
SECTION – A

There are **FOUR** questions in this section. Answer **Q. No. 1** and any **TWO** questions from the rest.

1. (a) The order of diffraction refers to the number of times a wave is diffracted or bent as it passes through a narrow opening or around an obstacle. To understand higher order diffraction often first order diffraction is considered. Explain how higher order diffraction can be studied through first order diffraction only. Use necessary mathematical expressions to support this statement. (13)
- (b) X-rays of an unknown wavelength is diffracted by a gold sample. The 2θ angle was 64.582° for the {220} planes. Calculate the wavelength of the X-rays used? (The lattice constant of gold = 0.40788 nm; assume first-order diffraction, $n = 1$). (12)
- (c) Diffraction peaks are not observed for all the crystallographic planes for different Bravais lattices. Arrange the crystallographic planes with decreasing interplanar values and categorize them based on the observed diffraction peaks for SC, BCC and FCC crystals. The planes are: (300), (100), (310), (200), (210), (211), (110), (220), (221), (111). (10)
2. (a) In stereographic projection all the crystallographic planes maintain specific angular relation. This is reflected from pole diagram and finally in the stereographic projection. Using neat sketches illustrate how stereographic projection of a great circle is either a circle or straight line. (20)
- (b) A crystal is associated with two lattices: real lattice and reciprocal lattice. Correlate both the lattices with necessary vector relationships. The reciprocal lattice plays a fundamental role in the most analytic studies of periodic structures, particularly in the theory of diffraction. Schematically demonstrate that the reciprocal lattice of a BCC crystal is FCC, and the reciprocal lattice of an FCC crystal is BCC. (15)
3. (a) Dislocations are defects in crystals. Dislocations are areas where the atoms are out of position in the crystal structure. Distinguish between deformation behaviour of edge and screw dislocations with sketches showing the mutual alignment of Burgers vector and slip line. Also, illustrate the stress distribution in the crystal with positive and negative edge dislocations. (20)

MME 211

Contd ... Q. No. 3

(b) Vacancy, in crystallography, means absence of an atom or molecule from a point that it would normally occupy in a crystal. Such an imperfection (crystal defect) in the regular spacing of atoms changes the electrical and optical properties of the crystal. Explain how temperature plays role on vacancy concentration for different metals with different melting temperature and comment on the final vacancy concentration for different metals near their melting temperatures. Show how electronic charge is balanced during formation of different types of vacancies. (15)

4. Demonstrate the following crystal structures using neat sketches: (35)

- (a) Zinc Blende (ZnS, sphalerite)
- (b) Zinc Blende (ZnS, wurtzite)
- (c) Two basic unit cells (one-eighth) of Spinel (AB₂O₄)
- (d) Antifluorite (Na₂O)

SECTION – B

There are **FOUR** questions in this section. Answer any **THREE**.

5. (a) After filling up lattice points of BCC site, you have filled up all octahedral sites of BCC with maximum-size ellipsoid-shaped atoms. Formulate the problem and solve the problem for atomic packing factor (APF) of the modified structure and eccentricity of the ellipsoid/(s). Remember, ellipsoid volume with *a, b, c* 'diameters' is $\frac{\pi}{6} abc$. (10+7=17)

(b) In 3D, devise a crystal structure-centering combination that doesn't provide any unique symmetry, other than Face-Centered Tetragonal (FCT). For this crystal structure, illustrate with proper labels the 'incorrect' structures' unit cell side-by-side with symmetry-corrected and correctly named unit cell. You may take help from the chart below. (6)

Crystal system	Bravais lattice
Triclinic	Primitive
Monoclinic	Primitive
	Base centered
Orthorhombic	Primitive
	Base centered
	Body centered
	Face centered
Rhombohedral	Primitive
Hexagonal	Primitive
Tetragonal	Primitive
	Body centered
Cubic	Primitive
	Body centered
	Face centered

MME 211**Contd ... Q. No. 5**

(c) Consider this hypothetical scenario. A stream of minute (circularly polarized) particles is passing through crystallographic-level channels of single crystal of an FCC material. If the particles are subjected to atomic structure with glide symmetry on its path exactly matching with its polarization, then the particles pass through with little dissipation. Conclude whether the channel exists or not, and with proper sketches, relate the parameters of glide you have found with the optimum wavelength and circular polarization of particle stream. (4+8=12)

