Syllabus for MRFT

MATERIAL SCIENCE

UNIT-I: Mathematics for Material Science

Linear Algebra (Algebra of real matrices: Determinant, inverse and rank of a matrix; System of linear equations (conditions for unique solution, no solution and infinite number of solutions); Eigen values and eigenvectors of matrices; Properties of Eigen values and eigenvectors of symmetric matrices, diagonalization of matrices; Cayley-Hamilton Theorem),

Calculus and Vector Calculus (Functions of single variable: Limit, indeterminate forms and L'Hospital's rule; Continuity and differentiability; Mean value theorems; Maxima and minima; Taylor's theorem; Fundamental theorem and mean value theorem of integral calculus; Evaluation of definite and improper integrals; Applications of definite integrals to evaluate areas and volumes (rotation of a curve about an axis). Functions of two variables: Limit, continuity and partial derivatives; Directional derivative; Total derivative; Maxima, minima and saddle points; Method of Lagrange multipliers; Double integrals and their applications. Sequences and series: Convergence of sequences and series; Tests of convergence of series with nonnegative terms (ratio, root and integral tests); Power series; Taylor's series; Fourier Series of functions of period 2π, Gradient, divergence and curl; Line integrals and Green's theorem)

Complex variables (Complex numbers, Argand plane and polar representation of complex numbers; De Moivre’s theorem; Analytic functions; Cauchy-Riemann equations)

Ordinary Differential Equations & Partial Differential Equations: First order equations (linear and nonlinear); Second order linear differential equations with constant coefficients; Cauchy-Euler equation; Second order linear differential equations with variable coefficients; Wronskian; Method of variation of parameters; Eigen value problem for second order equations with constant coefficients; Power series solutions for ordinary points. Classification of second order linear partial differential equations; Method of separation of variables: One dimensional heat equation and two dimensional Laplace equations. Probability and Statistics Axioms of probability; Conditional probability; Bayes' Theorem; Mean, variance and standard deviation of random variables; Binomial, Poisson and Normal distributions; Correlation and linear regression.   rule; Numerical solutions of first order differential equations by explicit Euler's method)

UNIT-II: Quantum Mechanics

Planck's hypothesis, wave-particle duality, introduction to quantum theory, de-Broglie concept of matter waves, Heisenberg's uncertainty principle, Schrodinger's time independent and time dependent wave equations, application of Schrodinger wave equation for physical significance and properties of the wave functionψ, application of Schrodinger wave equation for particle in one, two, and three dimensional well – Eigen wave functions and energy Eigen values of the particle

Operator and Operator algebra, eigen function and eigen values, expectation values, Dirac brakets, Completeness and closure property.

Some bound state problems: Linear harmonic oscillator, spherically symmetric potential, the hydrogen atom, particle in spherical cavity, Matrix representation of Angular momentum operator, Pauli matrices, Addition of angular momentum, Clebsch-Gordan coefficients.

Approximation methods for bound states: Stationary perturbation theory-non-degenerate and degenerate cases, Stark effect, LS and J-J coupling, Spectroscopic notation strong and weak field Zeeman effect.

Time dependent perturbation, transition probability, semi-classical treatment of radiation. Intensity ration of transition in alkali atoms.

UNIT III: Introduction to Material Science

The Structure of Crystalline Solids, Fundamental Concepts of Unit Cells, Metallic, Crystal Structures Density Computations, Polymorphism and Allotropy, Crystal Systems, Point Coordinates, Crystallographic Directions, Crystallographic Planes, Linear and Planar Densities, Close-Packed Crystal Structures, Crystalline and Noncrystalline Materials, Single Crystals, Polycrystalline Materials.

Defects in crystalline materials: 0-D, 1-D, and 2-D defects; vacancies, interstitials, configurational entropy, Frenkel and Schottky defects; dislocations; grain boundaries, twins, stacking faults; surfaces and interfaces.

Reciprocal lattice of cubic system, Ewald's construction, Laue, Rotation, powder method of X-ray diffraction, interpretation of diffraction pattern, cell parameter determination.

