U(r) = 2\epsilon(-3.688)$$

Problem: 3.4- Calculate the intermolecular potential between two Argon (Ar) atoms separated by a distance of 4.0 Angstroms (use $\epsilon = 0.997kJ/mol$ and $\sigma = 3.40$ Angstroms).

Solution

$$\begin{aligned}
\epsilon &= 0.997kJ/mol \\
\sigma &= 3.40 \text{ Angstroms} \\
r &= 4.0 \text{ Angstroms} \\
V(r) &= ?
\end{aligned}$$

To solve for the intermolecular potential between the two Argon atoms, we use equation where V is the intermolecular potential between two non-bonding particles.

$$\begin{aligned}
V(r) &= 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \\
V(r) &= 4 \times 0.997\left[\left(\frac{3.40}{4}\right)^{12} - \left(\frac{33.40}{4}\right)^{6}\right] \\
V(r) &= 3.988(0.14 - 0.38) \\
V(r) &= 3.988(0.24) \\
V(r) &= -0.96\ kJ/mol
\end{aligned}$$

Problem: 3.5- Calculate the modulus of liquid elasticity that reduced 0.035 per cent of its volume by applying a pressure of 5 Bar in a s slow process.

Solution

$$\begin{aligned}
B &= 2.15 \times 10^{9} \\
V &= 5 \\
\partial V &= 0.00035 \\
\Delta P &= ?
\end{aligned}$$

Using the definition for the bulk modulus

$$
\begin{aligned}
B &= -V\frac{\partial P}{\partial V}\\
B &\cong \frac{V}{\partial V}\varDelta P\\
\varDelta P &= B\frac{\partial V}{V}\\
\varDelta P &= 2.15\times 10^{9}\times\frac{0.00035}{5}\\
\varDelta P &= 14285.714 \text{ Bar}
\end{aligned}
$$

Chapter 4

Crystal Vibrations: Phonon-I

SOLVED PROBLEMS

Problem: 4.1- If velocity of sound in a solid is taken to be 3×10^3m/s and inter-atomic distance as 3×10^{-10}m, calculates the value of cut off frequency assuming a linear lattice.

Solution

$$\text{speed of sound} = v = 3 \times 10^3 \text{m/s}$$
$$\text{Inter-atomic distance} = a = 3 \times 10^{-10} \text{m/s}$$
$$\text{cut-off frequency} = f = ?$$

using

$$v = f\lambda$$
$$f = \frac{v}{\lambda}$$
$$f = \frac{v}{2a} = \frac{3 \times 10^3 \text{m/s}}{2 \times 3 \times 10^{-10} \text{m/s}}$$
$$f = 5 \times 10^{12} Hz$$

Problem: 4.2- We suppose that the interplaner force constant C_p, between planes s and $s+p$ of form;

$$C_p = \frac{\sin pk_o a}{pa}$$

A and k_o are constants and p runs over all integers. Such a form is expected in metals. Find an expression for ω^2 and for $\frac{\partial \omega^2}{\partial k}$. Prove that $\frac{\partial \omega^2}{\partial k}$ is infinite when $k = k_o$.

Solution

Dispersion relation is,

$$\omega^2 = \frac{2A}{M} \sum_{p>0} C_p (1 - \cos pka)$$

$$\omega^2 = \frac{2A}{M} \sum_{p>0} \frac{\sin pk_o a}{pa} (1 - \cos pka)$$

$$\frac{\partial \omega^2}{\partial k} = \frac{2A}{M} \sum_{p>0} \sin pk_o a \sin pka$$

$$At\ k = k_o \qquad \frac{\partial \omega^2}{\partial k} = \frac{2A}{M} \sum_{p>0} \sin^2 pk_o a$$

This is divergent series because $\sum_{p=0} 1$ diverges.

Problem: 4.3- If velocity of a sound in a solid is of order of 10^3m/s, find the frequency of sound wave $\lambda = 10A^o$ for a mono atomic system.

