42

RAJARATA UNIVERSITY OF SRI LANKA
FACULTY OF APPLIED SCIENCES

B.Sc. Honours in Chemistry
Fourth Year - Semester I Examination – January / February 2021

CHE 4215 – SOLID STATE CHEMISTRY

Time: Two (02) hours

Answer **any four (04)** questions.

All symbols given are as of their usual meaning.

Use of a non -programmable calculator is permitted.

---

01. a) Define the following terms.
    i. Unit cell
    ii. Amorphous solid (20 marks)

b) i. What information could be obtained from the following symbols used in crystallography?
(111), [111], {111}, <111> (10 marks)

ii. Draw the following information in separate cubic unit cells.
[212], [111], [110], (100), (110), (010) (15 marks)

c) The magnitude of the distance between two adjacent and parallel planes of atoms with the same Miller indices is called "interplanar spacing, d_{hkl}". The interplanar spacing in cubic crystals is given by the general equation,

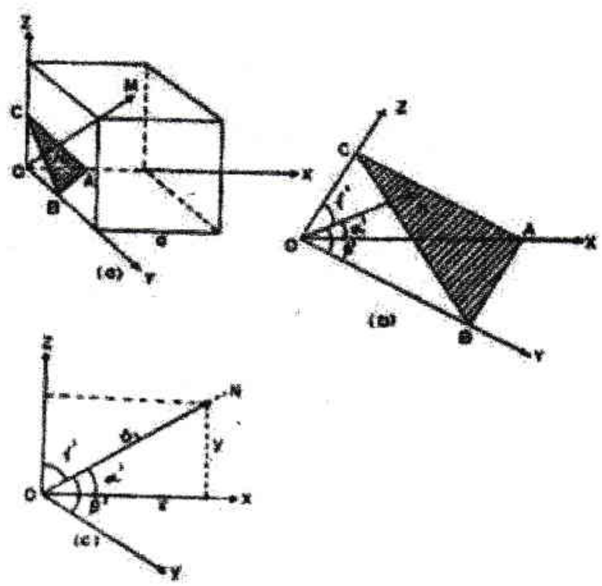
$$d_{hkl} = \frac{a}{\sqrt{(h^2+k^2+l^2)}}$$

in which **a** is the lattice parameter (unit cell edge length) and h, k, and l represent the Miller indices of the adjacent planes being considered.

Cont'd.

43

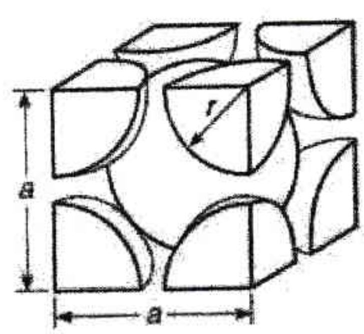
i. Derive the interplanar spacing formula for simple cubic unit cell using following diagram.



(40 marks)

ii. Determine the perpendicular distance between the two planes indicated by the Miller indices (1 2 1) and (2 1 2) in a unit cell of a cubic lattice with a lattice constant parameter 'a'. (15 marks)

02. a) Following question is based on the BCC lattice structure depicted in the figure.



i. Determine the number of equivalent whole atoms in the unit cell.
ii. Execute the relation between a and r.
iii. Calculate the atomic packing factor, APF for the simple cubic lattice structure shown in the above figure. (40 marks)

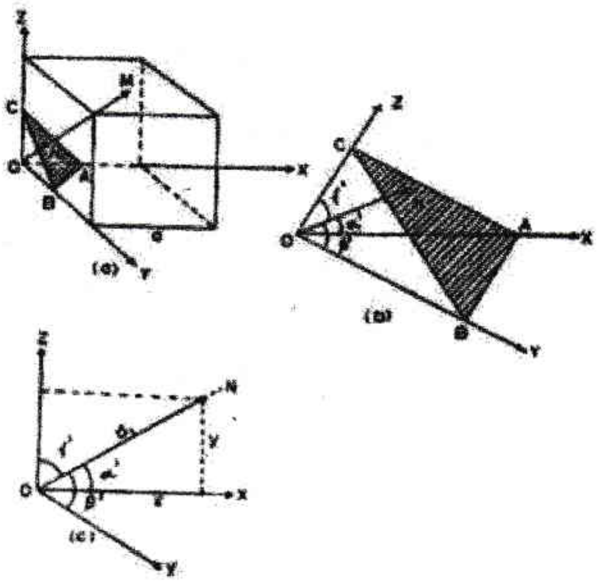
b) Calculate the volume of the unit cell of iron (Fe) in cubic meters, given that iron has a body-centered cubic crystal structure and an atomic radius of 0.124 nm. (15 marks)

c) If aluminum (Al) has an FCC crystal structure and an atomic radius of 0.143 nm, calculate the volume of its unit cell in cubic meters. (15 marks)

Cont'd.

43

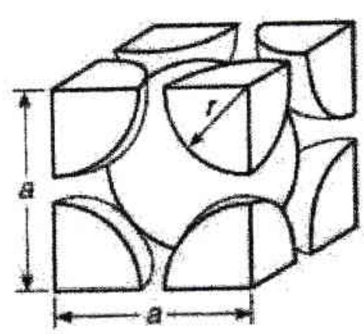
i. Derive the interplanar spacing formula for simple cubic unit cell using following diagram.