Solid solutions in metals, ceramic, and alloys - Phase diagrams - Gibbs phase rule – Single component systems – Eutectic phase diagram – lever rule - Study of properties of phase diagrams - Phase transformation - Nucleation kinetics and growth.

UNIT-IV: Thermodynamics

Continuum and macroscopic approach; thermodynamic systems (closed and open); thermodynamic properties and equilibrium; state of a system, state postulate for simple compressible substances, state diagrams, paths and processes on state diagrams; concepts of heat and work, different modes of work; zeroth law of thermodynamics; concept of temperature. Concept of energy and various forms of energy; internal energy, enthalpy; specific heats; first law applied to elementary processes, closed systems and control volumes, steady and unsteady flow analysis.

Limitations of the first law of thermodynamics, concepts of heat engines and heat pumps/refrigerators, Kelvin-Planck and Clausius statements and their equivalence; reversible and irreversible processes; Carnot cycle and Carnot principles/theorems; thermodynamic temperature scale; Clausius inequality and concept of entropy; microscopic interpretation of entropy, the principle of increase of entropy, T-s diagrams; second law analysis of control volume; availability and irreversibility; third law of thermodynamics.

Thermodynamic properties of pure substances in solid, liquid and vapor phases; P-V-T behaviour of simple compressible substances, phase rule, thermodynamic property tables and charts, ideal and real gases, ideal gas equation of state and van der Waals equation of state; law of corresponding states, compressibility factor and generalized compressibility chart.

T-ds relations, Helmholtz and Gibbs functions, Gibbs relations, Maxwell relations, Joule-Thomson coefficient, coefficient of volume expansion, adiabatic and isothermal compressibilities, Clapeyron and Clapeyron-Clausius equations.

Carnot vapor cycle, ideal Rankine cycle, Rankine reheat cycle, air-standard Otto cycle, air-standard Diesel cycle, air-standard Brayton cycle, vapor-compression refrigeration cycle. Ideal Gas Mixtures Dalton's and Amagat's laws, properties of ideal gas mixtures, air-water vapor mixtures and simple thermodynamic processes involving them; specific and relative humidities, dew point and wet bulb temperature, adiabatic saturation temperature, psychrometric chart.

UNIT-V : Processing, Properties, and Application of material

Mechanical properties of metals, ceramics, polymers and composites at room temperature; stress-strain response (elastic, inelastic and plastic deformation).

Electronic properties: free electron theory, Fermi energy, density of states, elements of band theory, semiconductors, Hall effect, dielectric behaviour, piezo- and ferro-electric behaviour. Magnetic properties: Origin of magnetism in materials, para-, dia-, ferro- and ferri-magnetism.

Thermal properties: Specific heat, heat conduction, thermal diffusivity, thermal expansion, and thermoelectricity. Optical properties: Refractive index, absorption and transmission of electromagnetic radiation. Examples of materials exhibiting the above properties, and their typical/common applications.

X-ray diffraction; spectroscopic techniques such as UV-Vis, IR and Raman; optical microscopy, electron microscopy, composition analysis in electron microscopes. Tensile test, hardness measurement. Electrical conductivity, carrier mobility and concentrations. Thermal analysis techniques: thermogravimetry and calorimetry.

Heat treatment of ferrous and aluminium alloys; preparation of ceramic powders, sintering; thin film deposition: evaporation and sputtering techniques, and chemical

UNIT VI : Tools and Technique-I

Thermal Analysis: Introduction, Thermogravimetric analysis (TGA)-instrumentation-determination of weight loss and decomposition products-application, differential thermal analysis (DTA)-cooling instrumentation- curves-application, differential Scanning calorimetry (DSC)-instrumentation-specific heat measurement-thermo-mechanical parameters.

Electrical Property Evaluation: Introduction, Two probe and Four Probe method-Vander-Pauw method, Hall probe method and measurement- Scattering mechanism, I-V characteristics, Electrical transport and Magento-transport measurement.