Solution

$$\text{speed of sound} = v = 10^3 \text{m/s}$$

$$\text{wavelength} = \lambda = 10 \times 10^{-10} m$$

$$\text{frequency} = \omega = ?$$

For mono atomic lattice frequency is,

$$\omega = vk$$

$$= v\frac{2\pi}{\lambda}$$

$$
\begin{aligned}
=&10 \times 3m/s \times \frac{2\pi}{10 \times 10^{-10}m} \\
=&6.28 \times 10^{12} rad/s
\end{aligned}
$$

Problem: 4.4- For the problem of diatomic molecule, find amplitude ratio $\frac{u}{v}$ for the branches at $k_{max} = \frac{\pi}{a}$. Show that at this value of k the two lattices act as if decoupled: one lattice remains at rest while the other lattice moves.

Solution

In deriving dispersion relation for diatomic molecules, we proved that

$$
\begin{aligned}
-\omega^2 M_1 u =& Cv\left(1 + e^{-ika}\right) - 2Cu \\
-\omega^2 M_2 v =& Cu\left(1 + e^{ika}\right) - 2Cv
\end{aligned}
$$

At $k = \frac{\pi}{a}$, we obtain

$$
\begin{aligned}
-\omega^2 M_1 u =& -2Cu \\
-\omega^2 M_2 v =& -2Cv
\end{aligned}
$$

Thus the two lattices are decoupled form one another, each move independently. At $\omega^2 = \frac{2C}{M_2}$ the motion in lattice is described by displacement v and at $\omega^2 = \frac{2C}{M_1}$, thus lattice u moves.

Problem: 4.5- The unit cell parameter of $NaCl$ crystal is $5.6A^o$ and modulus of elasticity along [100] direction is $5 \times 10^{10} N/m^2$. Estimate the wavelength at which an electromagnetic radiation is strongly reflected by the crystal. Atomic weight of Na is 23 and that of Cl is 37amu.

Solution

$$
\begin{aligned}
\text{Unit cell parameter} = a =& 5.6 \times 10^{-10} m \\
\text{Modulus of elasticity} = Y =& 5 \times 10^{10} N/m^2 \\
M_1 =& 37 \\
M_2 =& 23
\end{aligned}
$$

The maximum frequency of radiation in optical range is,

$$
\begin{aligned}
(\omega_+)_{max} =& \sqrt{2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)} \\
=& \sqrt{2aY\left(\frac{1}{M_1}+\frac{1}{M_2}\right)} \\
=& \sqrt{2\times 5\times 10^{10}Nm^{-2}\times 5.6\times 10^{-10}m\left(\frac{1}{37}+\frac{1}{23}\right)} \\
=& 4.86\times 10^{13} rad/s
\end{aligned}
$$

The wavelength at which radiation is strongly reflected is,

$$
\begin{aligned}
\lambda =& \frac{c}{f} = \frac{2\pi C}{\omega} \\
=& \frac{2\pi \times 3\times 10^{8} m/s}{4.86\times 10^{13} rad/s} \\
=& 3.88\times 10^{-5} m
\end{aligned}
$$

Chapter 5

Thermal Properties: Phonon-II

SOLVED PROBLEMS

Problem: 5.1- Calculate the highest possible frequency for copper and silicon if their Debye temperatures are 350 K and 550 K respectively.

Solution

$$\theta_1 = 350 \text{ K}$$
$$\theta_2 = 550 \text{ K}$$
$$k = 1.38 \times 10^{-23} \text{ JK}^{-1}$$
$$h = 6.63 \times 10^{-34} \text{ Js}$$
$$\nu_1 = ?$$
$$\nu_2 = ?$$

Since we know that,

$$h\nu = k\theta$$
$$\nu = \frac{k\theta}{h}$$

For Cu,

$$\nu_1 = \frac{1.38 \times 10^{-23} \times 350}{6.63 \times 10^{-34}}$$
$$\nu_1 = 7.2895 \times 10^{12}\ s^{-1}$$

For Si,

$$\nu_2 = \frac{1.38 \times 10^{-23} \times 550}{6.63 \times 10^{-34}}$$
$$\nu_1 = 11.45 \times 10^{12}\ s^{-1}$$

Problem: 5.2- Calculate the specific heat of lead at 10 K if its Debye temperature is 105 K. Also determine the highest frequency which the sample allows to propagate through it.

