

M. TECH – MATERIALS SCIENCE AND ENGINEERING

Center for Excellence in Advanced Materials and Green Technologies

The M.Tech. Materials Science and Engineering program is offered at Amrita Vishwa Vidyapeetham by the Center of Excellence in Advanced Materials and Green Technologies established in May 2013, based on a grant awarded by the Ministry of Human Resource Development (MHRD). The center has numerous ongoing research projects covering materials for fuels/energy, electricity, construction, and water.

The program is designed to produce graduates that can apply fundamental knowledge of mathematics, physics & chemistry of materials, and statistics, to model and solve problems related to design, synthesis, performance enhancement, and optimization of materials. Recognizing the multidisciplinary nature of the field, the teaching and project guidance will be accordingly delivered by highly qualified, world-class faculty from various departments including, chemical engineering, chemistry, physics, & aerospace engineering.

With a view towards developing both science and engineering skills, the program curriculum has been framed so as to incorporate and deliver on experimental, analytical, statistical, and computational tools & educational components of globally accepted standards in the materials discipline. The core courses include: Materials Science I & II, Materials Thermodynamics, Statistical Design of Experiments, Materials Characterization Techniques, Nanoscience and Nanotechnology, Materials Design, and Polymer Materials. While the labs cover important aspects of synthesis, testing, and characterization, the electives are structured in such a way as to offer opportunities for acquisition of specialized and advanced knowledge in sub-disciplines such as electronic materials, biomaterials, and materials for energy systems. Students have the opportunity to pursue their projects either in-house (research in the departments of chemical engineering, chemistry, physics, aerospace engineering, and the center for excellence in advanced materials & green technologies), or outside in reputed industrial or R&D institutions.

With a strong focus on developing research skills among the students, in frontier areas, the program includes educational components that would make the graduates suited to, and employable in, industrial, government R&D, and academic settings, spanning diverse areas such as electronics & communications, energy, chemicals, medicine, and transportation.

CURRICULUM

First Semester

Course Code	Type	Course	L T P	Cr
MA621	FC	Mathematical Foundations for Materials Science	3-0-0	3
MS602	FC	Materials Science I	4-0-0	4
MS603	FC	Materials Thermodynamics	3-1-0	4
MS611	SC	Materials Characterization Techniques	4-0-0	4
MS612	SC	Advanced Materials I	3-0-0	3
MS621	SC	Materials Synthesis Lab I	0-0-1	1
HU601	HU	Cultural Education*		P/F
			Credits	19

* Non Credit Course

Second Semester

Course Code	Type	Course	L T P	Cr
MS604	FC	Materials Science II	4-0-0	4
MS605	FC	Statistical Design of Experiments	3-0-0	3
MS613	SC	Materials Design	3-0-0	3
MS614	SC	Advanced Materials II	3-0-0	3
MS615	SC	Transport Processes in Materials Engineering	4-0-0	4
MS622	SC	Materials Synthesis Lab II	0-0-1	1
EN600	HU	Technical Writing**		P/F
			Credits	18

** Non Credit Course

Third Semester

Course Code	Type	Course	L T P	Cr
	E	Elective I	3-0-0	3
	E	Elective II	3-0-0	3
MS623	SC	Materials Performance Analysis Lab	0-0-1	1
MS799	P	Dissertation		8
			Credits	15

Fourth Semester

Course Code	Type	Course	L T P	Cr
MS799	P	Dissertation		14
			Credits	14

Total Credits 66

**List of Courses
Foundation Core**

Course Code	Course	L T P	Cr
MA621	Mathematical Foundations for Materials Science	3-0-0	3
MS602	Materials Science I	4-0-0	4
MS603	Materials Thermodynamics	3-1-0	4
MS604	Materials Science II	4-0-0	4
MS605	Statistical Design of Experiments	3-0-0	3

Subject Core

Course Code	Course	L T P	Cr
MS611	Materials Characterization Techniques	4-0-0	4
MS612	Advanced Materials I	3-0-0	3
MS613	Materials Design	3-0-0	3
MS614	Advanced Materials II	3-0-0	3
MS615	Transport Processes in Materials Engineering	4-0-0	4
MS621	Materials Synthesis Lab I	0-0-1	1
MS622	Materials Synthesis Lab II	0-0-1	1
MS623	Materials Performance Analysis Lab	0-0-1	1

