University of Anbar

College of Science

Department of Physics

فيزياء الحالة الصلبة

Solid state Physics

المرحلة الرابعة

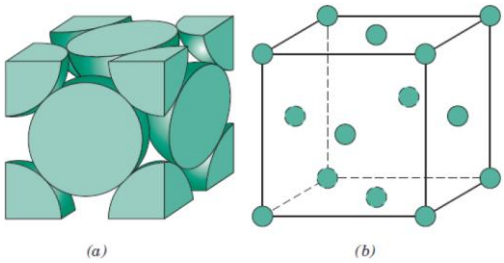
الكورس الاول

صلبة 1

Syllabus of this course مفردات الكور س

1- crystal structure
2- x-ray diffraction
3- lattice vibration
4- thermal properties in solids
5- free electron model

The Face-Centered Cubic Crystal Structure



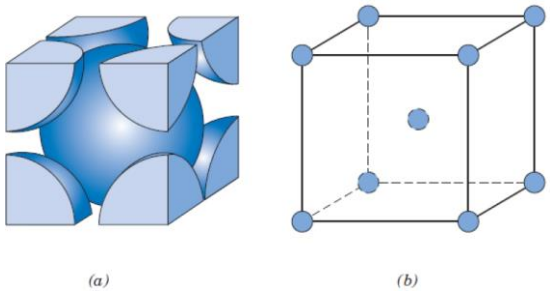
The cube edge length a and the atomic radius R are related through

$$a = 2R\sqrt{2}$$

The atomic packing factor (APF). The APF is the sum of the sphere volumes of all atoms within a unit cell divided by the unit cell volume that is

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

The Body-Centered Cubic Crystal Structure



The unit cell length a and atomic radius R are related through

$$a = \frac{4R}{\sqrt{3}}$$

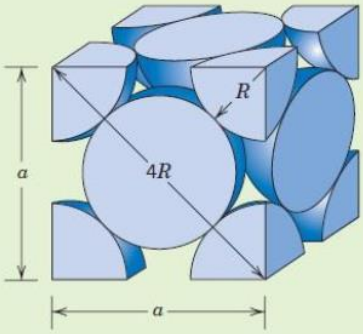
Example 1

Determination of FCC Unit Cell Volume

Calculate the volume of an FCC unit cell in terms of the atomic radius R.

Solution

In the FCC unit cell illustrated,



the atoms touch one another across a face-diagonal the length of which is $4R$. Because the unit cell is a cube, its volume is a^3, where a is the cell edge length. From the right triangle on the face,

$$a^2 + a^2 = (4R)^2$$

or, solving for a,

$$a = 2R\sqrt{2}$$

The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

Example 2

Computation of the Atomic Packing Factor for FCC

Show that the atomic packing factor for the FCC crystal structure is 0.74.

Solution

The APF is defined as the fraction of solid sphere volume in a unit cell, or

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

Both the total atom and unit cell volumes may be calculated in terms of the atomic radius R. The volume for a sphere is $\frac{4}{3}\pi R^3$, and because there are four atoms per FCC unit cell, the total FCC atom (or sphere) volume is

$$V_S = (4)\tfrac{4}{3}\pi R^3 = \tfrac{16}{3}\pi R^3$$

From Example Problem .1, the total unit cell volume is

$$V_C = 16R^3\sqrt{2}$$

Therefore, the atomic packing factor is

$$\text{APF} = \frac{V_S}{V_C} = \frac{(\frac{16}{3})\pi R^3}{16R^3\sqrt{2}} = 0.74$$

Theoretical density ρ of the crystal structure of a metallic solid.

$\rho = \frac{nA}{V_c N_A}$ for atoms

or

$\rho = \frac{n\,M_A}{V_c N_A}$ for molecular

Where

n= number of atoms associated with each unit cell.

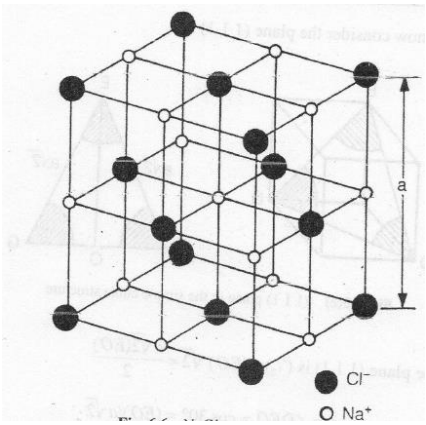
A= atomic weight or M_A molecular weight

V_c= volume of the unite cell

N_A= Avogadro's number (6.022×10^{23} atoms/mol)

Example 3

The crystal structure for NaCl is a cubic lattice the successive lattice sites being occupied by Na and Cl ions respectively. If the molecular weight of NaCl is 58.5, Calculate the spacing between the nearst neighbouring ions. Take the denstiy of the NaCl as 2180 kilogram/m^3 .