Solution

$$T = 10 \text{ K}$$
$$\theta = 105 \text{ K}$$
$$N = 6.023 \times 10^{23}$$
$$k = 1.38 \times 10^{-23} \text{ JK}^{-1}$$
$$C_V = ?$$
$$\nu = ?$$

Since we know that

$$C_V = \frac{12}{5}\pi^4 R \left(\frac{T}{\theta}\right)^3$$
$$C_V = \frac{12}{5}\pi^4 Nk \left(\frac{T}{\theta}\right)^3 \qquad \because Nk = R$$
$$C_V = \frac{12}{5}(3.14)^4 \times 6.023 \times 10^{23} \times 1.38 \times 10^{-23} \left(\frac{10}{105}\right)^3$$
$$C_V = 1678 \text{ JK}^{-1}/\text{mol}$$

Now,

$$\nu = \frac{k\theta}{h}$$
$$\nu = \frac{1.38 \times 10^{-23} \times 105}{6.63 \times 10^{-34}}$$
$$\nu = 21.87 \times 10^{11}\ s^{-1}$$
$$\nu = 2.187 \times 10^{12}\ s^{-1}$$

Problem: 5.3- A system consists of 10^{25} atoms which act as simple harmonic oscillator's each having a frequency of $10^{12}\ Hz$. Calculate the zero point energy and the mean thermal energy of system at 2.5 K 25 K 250 K and 2500 K.

Solution

$$N = 10^{25} \text{ atoms}$$
$$\omega = 10^{12}\ Hz$$
$$h = 6.63 \times 10^{-34} \text{ Js}$$
$$k_B = 1.38 \times 10^{-23} \text{ JK}^{-1}$$
$$T_1 = 2.5 \text{ K}$$
$$T_2 = 25 \text{ K}$$
$$T_3 = 250 \text{ K}$$
$$T_4 = 2500 \text{ K}$$
$$E = ?$$

Since, the thermal energy will be

$$E = 3N\bar{E}$$
$$E = 3N\left[\frac{h\omega}{e^{\left(\frac{h\omega}{k_B T}\right)-1}}\right]$$
$$E = 3 \times 10^{25}\left[\frac{6.63 \times 10^{-34} \times 10^{12}}{e^{\left(\frac{6.63\times10^{-34}\times10^{12}}{1.38\times10^{-23}\times T}\right)-1}}\right]$$

Now, at $T = 2.5$ K,

$$
\begin{aligned}
E &= 3\times 10^{25}\left[\frac{6.63\times 10^{-34}\times 10^{12}}{e^{\left(\frac{6.63\times 10^{-34}\times 10^{12}}{1.38\times 10^{-23}\times 2.5}\right)-1}}\right]\\
E &= 3\times 10^{25}\left[\frac{6.63\times 10^{-22}}{e^{19.2}-1}\right]\\
E &= 3\times 10^{25}\left[\frac{6.63\times 10^{-22}}{2.06\times 10^{8}}\right]\\
E &= 3\times 10^{25}\times 3.21\times 10^{-30}\\
E &= 9.65\times 10^{-5}\text{ J}
\end{aligned}
$$

At, $T = 25$ K,

$$E = 3.41\times 10^{3}\text{ J}$$

At, $T = 250$ K,

$$E = 9.39\times 10^{4}\text{ J}$$

and, at $T = 2500$ K,

$$E = 1.03\times 10^{6}\text{ J}$$

Problem: 5.4- Using Debye approximation, show that the heat capacity of a linear monoatomic lattice at temperatures,

$$T << \theta$$

is proportional to $\frac{T}{\theta}$. The effective Debye temperature is one dimensional may be expressed as

$$\theta = \frac{\hbar\omega}{k_B} = \frac{\pi\hbar\nu}{k_B a}$$

Solution As,

$$\theta = \frac{\hbar\omega}{k_B}$$

where heat capacity is,

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V$$

where,

$$E = 9Nk_BT\left(\frac{T}{\theta}\right)^3 \int_0^{\theta/T} \frac{x^3}{e^x-1}dx$$

$$C_V = \frac{9N}{\omega^3}\frac{\partial}{\partial T}\int_0^{\omega}\left(\frac{\hbar\omega^{33}}{e^{\hbar\omega/k_BT}}-1\right)d\omega$$

put, $x = \frac{\hbar\omega}{k_BT} \Rightarrow$

$$x = \frac{\hbar\omega}{k_BT}$$
$$\Rightarrow \omega = \frac{k_BT}{\hbar}x$$
$$\Rightarrow d\omega = \frac{k_BT}{\hbar}dx$$
$$\text{and} \quad \omega = \frac{\theta k_B}{\hbar}$$