List of Electives

Course Code	Course	L T P	Cr
MS701	Polymer Processing	3-0-0	3
MS702	Electrochemistry and Corrosion	3-0-0	3
MS703	Catalytic Chemistry	3-0-0	3
MS704	Carbon Nanomaterials	3-0-0	3
MS705	Interfacial Science and Engineering	3-0-0	3
MS706	Waste to Energy	3-0-0	3
MS707	Solar Energy	3-0-0	3
MS708	Energy Storage Technologies	3-0-0	3
MS709	Molecular Simulation	3-0-0	3
MS710	Design for Sustainable Development	3-0-0	3

Mathematical representation of problems – Vector & Matrix Algebra: Vector spaces, Linear independence, Basis of a space, Basics of Matrix Algebra, Eigenvalues & Eigenvectors; Basics of Numerical Analysis: Error analysis, Computations of errors of algorithms, Stiffness of algorithms, Interpolation (Lagrange approximation), Polynomial approximation and curve fitting (Newton method), Numerical differentiation and integration (Trapezoidal and Simpson's rules); Linear Algebraic Equations: $Ax = b$ (Gauss-Jordan and Gauss-Siedel), Numerical techniques for ODEs (Euler method, Runge-Kutta method); Partial Differential Equations: Numerical techniques for parabolic and elliptic equations – finite differences

TEXT BOOKS/REFERENCES:

1. A. K. Ray and S. K. Gupta, *Mathematical Methods in Chemical and Environmental Engineering*, Second Edition, Cengage Learning Asia, 2003.
2. E. Kreyszig, *Advanced Engineering Mathematics*, Ninth Edition, John Wiley & Sons, 2006.
3. V. G. Jenson and G. V. Jeffreys, *Mathematical Methods in Chemical Engineering*, Second Edition, Academic Press, San Diego, 1978.
4. M. K. Jain, S. R. K. Iyengar and R. K. Jain, *Numerical Methods for Scientific and Engineering Computation*, Fifth Edition, New Age International, New Delhi, 2008.
5. P. Ahuja, *Introduction to Numerical Methods in Chemical Engineering*, Prentice Hall India, 2010

Materials Structure and Mechanical Behaviour Of Materials: crystal systems- space lattice- miller indices of atomic planes and directions- small problems in crystallography- crystal defects- point, line and surface defects- elastic deformation- characteristics of elastic deformation- atomic mechanism of elastic deformation- inelastic deformation- strain – time curves plastic deformation- mechanism of plastic deformation- slip and twinning- Strengthening mechanisms: Work hardening- grain boundary hardening, dispersion hardening, Recovery and Recrystallization; Mechanical testing: Tensile -Impact- Hardness Creep: Primary, secondary and tertiary creep- Fatigue: S-N curves- endurance limit Fracture: Ideal fracture stress- brittle fracture- Griffith's theory- cup and cone type fracture, Schmidt's law- critical resolved shear stress Phase diagrams: solid solution- inter-metallic compound, cooling curves, phase rule - isomorphous- eutectic- peritectic and eutectoid reactions with examples non-equilibrium cooling--Iron- Iron carbide phase diagram. Austenite transformation-TTT and CCT diagrams.. Engineering materials: steels and cast irons- properties and applications- effect of alloying elements on steel

TEXT BOOKS/REFERENCES:

1. W.D. Callister, *Materials Science and Engineering*, Sixth Edition, John Wiley & Sons, 2003.
2. W.F. Smith, J. Hashemi and R. Prakash, *Materials Science and Engineering*, Fourth Edition, Tata Mc Graw Hill, 2008.
3. S.H. Avner, *Introduction to Physical Metallurgy*, Second Edition, McGraw Hill, 1997.
4. V. Raghavan, *Materials Science and Engineering: A First Course*, Fifth Edition, Prentice Hall India, 2004.

Entropy – Statistical Meaning; Combined First and Second Laws; Physical Meaning of Entropy, Pressure, and Chemical Potential; Postulational Approach to Thermodynamics: Criteria for Thermodynamic Equilibrium, Euler and Gibbs-Duhem Equations, Phase Rule, Thermodynamic

Potentials, and Criteria for Stability; Solid Equilibria; Mixtures and Solutions: Raoult's and Henry's Laws; Gibbs Free Energy of Solution; Activity Coefficients and Models; Regular Solutions, Criteria for Phase Stability; Phase Diagrams; Reactions involving Pure Condensed Phases - Ellingham Diagrams, Effects of Phase Transformations; Phase Diagrams of Binary Systems - Isomorphous, Eutectic, and Peritectic Systems; Disorder-to-order transformations, ordered alloys, thermodynamics of point defects, surfaces, and interfaces, Glass science; First-order and other transitions; Amorphous and Glassy materials; Thermodynamics of Nucleation; Stability

TEXT BOOKS/REFERENCES:

1. D. R. Gaskell, *Introduction to the Thermodynamics of Materials*, Fifth Edition, Taylor & Francis, New York, 2008
2. A. Ghosh, *Textbook of Materials and Metallurgical Thermodynamics*, Prentice Hall India, 2002.
3. Y. A. Cengel and M. A. Boles, *Thermodynamics: An Engineering Approach*, Seventh Edition, Tata McGraw Hill, 2011.
4. Y.V.C. Rao, *Chemical Engineering Thermodynamics*, Universities Press, New Delhi, 1997.
5. J. P. O'Connell and J. M. Haile, *Thermodynamics: Fundamentals for Applications*, Cambridge University Press, 2005.

