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FIRST SEMESTER M.TECH. (NANO SCIENCE AND TECHNOLOGY)
DEGREE EXAMINATION, APRIL 2020

NST 104-INTRODUCTION TO NANOMATERIALS

(2019 Admissions)

Time: Three Hours Maximum: 60 Marks

Section A

Answer all questions.

2 marks each.

- 1. Why nanoparticles are thermodynamically unstable?
- 2. What is the significance of surface to volume ratio in nanoparticles?
- 3. What is anisotropic growth?
- 4. What is positive and negative masking in photolithography?
- 5 What is SEELFS?
- 6. Explain Wulff's theorem.
- 7. What is heterogeneous nucleation?
- 8. Discuss the variation of fraction of solid state transformation with respect to time of growth at constant temperature.

 $(8 \times 2 = 16 \text{ marks})$

Section B

Answer any five questions.

4 marks each.

- 9. Explain the significance of Wulff plot?
- 10. Differentiate Ostwald ripening and sintering.
- 11. How Gibb's free energy influence nucleation?
- 12. Discuss quantum tunneling? How it can be used for visualization of nanosystems.
- 13. How surface process influence the particle nanoparticle growth?
- 14. Describe the metal oxide nanobelt growth by evaporation-condensation.

- 15. Explain template based synthesis.
- 16. Explain surface plasmon resonance.

 $(5 \times 4 = 20 \text{ marks})$

Section C

2

Answer any four questions.

6 marks each.

- 17. Explain the influencing factors in metallic nanoparticle synthesis.
- Discuss the size dependent variation in transition energy in nanostructures with the help of infinite
 potential well model.
- 19. Explain interaction between nanoparticles with the help of DLVO theory.
- 20. What is quantum tunneling? How it can be used for visualizing the nanosystems.
- 21. What is Scanning Electron Microscopy (SEM)? What are the factors deciding the image resolution SEM?
- Explain different steps involved in a photolithographic process? Differentiate a positive and negative
 photoresist.
- Write advantages of E-beam lithography and explain how the scattering of electrons affects the resolution.
- 24. Write notes on: (a) Electrospinning; and (b) Hydrothermal solvothermal synthesis.

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FIRST SEMESTER M.TECH. (NANOSCIENCE AND TECHNOLOGY) DEGREE EXAMINATION, APRIL 2020

NST 103—COMPUTATIONAL METHODS AND DATA PROCESSING

(2019 Admissions)

Time : Three Hours Maximum : 60 Marks

Section A

Answer **all** questions. 2 marks each.

- 1. Define curve fitting.
- 2. Find a root of the equation $x \sin x + \cos x = 0$.
- 3. Evaluate the sum $S = \sqrt{3} + \sqrt{5} + \sqrt{7}$ to 4 significant digits and find its absolute and relative errors.
- 4. Define Trapezoidal rule.
- 5. What are the Cartesian co-ordinates?
- 6. Explain backward difference operator.
- 7. Find a real root of equation $x^3 x 11 = 0$ by bisection method.
- 8. Write any two advantages of origin.

 $(8 \times 2 = 16 \text{ marks})$

Section B

Answer any **five** questions. 4 marks each.

- 9. Find a root of the equation $x^4 x 10 = 0$ using bisection method and correct to 2 decimal places.
- 10. Give an expression for Newton's general, forward and backward interpolation formula.
- 11. Explain in detail the Simpson's 1/3 rule.
- 12. Describe in detail the House holder's equation.
- 13. Determine the root of the equation $\cos x x e^x = 0$ by the method of False position.
- 14. Describe in detail the necessity of pivoting.

- 15. Discuss in detail about Excel and also write its uses.
- 16. Explain in detail the importance of normalization.

 $(5 \times 4 = 20 \text{ marks})$

Section C

2

Answer any **four** questions. 6 marks each.

- 17. Explain in detail the bisection method with examples.
- 18. Describe in detail the iteration method and find a real root of $2x \log_{10} x = 7$.
- 19. Explain the computational procedure for the LU decomposition method.
- 20. Discuss in detail the Trapezoidal rule.
- 21. Write a detailed note on Cartesian co-ordinates and internal co-ordinates.
- 22. Describe the super molecule method.
- 23. Describe the features of X pert high score software.
- 24. Discuss in detail the features of Chem Sketch.

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FIRST SEMESTER M.TECH. (NANOSCIENCE AND TECHNOLOGY) DEGREE EXAMINATION, APRIL 2020

NST 102-STRUCTURE AND BONDING IN SOLIDS

(2019 Admissions)

Time: Three Hours Maximum: 60 Marks

Section A

Answer all questions.

Each question carries 2 marks.

- 1. What is the difference between Frenkel and Schottky defects in crystalline solids?
- 2. Describe the radius ratio criterion for six co-ordination (octahedral) in crystalline solids.
- 3. Explain the main difference between ionic and covalent bonding in solids.
- 4. What is an F center? Give an example.
- 5. Briefly describe the Young's modulus of elasticity.
- 6. What is co-ordination number? What factors control co-ordination number?
- 7. What are the Symmetry elements in a C_{4v} point group.
- 8. Give examples of four plastic deformations in crystalline solids.

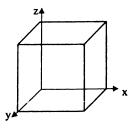
 $(8 \times 2 = 16 \text{ marks})$

Section B

Answer any five questions.