Now, we have

$$C_V = \frac{9\hbar^3N}{k_B^3\theta^3}\frac{\partial}{\partial T}\int_0^{\theta/T}\frac{\hbar x^3k_B^3T^3}{\hbar^3(e^x-1)}\times\frac{k_BT}{\hbar}dx$$

$$C_V = \frac{9Nk_B}{\theta^3}T^3\times\int_0^{\theta/T}\frac{x^3e^x}{e^x-1}dx$$

$$C_V = \frac{9Nk_B}{\theta^3}T^3\frac{\pi^4}{15} \qquad \because \frac{\pi^4}{15} = \int_0^{\theta/T}\frac{x^3e^x}{e^x-1}dx$$

$$C_V = 9Nk_B\frac{T^3}{\theta^3}\frac{\pi^4}{15}$$

$$C_V = \frac{9Nk_B\pi^4}{15}\left(\frac{T}{\theta}\right)^3$$

$$C_V = \text{constant}\left(\frac{T}{\theta}\right)^3 \qquad \because \frac{9Nk_B\pi^4}{15} = \text{constant}$$

$$C_V \propto \frac{T}{\theta}$$

Hence, this relation shows that the specific heat is proportional to $\frac{T}{\theta}$.

Problem: 5.5- $NaCl$ has the same structure as KCl. The Debye temperature of $NaCl$ and KCl are 281 K and 230 K respectively. If the lattice heat capacity of $NaCl$ is 1.6×10^{-2} J/mole-K at 5 K, estimate the heat capacity of KCl at 5 K and 3 K.

Solution As we know that the heat capacity is,

$$C_V = \frac{12}{5}\pi^4 R\left(\frac{T}{\theta}\right)^3$$

For $NaCl$, at $T = 5$ K and $\theta = 281$ K, then

$$C_V = 1.66 \times 10^{-2} \text{ J mol}^{-1} \text{ K}^{-1}$$

So, we can find R, then

$$\begin{aligned} 1.66 \times 10^{-2} &= \frac{12}{5} \times (3.14)^4 \times R\left(\frac{5}{281}\right)^3 \\ R &= \frac{0.66 \times 10^{-2}}{(3.14)^4} \times \left(\frac{281}{5}\right)^3 \\ R &= 1825.98 \times 0.66 \times 10^{-2} \\ R &= 12.05 \end{aligned}$$

For, KCl, we have

$$\begin{aligned} \theta &= 230 \\ T &= 3 \text{ K} \\ R &= 12.05 \end{aligned}$$

So,

$$\begin{aligned} C_V &= \frac{12}{5} \times (3.14)^4 \times 12.05\left(\frac{3}{230}\right)^3 \\ C_V &= 6.23 \times 10^{-3} \text{ J mol}^{-1} \text{ K}^{-1} \end{aligned}$$

Chapter 6

Crystal Imperfections

SOLVED PROBLEMS

Problem: 6.1- Determine the fraction of atoms in a given solid with energy equal to or greater than $1.5eV$ at room temperature $300K$.

Solution

$$E = 1.5eV$$
$$T = 300K$$

using

$$\frac{n}{N} = e^{-\frac{E}{k_B T}}$$
$$= e^{-\frac{1.5}{8.614 \times 10^{-5} \times 300}}$$
$$= 6.185 \times 10^{-26}$$

Problem: 6.2- The average energy required to create a Frenkel defect in an ionic crystal is $1.4eV$. Find ratio of Frenkel defects at $300K$ and $600K$ in 1g of crystal.

