Centre of Material Sciences
University of Allahabad

M. Sc. (Materials Science) Syllabus
(Curtailed for session 2020-21)

Semester - I

MSE - 501 –Quantum Mechanics

Application of Schrodinger wave equation: Schrodinger wave equation, Continuity equation and probabilistic interpretation, Uncertainty principle, Concept of Eigen value.Effect of the confinement of the particle in a box, Potential step, Potential barrier,Tunnel effect, Discussion on bound states, Degeneracy of states.
Hermite and Laguerre polynomials, Linear harmonic oscillator.
Angular Momentum: Rotation operators, Angular momentum operators, Commutationrules, Eigenvalues of angular momentum operator, Matrix representations, Addition oftwo angular momenta.
Scattering Theory: Centre of mass and Laboratory systems, Scattering amplitude andcross sections, Scattering of a wave packet, Born approximation, Validity.

Reference Books:

1. L. Schiff, Quantum Mechanics, McGraw-Hill Book Co., New York, 1996.
2. K. .Ziock, Basic Quantum Mechanics, John Wiley & Sons, New York, 1969.
3. Sathyaprakash, Quantum Mechanics, KedarnathRamnath& Co., Meerut, 1994.
4. Chatwal and Anand, Quantum Mechanics, Himalaya Publishing House, New Delhi, 1993.
5. P.M.Mathews and K.Venkatesan, A Text book of Quantum mechanics, Tata McGraw-Hill, New Delhi, 1977.
6. J.J.Sakurai, Modern Quantum Mechanics, Addison Wesley, Tokyo, 1994.
7. E.Merzbacher, Quantum Mechanics, Wiley International, New York, 1970.
8. A.K.Chandra, Introductory Quantum Chemistry, Tata McGraw-Hill, New Delhi, 1983.

MSE - 502 – Crystallography and Diffraction Techniques

Symmetry elements and Symmetry operations, Classification of molecules based on symmetry, Point group and space group
Crystal structure- Primitive lattice cell, Fundamental type of lattices, Crystal systems, Close packing in crystals, Lattice planes, Miller indices of planes and directions, Bragg's Law, Reciprocal lattice, Ewald sphere, Atomic scattering factor, Structure factor,
X-ray Diffraction- Powder, Laue and Rotation methods.

Reference Books:

1. J.A.K .Tareen, & T.R.N. Kutty, , A basic course in crystallography, University Press, 2001.
2. O N Srivastava A R Verma, Crystallography Applied To Solid State Physics 2e, New Age International (p) Limited, 2008
3. A. R West, Solid State Chemistry & Its Applications, John Wiley & Sons Inc (sea) Pte Ltd

4. G.H. Stout, L. Jensen, X-ray structure determination, A Practical Guide, Macmillan, Newyork,1989.
5. B.D Cullilty,. Elements of X-ray diffraction, Addison-Wesley, Reading, MA,1978.
6. R.A. Young, The Rietveld method, IUCR-Oxford University Press, 1995.
7. L.V. Azaroff, Elements of X-ray crystallography, McGraw-Hill,NY,1968.

MSE - 503 – Materials: Introduction, Synthesis and Processing

Introduction to materials science, Types of materials-Metals and alloy, Ceramics, Composites and Nano-materials.

Diffusion: Laws of diffusion,Types of diffusion, Fick's law, Diffusion in ionic solids, Role of diffusion in solid state reactions and sintering.

Ceramic powder synthetic methods: Solid state reaction method, Sol-gel method, Hydrothermal, Combustion and Microwave synthesis.

Synthesis and stabilization of nanoparticles: Chemical reduction, Reactions in micelles, Emulsions and dendrimers, Photochemical and radiation chemical reduction, Sonochemical methods.

Synthetic techniques for carbon nanomaterials: Chemical vapor deposition (CVD), Laser ablation, Arc-discharge, Ball-milling, Thermal decomposition, High-pressure CO disproportionation process (HiP_{CO} Process).

Thin film preparation methods: Physical vapor deposition, Sol-gel film and Langmuir-Blodgett films.