MS604

MATERIALS SCIENCE II

4-0-0-4

Electrical conduction in solids – metals, semiconductors, ionic solids; Drude model, Factors affecting resistivity, thin film conduction; Basic Quantum Physics - atomic structure, Band theory and occupation statistics in metals and nonmetals, molecular orbital theory. Thermal conduction, Hall Effect and Hall Devices; Working of Semiconductor Devices using band diagrams and their electrical characteristics: pn junctions, BJT, MOSFET. Use of band theory to explain optoelectronic properties of materials and optoelectronic devices: LEDs, Solar Cells, Lasers, pin diodes, photodiodes; Magnetic properties and Superconductivity: Magnetic moments and Magnetic Permeability, types of magnetism, saturation magnetization, magnetic domains, soft and hard magnetic materials, superconductivity and its origin, Giant Magneto Resistance, Josephson effect, Energy band diagrams and Magnetism, Applications of magnetic materials - Magnetic recording materials; Optical Properties of Materials: Reflection, Refraction, Dispersion, Refractive Index, Snells Law, Light Absorption and Emission, Light Scattering, Luminescence, Polarization, Anisotropy, Birefringence; Dielectric Properties of Materials: Polarization and Permittivity, Mechanisms of polarization, dielectric properties-dielectric constant, dielectric loss, dielectric strength and breakdown, Piezoelectricity, Ferroelectricity, and Pyroelectricity, Dielectric Materials; Ceramic Materials: Silicate Ceramics, Carbon, Imperfections in Ceramics, Diffusion in Ionic Materials, Ceramic Phase Diagrams, Mechanical Properties, Types and Applications of Ceramics - Glass, Clay, Refractories, Abrasives, Cements; Fabrication and Processing of Ceramics

TEXT BOOKS/REFERENCES:

1. S. O. Kasap, *Principles of Electronic Materials and Devices*, Third Edition, Tata McGraw Hill, 2006.
2. W. D. Callister, Jr., *Materials Science and Engineering*, Sixth Edition, Wiley India, 2006.
3. D. Jiles, *Introduction to the Electronic Properties of Materials*, Chapman & Hall. 1994.

MS605

STATISTICAL DESIGN OF EXPERIMENTS

3-0-0-3

PLANNING: Framing objectives & hypothesis statements, identifying metrics, and creating experimental plan; Introduction to the role of experimental design; basic statistical concepts; sampling and sampling distributions; ANALYSIS: Statistical testing of hypotheses; Principle of

Least Squares and Linear Regression; DESIGN & ANALYSIS: 2^k Factorial and Fractional Factorial Designs (Plackett-Burman) – case studies and hands-on applications; Response Surface Methodology – central composite designs (structure, rotatability, orthogonality, types of CCD, analysis) & Box-Behnken designs – case studies and hands-on applications; Mixture designs – structure, analysis, and applications – case studies and hands-on applications

TEXT BOOKS/REFERENCES:

1. Montgomery and Douglas C., *Design and Analysis of Experiments*, Sixth Edition, John Wiley & Sons, Incorporated, New York, 2005.
2. Box, Hunter, and Hunter, *Statistics for Experiments*, Second edition. Wiley-Interscience, 2005.
3. Jiju Antony, *Design of Experiments for Engineers & Scientists*, Butterworth-Heinemann, 2003.
4. Zivorad Lazic, *Design of Experiments in Chemical Engineering*. Wiley-VCH, Weinheim, 2004.

MS611

MATERIALS CHARACTERIZATION TECHNIQUES

4-0-0-4

Imaging Microscopies and Image Analysis: Optical Microscopy, Scanning Electron Microscopy, Scanning Probe Microscopy, Image Analysis; X-ray and Electron Diffraction: Properties of X-Rays, Review of Crystal Systems and Miller Indices, Stereographic Projections, The Reciprocal Lattice, Laue Equations, Diffraction Methods, Scattered Intensities, Phase Identification, Small angle scattering; Spectroscopic Techniques: Energy Dispersive X-ray Spectroscopy, X-ray Photoelectron Spectroscopy; Thermal and Thermomechanical Techniques: Differential Scanning Calorimetry and Differential Thermal Analysis, Thermogravimetric Analysis, Dynamic Mechanical Analysis and Thermomechanical Analysis.