6. (a) Calculate ideal C-C single bond length. Pure diamond's specific gravity is 3.52. Lonsdaleite, another allotrope of Carbon, crystallizes in crystal structure similar to hexagonal ZnS but C in place of both Zn and S. Find density of that allotrope, and hence calculate density ratio of these two allotropes. Does this ratio depend on C-C bond-length or atomic mass of carbon, or neither? (7+7+3=17)
- (b) Compare the smallest angle between two densest lines on same densest plane of BCC, and the smallest angle between two densest planes sharing same densest line of BCC. Which of these two angles is smaller? Show the calculation with appropriate sketches. (5×2+2+3×2=18)

7. You have a BCC lattice with atomic radius r_0 . How to fill up all lattice points, octahedral sites and tetrahedral sites of BCC simultaneously, and maximize Atomic Packing Factor (APF)? You thought, but you came across three obvious limitations. You need to convert these limitations into equations or inequalities first to solve the problem.

(i) Tetrahedral site atomic radius r_4 must be smaller than or equal to tetrahedral void itself. This means, $\frac{r_4}{r_0} \leq A_4; A_4 \text{ const.}$

(ii) Octahedral site atomic radius r_8 must be smaller than or equal to octahedral void itself. This means, $\frac{r_8}{r_0} \leq A_8; A_8 \text{ const.}$

(iii) Sum of r_8 and r_4 must be less than or equal to distance between tetrahedral and octahedral sites. This means, $\frac{r_4 + r_8}{r_0} \leq A_{48}; A_{48} \text{ const.}$

You approach the problem as follows:

- (a) Devise an equation for APF of BCC if lattice sites, tetrahedral sites, octahedral sites - all three are filled with three different atomic radius (r_0, r_4, r_8) respectively. Write APF as function of $\frac{r_4}{r_0}$ and $\frac{r_8}{r_0}$. (9)

- (b) Rewrite the three inequalities mentioned before (i, ii, iii) in equation form, mentioning values of A_4, A_8, A_{48} . (3×3=9)

MME 211

Contd ... Q. No. 7

(c) Now, do the following. Solve equations (i) and (iii), and find $\left(\frac{r_4}{r_0}, \frac{r_8}{r_0}\right)$. Put these values in equation of APF at (a), and calculate value of APF. Do the same for solving equations (ii) and (iii) simultaneously, and find APF for that case as well. Find the scenario with higher APF and whether the values of radii are feasible. You may draw a diagram showing the equations or inequalities (i, ii, iii) in $(x, y) = \left(\frac{r_4}{r_0}, \frac{r_8}{r_0}\right)$ plane, if convenient for you to draw conclusion. (17)

8. (a) For HCP, the nearest neighbours are 6 in-plane atoms, 3 atoms above and 3 below. But what are 2nd and 3rd nearest neighbours? Calculate their numbers and center-to-center distances. (4+7=11)
- (b) Calculate three angles of the triangular face that is shared by distorted octahedral site and distorted tetrahedral site of BCC, with proper coordinates if necessary. (3×2=6)
- (c) What is the position of improper rotation axis of a HCP lattice? How can you represent that axis with help of Rotation-reflection and Rotation-inversion? Explain and illustrate with proper image and labelling. (6+6+6=18)
-

BANGLADESH UNIVERSITY OF ENGINEERING AND TECHNOLOGY, DHAKA

L-2/T-1 B. Sc. Engineering Examinations 2022-2023

Sub: **MME 215** (Thermodynamics of Materials)

Full Marks: 210

Time: 3 Hours

The figures in the margin indicate full marks.

USE SEPARATE SCRIPTS FOR EACH SECTION

SECTION – A

There are **FOUR** questions in this section. Answer **Question # 1** and any **Two** questions from the rest. **Question # 1 is COMPULSORY.**

1. Give the required definitions, principles, or mathematical expressions for any fifteen (15) of the following questions. Be sure to carefully define any symbols if used. (45)
 - (i) A state function.
 - (ii) The mathematical expression of the second law of thermodynamics.
 - (iii) The third law of thermodynamics.
 - (iv) The work function.
 - (v) The maximum non-mechanical work obtainable from a process under constant temperature and pressure conditions.
 - (vi) The conditions for equilibrium of binary iron- carbon alloy having ferrite (α) and pearlite (P) phases in the system.
 - (vii) The activity of a component in solution.
 - (viii) The partial molar enthalpy of A in terms of the molar enthalpy of A-B solution.
 - (ix) The metastable equilibrium.
 - (x) An expression for activity of Si in a dilute solution of Fe-C-Si-Mn alloy.
 - (xi) The change in entropy during mixing of A-B real solution.
 - (xii) The chemical affinity of a reaction.
 - (xiii) The equation for ice-steam equilibrium in a pressure – temperature diagram.
 - (xiv) Richards' rule.
 - (xv) The general equilibrium condition for the reaction $A + 2B \leftrightarrow C$.
 - (xvi) Kirchoff's equation.
 - (xvii) An equation that shows the relationship between the equilibrium constant and temperature of a chemical reaction.
 - (xviii) Langmuir adsorption isotherm.
 - (xix) Phenomenological thermodynamics.
 - (xx) The conditions for equilibrium in statistical thermodynamics.