Reference Books:

1. V. Raghavan, Materials Science And Engineering: A First Course, Prentice-hall India Pvt. Ltd.
2. W. D. Callister, Materials Science And Engineering: An Introduction, 7th Ed, Wiley India
3. W.O. Gonzalez -. Vinas, Hector L. Mancini, An Introduction To Materials Science, Princeton University Press, 2004
4. C.N.R. Rao, P. John Thomas, G.U. Kulkarni, Nanocrystals:: Synthesis, Properties and Applications, Springer, 2011

MSE - 504 – Data Analysis and Computational Techniques

System of Equations: Roots of equations, Methods of bisection and false position, Newton-Raphson method, Solution of simultaneous linear algebraic equations, Gauss elimination, Gauss Jordan methods, Matrix inversion and LU decomposition methods, Eigenvalues of matrices, Power method.

Interpolation and Curve Fitting and Error Analysis: Newton's forward and backward interpolation formulae, Lagrange's method, Lagrange's inverse interpolation, Curve fitting, principle of least squares.

Numerical Differentiation and Integration: Newton's forward and backward difference formulae, Numerical integration, Trapezoidal rule and Simpson's rule, Numerical solution of ordinary differential equations, Taylor series, Euler's method, Improved and modified methods, Runge-Kutta methods.

Probability, Statistics and Error Analysis: Probability concepts, Binomial, Poisson, Exponential and normal distribution, Tests of hypothesis (small and large samples) based on student's 't' and chi-square distribution, Testing goodness of fit, Accuracy and precision, Significant figures.

Reference Books:

1. M.K.Venkatraman, "Numerical Methods in Science and Engineering", National Publishing Company, Madras, 1996
2. S.S.Sastry, "Introductory Methods of Numerical Analysis", Prentice Hall of India, New Delhi, 1992.
3. E.Walpole, R.M Myers, S.L.Myers and K.Ye, "Probability & Statistics for Engineers and Scientists", Pearson Education, 2002.
4. B.S.Grewal, Numerical Methods in Engineering and Science, Khanna Publishers, New Delhi, 2006.

MSE -531: Material Science Lab – I

Semester – II

MSE – 505- Group Theory and Spectroscopy:
Definition of group, representation of group and cyclic group, the great orthogonality theorem, reducible and irreducible representation, transformation of coordinate matrices, matrix representation of symmetry operation, character table, direct product.
Electronic structures of free atoms and ions, splitting of levels and terms in chemical environment, construction of energy level diagram, relation of energy level diagrams to spectral properties, selection rules and polarization in electronic transitions, vibronic transitions. Classical description of molecular vibrations, symmetry of normal vibrations, determination of symmetries of the normal modes, use of internal coordinates to normal modes, selection rules for fundamental vibrational (infrared and Raman) transitions with illustrative examples, mutual exclusion principle, Fermi resonance.

Reference Books:

1. J. L. Mchale, Molecular Spectroscopy, Dorling Kindersley (india) Pvt Ltd, 2008
2. Banwell, Fundamentals Of Molecular Spectroscopy, Tata Magraw Hill, 2008
3. H.Friebolin, Basic One- and Two-Dimensional NMR Spectroscopy, Wiley-VCH Verlag GMBH Co., 2011
4. T. E. Cranshaw, B. W. Dale, G. O. Longworth and C. E. Johnson,Mössbauer Spectroscopy and its Applications, Cambridge University Press, 1986
5. R. L. Carter, Molecular Symmetry and Group Theory, Wiley, 1997

MSE - 506 –Physics of Solid State Materials
Bonding and Lattice Dynamics: Types of bonding, Lattice energy, Madelung constants, Vibration of crystal with monoatomic and diatomic lattices, Quantization of elastic waves, Phonon momentum, Inelastic scattering by phonons, Harmonic approximation, Phonon frequencies and density of states, Einstein and Debye theories of lattice energies and phonon dispersion curves, Anharmonic effects, Thermal expansion, Thermal conductivity.
Free Electron Theory: Energy level in one dimension, Free electron gas in three dimension, Heat Capacity and electron gas, Experimental heat capacity of metals, Electrical conductivity and Ohms law, Experimental electrical resistively of metals, Motion of electron in magnetic field, Hall effect.
Periodic Potential and Energy Band: Nearly free electron model, Bloch function, Kronig Penny model, Formation of energy bands and gaps, Brillouin zones and boundaries, Effective mass of electrons and concept of holes, Wave equation of electron in Periodic potential, Number of orbital in a band, Classifications into insulators, conductors, semiconductors and semimetals.