Each question carries 4 marks.

9. Using the following diagram as basis, mark the following planes in a cubic crystal (202), (001).



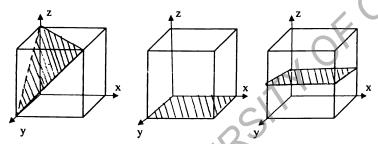
10. The molecular weight of a material is 223. It has a cubic structure with a = 4Å. Calculate the density of the material.

Turn over

- 11. Draw the M.O. diagram for a heteronuclear diatomic molecule. (eg: CO)
- 12. Illustrate the energy level diagram of a n-type semiconductor including the Fermi level.

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- 13. Describe briefly VSEPR rule with an example.
- 14. Describe direct and indirect band gap semiconductors with examples.
- 15. In a cube, mark the (110) and (111) planes and calculate the angle between them.
- 16. Identify the crystallographic planes in the following diagrams:



 $(5 \times 4 = 20 \text{ marks})$

Section C

Answer any **four** questions.

Each question carries 6 marks.

- 17. Describe edge and screw dislocations in a crystal.
- 18. Calculate the radius ratio rules for a typical structure with octahedral co-ordination. Give an example of a solid adopting this structure.
- ZnO has a hexagonal structure having the lattice parameter, a = 4Å and c = 5Å. Calculate the unit cell volume.
- Calculate the radius ratio rules for a typical structure with tetrahedral co-ordination. Give an example of a solid adopting this structure.
- 21. Draw the structure of a molecule adopting D_{4th} symmetry and mark all the proper axes.
- 22. Describe the different elements of symmetry in crystallography.
- A molecule with the general formula ABO₃ adopts cubic structure. Mark the probable positions of A, B and O in a cubic unit cell.
- 24. Explain the difference between hexagonal close packing and cubic close packing.

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FIRST SEMESTER M.TECH. (NANOSCIENCE AND TECHNOLOGY) DEGREE EXAMINATION, APRIL 2020

NST101-QUANTUM MECHANICS

(2019 Admissions)

Time: Three Hours Maximum: 60 Marks

Section A

Answer all questions.

2 marks each.

- 1. What is Hermitian operator? Why it is significant in Quantum mechanics?
- 2. What is eigen values and expectation values?
- 3. What is probability density?
- 4. Explain superposition theorem
- 5. What is the significance of group velocity and particle velocity in quantum mechanics?
- 6. Write the Schrödinger equation for a free electron. Discuss the possible solutions.
- 7. What is mean by linear operator? Prove Schrödinger equation is linear.
- 8. Prove nonexistence of a electron inside nucleus.

 $(8 \times 2 = 16 \text{ marks})$

Section B

Answer any five questions.

4 marks each.

- 9. State uncertainty principle and prove with single slit diffraction.
- 10. Explain the concept of normalization of wave functions. Normalize the wave function $\psi = Ae^{i(\omega t kx)}$ where A, k and ω are real positive constants.
- Compare the uncertainties in the velocities of an electron and a proton confined to a box of width 10 A⁰.

12. Consider an electron in a three-dimensional cubic box of side length L. The walls of the box are presumed to correspond to infinitely high potentials. Find an expression for the allowed energies of the electron in this box. (i) Express your result in terms of the lowest allowed energy, of a particle in a one-dimensional box. (ii) State the energies and describe the form of the wavefunctions for the 4 lowest energy states.

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- Write the radial equation of Hydrogen atom in spherical polar co-ordinates and derive an expression for energy eigen values.
- 14. Discuss quantum tunnelling. An electron wave of energy 0.5 eV is incident on an infinitely thick potential barrier of height 1 eV. Is the electron more likely to be found (a) within the first 1 Ångstrom of the barrier, or (b) somewhere further into the barrier?
- Write down the Schrödinger equation for harmonic oscillator. Derive an expression for energy eigen values.
- 16. Consider Schrödinger's time-dependent equation for an electron, with a potential that is uniform and constant at a value V_0 , with a solution of the form $\exp\left[(ikz \omega t)\right]$. Deduce the relationship giving k in terms of ω and V_0 , and deduce under what conditions there is a solution for real k.

 $(5 \times 4 = 20 \text{ marks})$

Section C

Answer any four questions 6 marks each.

- 17. Explain the concept of wave packet? What is mean by wave velocity and group velocity? An electron eigen energy is given as $E = \frac{\hbar^2 k^2}{2b}$, k is the wave vector in z direction and b is a positive constant. If a wave packet created with wave vectors with in small range of k, determine whether the wave is moving in positive or negative direction.
- 18. Write down the Schrödinger equation for particle confined in a one dimensional infinite potential well of width L. Derive the expressions for eigen states and eigen values. Find the expectation value for momentum in the ground state.
- 19. What is the position of maximum probability density of linear harmonic oscillator of potential energy $\frac{1}{2}Kx^2$ in its ground state? What is the value of maximum probability density.

20. Apply the variation function $\varphi = e^{-cr}$ to the hydrogen atom; choose the parameter c to minimize the variational integral.

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- 21. Explain, how Hatree-Fock self-consistent field method can be used to solve Hydrogen molecule problem?
- 22. If the kinetic energy of an electron known to be about 1eV, must be measured to with in 0.0001 eV, to what accuracy can its position be measured simultaneously.
- 23. Explain time dependent perturbation theory.