2. (a) Develop an expression for the change in volume of a system for a process in which the pressure of the system is changed at constant entropy. (20)

- (b) Twenty litres of ideal gas at 27°C and 50 atm expands reversibly and adiabatically to 200 litres. Determine the change in internal energy of the gas for the process. (10)

MME 215

3. (a) Use the equilibrium principle (i.e., criterion for equilibrium) governing equilibrium under constant entropy, pressure, and number of moles to determine the conditions for equilibrium for unary two-phase system. (20)
- (b) The pressure of 5 moles of diatomic gas is increased from 1 atm to 100 atm inside a rigid container. Determine the change in entropy of the system. (10)
4. (a) "Although imaginary and does not exist in nature, a reversible process is vitally important for the development of classical thermodynamics." Explain this assertion. (10)
- (b) Derive the expression $(\partial U / \partial T)_p = C_p - P(\partial V / \partial T)_p$ (10)
- (c) Explain the term metastable equilibrium. Using suitable examples, analyse its importance in materials science and engineering. (10)

SECTION - B

There are **FOUR** questions in this section. Answer any **THREE**.

5. (a) Deduce an expression indicating the temperature dependence of equilibrium constant. (10)
- (b) Explain how the concept of equilibrium constant can be used in deoxidation of steelmaking process. (10)
- (c) Will a blast furnace gas analyzing 28% CO, 13% CO₂ and 59% N₂ reduce FeO at 727°C? Given data: (15)
- $$\langle \text{Fe} \rangle + 1/2 (\text{O})_2 = \langle \text{FeO} \rangle ; \Delta G_0 = -62050 + 14.95 T \text{ cal}$$
- $$\langle \text{CO} \rangle + 1/2 (\text{O})_2 = \langle \text{CO}_2 \rangle ; \Delta G_0 = -62750 + 20.75 T \text{ cal}$$
6. (a) Explain how interfacial tension controls the shapes of a precipitate. How does the addition of manganese in steel eliminate the harmful effect of sulphur? (15)
- (b) Explain how the concept of adsorption is used to manufacture cutting fluid solution. (10)
- (c) A liquid silicate with surface tension of 500 ergs cm⁻² makes contact with a polycrystalline oxide with an angle $\theta = 45^\circ$ on the surface of the oxide. If mixed with the oxide, it forms liquid globules at three grain intersections. The average dihedral angle ϕ is 90°. If we assume the interfacial tension of the oxide-oxide interface, without the silicate liquid is 1000 dyne cm⁻¹, compute the surface tension of the oxide. (10)
7. (a) X_A moles of A and X_B moles of B are mixed to form a regular binary AB solution. Deduce an expression for the Gibbs free energy change of mixing of this solution. What would be the expression if the solution formed were an ideal solution? (20)

MME 215

Contd ... Q. No. 7

(b) Explain the principal characters of a dilute solution. (10)

(c) Give the mathematical expression of the partial molar Gibbs free energy of carbon in Fe-C-Si alloy. (5)

8. (a) Platinum (Pt) may exist as a solid, a liquid or a vapour. The vapour pressure for the solid and liquid are given below: (20)

$$\text{Solid Pt: } \log p = -28460/T - 1.27 \log T + 14.33 \text{ (mm Hg)}$$

$$\text{Liquid Pt: } \log p = -27890/T - 1.77 \log T + 15.71 \text{ (mm Hg)}$$

Calculate:

- (i) The normal boiling point of Pt,
- (ii) The triple point temperature and pressure,
- (iii) The enthalpy of evaporation of Pt at the normal boiling temperature,
- (iv) The enthalpy of fusion of Pt at the triple point temperature,
- (v) The difference between the constant-pressure heat capacities of solid and liquid Pt.