X-ray Diffraction: Introduction, Production, discovery & applications of cathode rays & x-rays, Properties of x-rays. Emission, absorption, detection & safety precautions. Crystal lattices and their symmetry. Space groups. The reciprocal lattice and stereographic projection. Diffraction, constructive & destructive interference, Bragg's Law. Experimental methods for single & polycrystalline samples, effect of crystallite size (thickness) per Scherrer's eqn. Scattering of x-rays by electrons, atoms and unit cells. Structure factor for various crystals, other factors affecting intensity of diffracted beams, application to powder diffraction. Use of CaRIne or Powder Cell software. Use of intensity ratios to determine volume fractions of phases present, Indexing of diffraction patterns and determination of crystal structure. Precise determination of lattice parameters. Determination of phase diagrams. Ordered and disordered alloys. Measurement of micro-strain and residual macro-stress. Separation of line broadening due to micro-strain and crystallite size. Comparison of x-ray, electron & neutron diffraction methods; scattering factors for electrons; Ewald construction in reciprocal space

Optical microscopy : Introduction, Optical microscopy techniques, Bright field and Dark Field Optical microscopy, Dispersion Staining Microscopy, Phase contrast microscopy, differential interference contrast microscopy, confocal microscopy. vapour deposition, thin film growth phenomena.

UNIT-VII: Tools and technique-II

Principle, instrumentation, measurement and analysis of High Resolution **Scanning Electron Microscopy** (SEM), High Resolution **Transmission Electron Microscopy** (TEM), **UV-Visible spectroscopy, IR spectroscopy Raman spectroscopy**

UNIT-VIII: Mechanical Behaviour of material

Definition of stress, strain, transformation of coordinate systems, tensor notations, relationship between stress and strain in elastic materials, concept of principal stress and principal strain, stress invariants, modulus, Hook's law and understanding of stiffness and compliance tensors, elastic anisotropy.

Yield criteria, equivalent stress and plastic strain, Theoretical shear of perfect crystal, Mohs circle, concept of dislocations and dislocation theory, edge and screw dislocations, dislocation interactions, kink and jog, sessile and glissiles, partial dislocations, dissociation of dislocations, Thomson tetrahedral, Lomer-Cottress barriers.

Strengthening mechanisms, work hardening, solid solution strengthening, grain boundary strengthening, particle hardening, polymer elasticity and viscoelasticity, types of reinforcements and their influence, types of composites, high temperature degradation, creep and stress rupture, deformation mechanism maps, superplasticity and hot working.

Hardness, types of hardness measurements, comparison among hardness methods and scales, nanoindentation, compression testing, comparison between tension and compression studies of materials, shear testing, shear modulus, torsion and twist.

Fatigue of materials, S-N curves, life data presentation, influence of stress, linear elastic fracture mechanics in fatigue, crack growth studies, Paris law, metallurgical aspects of fatigue failures, concepts of remedial measures, creep-fatigue interaction, theoretical strength, Griffith equation, Brittle fracture, ductile fracture, fracture maps.

UNIT-IX: Polymer Engineering and Technology

Monomers, functionality, degree of polymerizations, classification of polymers, glass transition, melting transition, criteria for rubberiness, polymerization methods: addition and condensation; their kinetics, metallocene polymers and other newer methods of polymerization, copolymerization, monomer reactivity ratios and its significance, kinetics, different copolymers, random, alternating, azeotropic copolymerization, block and graft copolymers, techniques for polymerization-bulk, solution, suspension, emulsion. Concept of intermolecular order (morphology) – amorphous, crystalline, orientation states. Factor affecting crystallinity. Crystalline transition. Effect of morphology on polymer properties. Solubility and swelling, Concept of molecular weight distribution and its significance, concept of average molecular weight, determination of number average, weight average, viscosity average and Z-average molecular weights, polymer crystallinity, analysis of polymers using IR, XRD, thermal (DSC, DMTA, TGA), microscopic (optical and electronic) techniques, Molecular wt. distribution: Broad and Narrow, GPC, mooney viscosity.

Commodity and general purpose thermoplastics: PE, PP, PS, PVC, Polyesters, Acrylic, PU polymers. Engineering Plastics: Nylon, PC, PBT, PSU, PPO, ABS, Fluoropolymers Thermosetting polymers: Polyurethane, PF, MF, UF, Epoxy, Unsaturated polyester, Alkyds. Natural and synthetic rubbers: Recovery of NR hydrocarbon from latex; SBR, Nitrile, CR, CSM, EPDM, IIR, BR, Silicone, TPE, Speciality plastics: PEK, PEEK, PPS, PSU, PES etc. Biopolymers such as PLA, PHA/PHB.