Solution

Number of ions in unit cell is

8x(1/8)x8=8 ions or 4 molecules

From equationf

$$\rho = \frac{n\,M_A}{V_c N_A}$$

with

(i) $M_A = 58.5$
(ii) $N_A = 6.02 \times 10^{26}$/kmol
(iii) $n = 4$
(iv) $\rho = 2180$ kilogram/metre^3

The volume Vc= a^3

$\rho = \frac{n\,M_A}{a^3 N_A}$ Therefore: $\rho\, a^3 N_A = n\, M_A$

$a^3 = \frac{n\,M_A}{\rho N_A}$,, $a = [\frac{n\,M_A}{\rho N_A}]^{1/3}$

$$a = [\frac{4 \times 58.5}{2180 \times 6.02 \times 10^{26}}]^{1/3} = 0.563 \times 10^{-9} metre = 0.563\, nm$$

The distance between the adjacent ions is r_o=a/2

$r_o = 0.563 \times 10^{-9}/2 = 0.282 nm$

Example 4:

Find the maximum radius of interstitial sphere that can just fit into the void at (½, ½, ½) between the body centred atoms of bcc structure. As shown in figure (5.1).

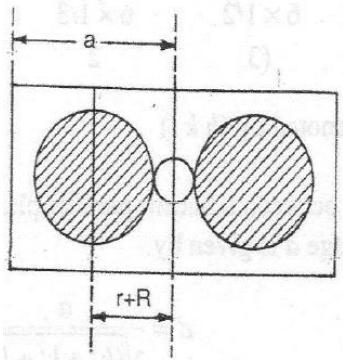


Figure 5.1

Solution:

Let r be the radius of the atom and R be the radius of the sphere that can just fit into the void.

r+R=a/2

R=(a/2)-r

For bcc structure

$$a = \frac{4r}{\sqrt{3}}$$

$$R = \frac{4r}{\sqrt{3}(2)} - r$$

$$R = \frac{2r}{\sqrt{3}} - r$$

$$R = \frac{r(2-\sqrt{3})}{\sqrt{3}} = 0.155r$$

Quantization Of Elastic Waves

The energy of a lattice vibration is quantized مكممة. The quantum of energy is called a phonon فونون in analogy with the photon of the electromagnetic wave. The energy of an elastic المرن mode of angular frequency ω is

$$\epsilon = (n + \tfrac{1}{2})\hbar\omega$$

when the mode is excited متهيجا to quantum number **n** that is when the mode is occupied محتل by **n** phonons. The term $\frac{1}{2}\hbar\omega$ is the zero-point energy of the mode. It occurs يحدث for both phonons and photons as a consequence نتيجة of their equivalence مكافئ to a quantum harmonic oscillator متذبذب هارموني of frequency ω, for which the energy eigenvalues القيم الذاتية are also (n+ $\frac{1}{2}$) $\hbar\omega$.

We can quantize the mean square phonon amplitude.

يمكننا تحديد متوسط سعة الفونون المربعة

$$u = u_0 \cos Kx \cos \omega t \ .$$

Here u is the displacement of a volume element from its equilibrium position at x in the crystal.

kinetic energy and half potential energy, when averaged over time.

The kinetic energy density is $\frac{1}{2}\rho(\partial u/\partial t)^2$ where ρ is the mass density

the volume integral of the kinetic energy is $\frac{1}{4}\rho V\omega^2 u_0^2 \sin^2 \omega t$.

The time average kinetic energy is

$$\tfrac{1}{8}\rho V\omega^2 u_0^2 = \tfrac{1}{2}(n + \tfrac{1}{2})\hbar\omega$$

because $\langle \sin^2 \omega t \rangle = \frac{1}{2}$. The square of the amplitude of the mode is

$$u_0^2 = 4(n + \tfrac{1}{2})\hbar/\rho V\omega \ .$$

A **phonon** of wavevector **K** will interact with particles such as **photons**, **neutrons**, and **electrons** as if it had a momentum $\hbar\boldsymbol{K}$.

The **elastic scattering** استطارة مرنة of an X-ray photon by a crystal is governed يحكم by **wavevector selection rule**

$$\mathbf{k}' = \mathbf{k} + \mathbf{G} \ ,$$

where **G** is a vector in the reciprocal lattice, **k** is the wavevector of the incident

photon, and $\mathbf{k}'$ is the wavevector of the scattered photon.
If the scattering استطارة of the photon is inelastic غير مرن with the creation خلق of a phonon of wavevector **K,** then the **wavevector selection rule** is

$$\mathbf{k}' + \mathbf{K} = \mathbf{k} + \mathbf{G}$$

If a phonon $\mathbf{K}$ is absorbed in the process, we have instead the relation

$$\mathbf{k}' = \mathbf{k} + \mathbf{K} + \mathbf{G}$$

References

1- Charles Kittel - Introduction to Solid State Physics-Wiley (2005)

2- J. S. Blakemore - Solid State Physics-Cambridge University Press (1985)

3- M. A. OMAR Elementary-solid-state-physics