(b) Indicate the conditions for equilibrium in a three-component, three-phase system. (5)

(c) Discuss the information one would gather when a phase diagram is constructed in a space where all the coordinates are thermodynamic potentials. What extra information one would muster if the coordinates are not thermodynamic potentials? (5+5=10)

SECTION – AThere are **FOUR** questions in this section. Answer any **THREE**.

Symbols have their usual meanings.

1. (a) State and explain the basic postulates of Einstein's special theory of relativity. (10)
 (b) Derive an expression for the relativistic kinetic energy of a particle and show that for smaller speeds it reduces to the classical expression. (17)
 (c) Calculate the mass of an electron when it is moving with a kinetic energy of 10 MeV. (8)
2. (a) Define photoelectric effect. What are photoelectric work function and threshold frequency? (8)
 (b) Show that the change in wavelength of an X-ray photon during Compton scattering is independent of the wavelength of the incident photon. On which condition does the greatest wavelength change occur? (19)
 (c) An X-ray photon of initial frequency 3.0×10^{19} Hz collides with an electron and is scattered through 90° . Find its new frequency. (8)
3. (a) What is radioactive series? Mention the name of the radioactive series with their parent and stable end product. (12)
 (b) Explain clearly what conclusions we get about the stability of the nucleus from the neutron-proton diagram. (15)
 (c) Half-life of ^{222}Rn is 3.8 d. Find the activity of 1.00 mg of ^{222}Rn . What will the activity of it be exactly one week later? (8)
4. (a) Describe a physical phenomenon that cannot be explained by classical mechanics but can be understood through the concepts of quantum mechanics. (10)
 (b) Show that infinite square-well energy quantization law can be obtained from the de Broglie hypothesis by fitting an integral number of half de Broglie wavelength $\lambda/2$ into the width ' a ' of the potential well. (15)
 (c) Determine the expectation value for the position of a particle confined within a box of width ' L '. (10)

PHY 201

SECTION – B

There are **FOUR** questions in this section. Answer any **THREE**.

5. (a) Write down expressions for time-independent and time-dependent forms of the Schrödinger equation. What are energy quantization and zero-point energy? (10)
- (b) Examine the differences between the wave function and the probability function concerning an electron in potentials of infinite and finite square wells. What conclusions can be drawn from these schematic diagrams? (20)
- (c) An eigenfunction of the operator d^2/dx^2 is $\Psi = e^{2x}$. Find the corresponding eigenvalue. (5)
6. (a) Draw schematically potential wells and energy levels of a hydrogen atom and a harmonic oscillator. In each case, show the energy levels corresponding to different quantum numbers. (10)
- (b) Explain the 'Quantum Mechanical Tunneling' effect and its significant application: (15)
- (c) Electrons with energies of 1.0 eV and 2.0 eV are incident on a barrier 10.0 eV high and 0.50 nm wide. (i) Find their respective transmission probabilities. (ii) How are these affected in the barrier is doubled in width? (10)
7. (a) Briefly state different nanomaterials according to the number of dimensions. (10)
- (b) Describe the working principle of high energy ball milling process. Explain the Factors upon which the process depends on. (15)
- (c) Distinguish the purposes of XRD, SEM, EDS and FTIR in determining the properties of nanostructured materials. (10)
8. (a) State Scherrer's formula and Bragg's law. (10)
- (b) Describe how the properties of a thin film depend on film thickness, film uniformity, reflectivity and yield. (15)
- (c) In a typical XRD diffraction pattern of cubic spinel ferrite, the first three characteristic peaks of (111), (220), (311), are observed in $2\theta = 18.33^\circ$, 30.14° and 35.49° , respectively. The wavelength of the Cu- K_α radiation is 1.54 Å. Calculate average inter-planer spacing (d) and the average lattice parameter for the cubic spinel ferrite. (10)
-

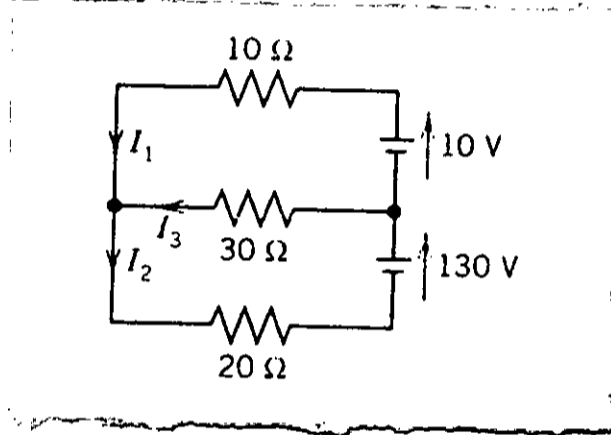
SECTION - A

There are **FOUR** questions in this section. Answer any **THREE**.