Reference Books:

1. W. Neil Ashcroft, Solid State Physics, Cengage Learning (Thompson), 2008
2. C.Kittel, Introduction to solid state physics, Wiley 7th edition, 1996.
3. V. Keer, Principles of solid state physics, Wiley - Eastern, 1993.
4. J. Patterson, Bernard Bailey, Solid-State Physics: Introduction to the Theory, Springer; 2nd ed. Edition, 2011

MSE - 507-Characterization Techniques for Materials:
X-ray photoelectron spectroscopy (XPS), Scanning electron microscopy (SEM), Auger electron spectroscopy (AES), Transmission electron microscopy (TEM), Atomic force microscopy (AFM), Thermo gravimetry analysis (TGA), Differential thermal analysis (DTA), differential scanning calorimetry (DSC),Raman spectroscopy, UV/Vis/Nir and FTIR spectroscopy.

Reference Books:

1. P. K. Ghosh, Introduction to Photoelectron Spectroscopy (Chemical Analysis Vol. 67) Wiley Interscience, 1983
2. J. F. Watts, John Wolstenholme, An Introduction to Surface Analysis by XPS and AES, John Wiley & Sons Ltd., 2003
3. R. Egerton,Physical Principles Of Electron Microscopy: An Introduction To TEM, SEM, And AEM; Springer, 2005
4. D. B. Williams, C. Barry Carter, Transmission Electron Microscopy: A Textbook For Materials Science, Springer, 2009
5. P. R. Buseck, John M. Cowley, Leroy Eyring, High-resolution Transmission Electron Microscopy: And Associated Techniques, Oxford University Press, 1989
6. GüntherHöhne, Wolfgang F. Hemminger and H.-J. Flammersheim, Differential Scanning Calorimetry, 2nd ed., Springer 2003
7. Ewen Smith , Geoffrey Dent, **Modern Raman Spectroscopy: A Practical Approach,** 1st edition, Wiley 2005
8. Edgar Bright Wilson, J. C. Decius and Paul C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Publications 1980.

MSE – 508-Thermodynamics and Phase Transformations

Statistical Thermodynamics: Helmholtz and Gibbs free energies, Thermodynamic reactions, Euler equation, Maxwell's relations and applications, Gibbs phase rule, Phase equilibrium (single and multicomponent systems, Clausius-Clayperon equation, Law of mass action, First order phase transition in single component systems.

Microcanonical, Canonical and grand canonical ensembles, Maxwell, Boltzmann, Bose- Einstein and Fermi-Dirac statistics, Comparison of MB, BE and FD statistics.

Phase Transformations: Classification, Nucleation, Growth models, Landau theory, Types of phase changes, Diffusion in solids, Nucleation and growth, Solidification, Pearlitic transformations, Martensitic transitions, Phase rule, Interpretation of phase diagrams, Binary and ternary Phase diagrams, Microstructural development, Heat treatment and kinetics of phase transformations, Phase transitions, Invariant reactions, Eutectic, Eutectoid, Peritectic and pertectoid reactions, Free energy composition curves, Iron-iron carbide phase diagram.

Reference Books:

1. M.C.Gupta, Statistical Thermodynamics, Wiley Eastern Ltd., New Delhi, 1993
2. B.K.Agarwal and Melvin Eisner, Statistical Mechanics by, Wiley Eastern Ltd., New Delhi –1988
3. H.B.Callen Thermodynamics by , John Wiley and Sons, New York 1960
4. Y.V.C. Rao, Introduction To Thermodynamics, An (second Edition), Universities Press, 2003
5. V. Raghavan, Solid State Phase Transformations, Prentice-hall of India Pvt Ltd, 2008

MSE -532: Material Science Lab – II