(40 marks)

ii. Determine the perpendicular distance between the two planes indicated by the Miller indices (1 2 1) and (2 1 2) in a unit cell of a cubic lattice with a lattice constant parameter 'a'. (15 marks)

02. a) Following question is based on the BCC lattice structure depicted in the figure.



i. Determine the number of equivalent whole atoms in the unit cell.
ii. Execute the relation between a and r.
iii. Calculate the atomic packing factor, APF for the simple cubic lattice structure shown in the above figure. (40 marks)

b) Calculate the volume of the unit cell of iron (Fe) in cubic meters, given that iron has a body-centered cubic crystal structure and an atomic radius of 0.124 nm. (15 marks)

c) If aluminum (Al) has an FCC crystal structure and an atomic radius of 0.143 nm, calculate the volume of its unit cell in cubic meters. (15 marks)

Cont'd.

44

d) Calculate the density of aluminum, given that it has an FCC crystal structure, an atomic radius of 0.143 nm and an atomic mass of 26.98 g/mol. (30 marks)
(Avogadro's Number = 6.022×10^{23} mol^{-1})

03. a) Explain AAAA, ABABA and ABCABC types of three-dimensional crystal packing using illustrations. (30 marks)

b) Identify the type of stochiometric defect present in following compounds and write short notes on each defect type.

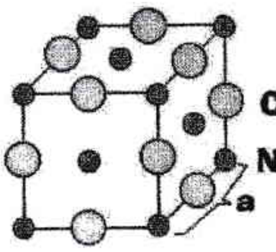
i. AgBr
ii. ZnS (20 marks)

c) Define each term of the following equation and calculate the number of vacancies in 1 cm^3 of Cu metal at room temperature (27 °C).

$$N_v = N_s exp^{\left(\frac{-Q_v}{k_b T}\right)}$$

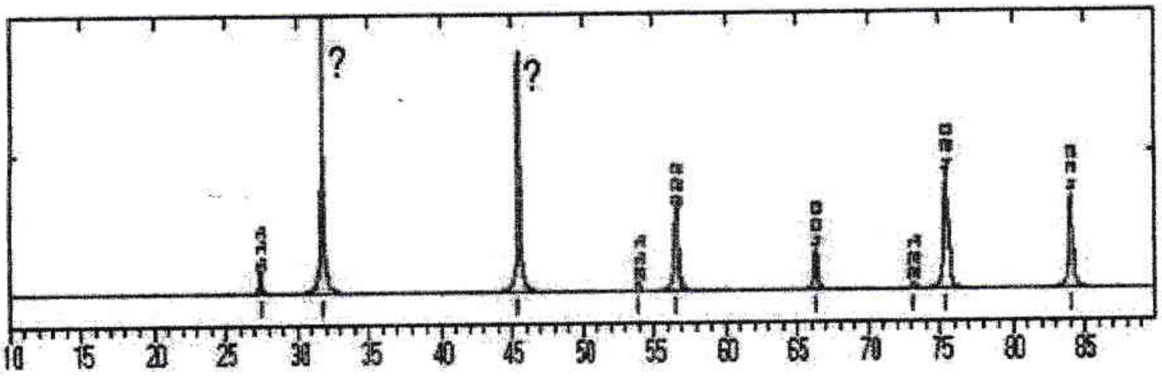
$k_b = 8.62 \times 10^{-5}$ eV $atom^{-1}$ K^{-1}, $Q_v = 0.9$ eV $atom^{-1}$, $N_A = 6.023 \times 10^{23}$ atoms mol^{-1},
$\rho = 8.4$ g cm^{-3}, $A_{cu} = 63.5$ g mol^{-1} (20 marks)

d) X-Ray diffraction is a technique used to determine the crystallographic structure of single crystal materials. The figure below shows the diffraction pattern of NaCl. X-ray diffraction peaks for NaCl are indicated in terms of their Miller indices. Determine unit cell length **a** (Å) and the missing Miller indices using following information.
($\lambda = 1.54056$ Å)



For a cubic system,

$$\sin^2\theta = \frac{\lambda^2}{4a^2}\left(h^2 + k^2 + l^2\right)$$



Cont'd.

Selected data from the NaCl diffractogram is given by the following table.

2θ (°)	h,k,l
27.47	111
31.82	?
45.62	?
56.47	222

(30 marks)

04. In a scanning electron microscope, a focused electron beam is scanned across a sample. The interaction between the electron beam and the sample leads to the emission of many different signals (electrons, X-rays, visible light) which can be detected to gain information about the sample. Each signal provides different information about the sample.

a) List the names of different types of signals and explain the origin of each signal and what information can be obtained about the sample from each signal. (25 marks)

b) Discuss the three modes used in in AFM (20 marks)

c) Sketch the main components of a SEM apparatus and explains how SEM functions. (35 marks)

d) Define what semiconductor is. Describe the two main types of semiconductors and contrast their conduction mechanism. (20 marks)

05. a) Describe the basic principles of DTA (45 marks)

b) Draw the TGA pattens for following conditions.

i. The sample undergoes no decomposition with loss of volatile products over the temperature range.

ii. The rapid initial mass loss is characteristic of desorption or drying.

iii. Multi-stage decomposition with relatively stable intermediates.

iv. Multi-stage decomposition no stable intermediate product.

v. Gain in mass due to reaction with atmosphere. (25 marks)

c) Pure $AgNO_3$ sample is analyzed by TG technique. Herein, the 50 mg of the $AgNO_3$ remains constant up to a temperature of 473 °C. At 473 °C it starts losing its weight and this indicates that the decomposition starts at this temperature. It decomposes to NO_2, O_2 and Ag. The loss in weight continues up to 608 °C and beyond this temperature the weight of the sample remains constant. Draw the thermogram of pure $AgNO_3$. (30 marks)

——END——