Difference between blends and composites, their significance, choice of polymers for blending, blend miscibility-miscible and immiscible blends, thermodynamics, phase morphology, polymer alloys, polymer eutectics, plastic-plastic, rubber-plastic and rubber-rubber blends, FRP, particulate, long and short fibre reinforced composites. Polymer reinforcement, reinforcing fibres – natural and synthetic, base polymer for reinforcement (unsaturated polyester), ingredients / recipes for reinforced polymer composite.

Polymer compounding-need and significance, different compounding ingredients for rubber and plastics (Antioxidants, Light stabilizers, UV stabilizers, Lubricants, Processing aids, Impact modifiers, Flame retardant, antistatic agents. PVC stabilizers and Plasticizers) and their function, use of carbon black, polymer mixing equipments, cross-linking and vulcanization, vulcanization kinetics.

Compression molding, transfer molding, injection molding, blow molding, reaction injection molding, filament winding, SMC, BMC, DMC, extrusion, pultrusion, calendaring, rotational molding, thermoforming, powder coating, rubber processing in two-roll mill, internal mixer, Twin screw extruder.

UNIT-X: Physical Metallurgy

Diffusion, energetic of solidification Nucleation and growth-dealing homogeneous and heterogeneous nucleations and growth of solids, dendritic growth in pure metals, constitutional super cooling and dendritic growth in alloys.

Phase diagrams – solid solution –types, Hume –Rothery rule. Phase diagrams – Binary- types – Lever rule. Solidification of different types of solid solutions – Iron-

Carbon diagram – Effect of alloying element on Iron-carbon diagram. Ternary phase diagrams- Understanding of isotherms and isopleths.

Heat treatment of ferrous alloys; Annealing, Normalising, TTT and CCT diagrams, Hardening – hardenability measurements, tempering. Thermo mechanical treatments. Heat treatment furnaces – atmospheres – quenching media – case hardening techniques. Basic concept of dislocations their types and its interactions. Dislocations and strengthening mechanisms strengthening by grain-size reduction, solid solution strengthening, strain hardening, dispersion hardening and other recent modes of hardening.

UNIT XI: Nano Science and technology

Nanoscale systems: Hetero-structures and band offset, Length, energy, and time scales-Quantum confinement of electrons in semiconductor nanostructures: Quantum confinement in 3D, 2D, 1D, and Zero dimensional structures-Size effect and properties of nanostructures-Landauer-Bvttiker formalism for conduction in confined geometries, Top down and bottom-up approach.

Basic properties of Nanoparticles: Size effect and properties of nanoparticles-particle size-particle shape-particle density-melting point, surface tension, wettability-specific surface area and pore size-Reason for change in optical, electrical, and mechanical properties-advantages.

Synthesis of Nanostructure materials:

Gas phase condensation-Vacuum deposition- Physical vapour deposition (PVD)-Chemical Vapor deposition (CVD)-Laser ablation-Sol-Gel-Ball milling-Electro deposition-Spray Pyrolysis-Plasma based synthesis process of nano wires by-solvohermal-template method (qualitative)-nanofibers-electrospinning techniques-hydrothermal synthesis.

Quantum Dots: Excitons and excitonic Bhor radius-difference between nanoparticles and quantum dots-preparation through colloidal methods-Epitaxial method-MOCVD and MBE growth of Quantum dots-Current-Voltage characteristics-magentotunneling measurements-Spectroscopy of Quantum dots: Absorption and Emission Spectra, Photoluminescence Spectroscopy-Optical Spectroscopy-Linear and non-linear optical spectroscopy.

Nanotechnology Applications: Application of nanoparticles, quantum dots, nanotubes, and nano-wires for nanodevice fabrication-Single electron transistors, Colulomb blockade effects in ultrasmall metallic tunnelling junctions-nanoparticles based solar cells and quantum dots based white LEDs-CNT based transistors-principle of dip pen lithography.