Solution

$$E_i = 1.4eV$$
$$\frac{\text{n at } 300K}{\text{n at } 600K} = ?$$

For Frenkel defect,

$$n = (NN)^{1/2} e^{-E_i/2Tk_B}$$

$$So, \qquad \frac{\text{n at } 300K}{\text{n at } 600K} = \frac{(NN)^{1/2} e^{-E_i/300k_B}}{(NN)^{1/2} e^{-E_i/600k_B}}$$

$$= \exp\left[\frac{E_i}{2k_B}\left(\frac{1}{600} - \frac{1}{300}\right)\right]$$

$$= 1.316 \times 10^{-6}$$

Problem: 6.3- Suppose that the energy required to remove a Sodium atom form the inside of a Sodium crystal to the boundary is 1eV. Calculate concentration of Schottky vacancies at $300K$.

Solution

$$E_v = 1eV$$

$$T = 300K$$

$$N = 2.5 \times 10^{22} \ atom/cm^3$$

For Schottky defect,

$$n = Ne^{-E_v/k_BT}$$

$$= 2.5 \times 10^{22} \times \exp\left(\frac{1}{8.61 \times 10^{-5} \times 300}\right) \approx 10^5 cm^{-3}$$

Problem: 6.4- The energy of formation of a vacancy in copper is $1eV$. Estimate the relative change in density of copper due to vacancy formation at a temperature just below its melting point $1356K$.

Solution

$$\text{Here,} \qquad E_v = 1eV$$

$$T = 1356K$$

$$\begin{aligned} \text{Using} \qquad n =& N e^{-E_v/k_BT} \\ =& 6.023 \times 10^{23} \times \exp\left(-\frac{1}{8.61 \times 10^{-5} \times 1356}\right) = 1.1528 \times 10^{20} \end{aligned}$$

Relative change in density of copper is,

$$\frac{n+N}{N} = \frac{6.0241528 \times 10^{23}}{6.023 \times 10^{23}} = 1.0001914 : 1$$

Problem: 6.5- The energy required to remove a pair of ions, Na^+ and Cl^-, from $NaCl$ is almost $2eV$. Evaluate approximate number of Schottky imperfections present in a $NaCl$ crystal at room temperature.

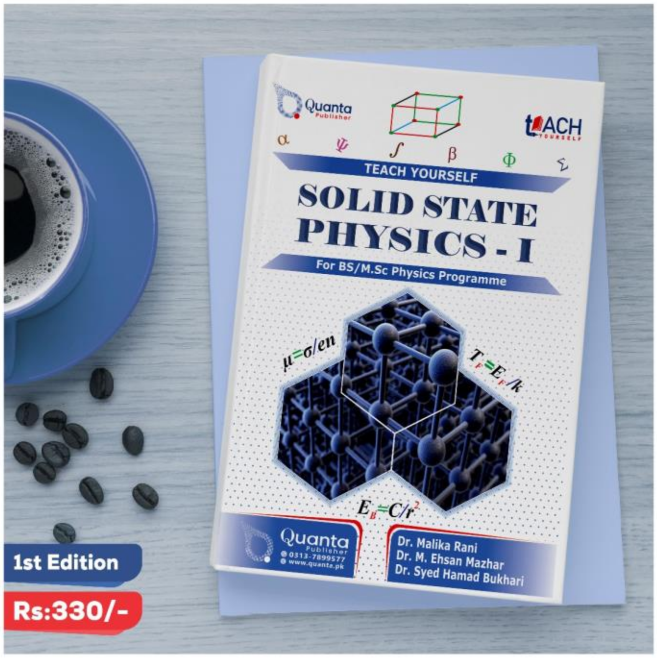
Solution

$$\begin{aligned} \text{Here,} \qquad E_p =& 2eV \\ T =& 300K \end{aligned}$$

$$\begin{aligned} \text{For Schottky defect,} \qquad n =& N e^{-E_v/k_BT} \\ =& 6.023 \times 10^{23} \times \exp\left(\frac{1}{2 \times 8.61 \times 10^{-5} \times 300}\right) = 9.42 \times 10^{6} \end{aligned}$$

since volume of one mole of crystal is $26.83cm^3$, so

$$n = \frac{9.42 \times 10^6}{26.83} = 0.35 \times 10^6 cm^{-3}$$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