1. (a) Define Hermitian and Nilpotent matrices with examples. For the matrix (17)

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 2 & 1 & 2 \\ 3 & 1 & 0 \end{bmatrix} \text{ verify that } A(\text{adj}A) = |A|I_3. \text{ Find the inverse of } A \text{ as well.}$$

- (b) Apply Kirchoff's laws to derive the system of linear equations and then find currents using matrix from the following diagram: (18)



2. (a) Reduce the matrix $\begin{bmatrix} 2 & 4 & 3 & 2 \\ 3 & 6 & 5 & 2 \\ 2 & 5 & 2 & -3 \\ 4 & 5 & 14 & 14 \end{bmatrix}$ into canonical form. Also, find rank. (17)

- (b) Factorize the matrix $\begin{bmatrix} 1 & 2 & 2 \\ 1 & 3 & 2 \\ 1 & 2 & 3 \end{bmatrix}$ into elementary matrices. (18)

3. (a) State and verify Cayley-Hamilton theorem for the matrix $B = \begin{bmatrix} 4 & -1 & 1 \\ -1 & 4 & -1 \\ 1 & -1 & 3 \end{bmatrix}$. Hence find B^4 . (17)

(b) Let the oldest age attained by the females in some animal population be 12 years. Divide the population into three age classes of 4 years each. Let the Leslie model

$$L = l_{jk} = \begin{bmatrix} 0 & 3.45 & 0.6 \\ 0.9 & 0 & 0 \\ 0 & 0.45 & 0 \end{bmatrix}, \text{ where } l_{1k} \text{ is the average number of daughters born to a single}$$

female during the time she is in age class k , and $l_{j,j-1}$ ($j = 2, 3$) is the fraction of females in age class that will survive and pass into class j . (18)

MATH 273

Contd ... Q. No. 3(b)

- (i) What is the number of females in each class after 4, and 8 years if each class initially consists of 500 females?
- (ii) For what initial distribution will the number of females in each class change by the same proportion? What is this rate of change?

4. (a) Check whether the matrix $\begin{bmatrix} 6 & 2 & -2 \\ 2 & 3 & -1 \\ -2 & -1 & 3 \end{bmatrix}$ is derogatory or not. If yes, then express

the characteristic polynomial as the product of minimal polynomial and a certain monic factor of it. (17)

- (b) Write the properties of eigen values of the matrix that exists in the positive and negative definite quadratic forms. Reduce the quadratic form $q = 4x_1^2 + 3x_2^2 - x_3^2 + 2x_2x_3 - 4x_3x_1 + 4x_1x_2$ to the canonical form. Hence find rank, index and signature of q . Write down the corresponding equations of transformation. (18)

SECTION - B

There are **FOUR** questions in this section. Answer any **THREE**.

5. (a) Graph the function $f(x) = \begin{cases} 1 & 0 < x < \pi \\ 0 & \pi < x < 2\pi \end{cases}$ then find Fourier series of $f(x)$. (18)

- (b) Find the Fourier half range cosine series of $f(x) = \begin{cases} 2x & 0 < x < 1 \\ 2(2-x) & 1 < x < 2 \end{cases}$. (17)

6. (a) Find the Fourier integral of $f(t) = \begin{cases} 1+t & |t| \leq 1 \\ 0 & |t| > 1 \end{cases}$ (17)

And hence evaluate $\int_0^\infty \left(\frac{\sin u}{u}\right)^2 du$.

- (b) Use finite Fourier transforms to solve the following boundary value problem: (18)

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 4, t > 0$$

Given that $U(0, t) = 0, U(4, t) = 0, U(x, 0) = 2x$.

7. (a) Solve the differential equation $(x^3 + 4x)y'' - 2xy' + 6y = 0$ by Frobenius Method. (25)

- (b) For Bessel's function show that $J_{\frac{3}{2}}(x) = \sqrt{\frac{2}{\pi x}} \left(\frac{\sin x}{x} - \cos x\right)$. (10)

8. (a) Prove the Rodrigues's formula for Legendre polynomials (12)

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n$$

- (b) For Bessel's function $J_n(x)$ show that $2nJ_n = x(J_{n-1} + J_{n+1})$. (12)

- (c) Prove that $J_n(x)$ and $J_{-n}(x)$ are linearly dependent when n is a positive or negative integer. (11)