TEXT BOOKS/REFERENCES:

1. B.D. Cullity and S.R. Stock, *Elements of X-ray Diffraction*, Third Edition, Prentice Hall Inc., New Jersey, 2001.
2. K.P. Menard, *Dynamic Mechanical Analysis; A Practical Introduction*, Chapter 3, CRC Press, Boca Raton, 1999.

MS612

ADVANCED MATERIALS – I

3-0-0-3

Nanotechnology fundamentals - Atoms, molecules and phases, top down and bottom up approach, Self-Assembly and Self-Organization, - Micro/Nano Fabrication Techniques: optical and electron beam lithography, molecular beam epitaxy, nanoparticle synthesis, sol-gel process, carbon nanotubes, - Nanotechnology Applications: molecular electronics, quantum computing, MEMS, NEMS, nanoscale optoelectronics(QDs and photonic crystals) - Smart Materials: chitosan-based gels, magnetorheological fluids, electrorheological materials; Alloys: shape memory alloys, ferrous and nonferrous alloys, super alloys; Ceramics and Glasses: crystal structures, silicate ceramics, imperfections in ceramics, diffusion in ionic materials, stress-strain behavior, glasses, glass-ceramics, fabrication and processing of glasses and glass-ceramics, advanced ceramics, piezoelectric ceramics.

TEXT BOOKS/ REFERENCES:

1. M.D. Ventra, S. Evoy and J. R. Heflin, *Introduction to Nanoscale Science and Technology*, Kluwer Academic Publishers, 2004.
2. M. Schwartz, *Smart Materials*, CRC Press, 2008.
3. W.D. Callister and D.G. Rethwisch, *Materials Science and Engineering - An Introduction*, Eighth Edition, John Wiley & Sons, 2010.

4. C.I. Contescu and K. Putyera, *DEKKER Encyclopedia of Nanoscience and Nanotechnology*, Second Edition, CRC Press, 2009.

MS613

MATERIALS DESIGN

3-0-0-3

Structure-Property-Function Relationships in Materials, Process-Property Interaction, Material Property Charts, Design through Materials Synthesis and Modification, Materials and Process Information for Design; Translation, Screening and Ranking of Materials, Manipulating Properties - Density, Mechanical, Thermal, Electrical, Magnetic, Optical, Reactivity, and Catalytic Properties; Selected Case Studies: Ball Milling, Sintering, Layered Compounds, Chemical Vapor Deposition of Solids, Crystal Growth, Hydrothermal Synthesis, Sol-Gel Process, Polymer Synthesis, Gas-Phase Pyrolysis for Liquids, Catalytic Control of Fischer-Tropsch Process for Engine-Grade Fuels, Nanomaterials: Nanoparticles, Soft Templating, Self-Assembled Monolayers, Hard Templating - Nanocasting, Nanowires using Templated Deposition, Chemical Synthesis of Graphene, Graphene Functionalization for Applications, Biomaterials: Designing Bone Scaffolds, Contact Lenses

TEXT BOOKS/REFERENCES:

1. M. Ashby, H. Shercliff and D. Cebon, *Materials: Engineering, Science, Processing and Design*, Second Edition, Butterworth-Heinemann, 2010
2. U. Schubert and N. Hüsing, *Synthesis of Inorganic Materials*, Third Edition, Wiley-VCH, 2012
3. Selected recent papers published in reputed international journals discussing materials design - for case studies.

MS614

ADVANCED MATERIALS – II

3-0-0-3

Polymers: introduction, thermoplastics, thermosets-Polymerization mechanisms: Overview of condensation, addition mechanisms-Polymerisation methods: Overview of bulk, solution, suspension and emulsion-Polymer structure and effects on properties: Molecular weight and distribution, intermolecular and supra-molecular forces, crystallinity, orientation, tacticity, glass and melt transitions-Polymer additives: fillers, process aids, stabilizers, curatives, etc-Polymer processing methods: Overview of injection molding, extrusion, compression molding, blow-moulding, thermoforming, solution processing, spinning, etc.- Polymer properties: mechanical, viscoelasticity, solubility, optical, calorimetric-Processing of elastomers: compounding, vulcanization-Polymer composites: Types of composites-Reinforcement types, mechanisms and effects on composite properties-Processing of Composites: hand lay-up, spray up, continuous sheet manufacturing, pultrusion, resin transfer molding, filament winding, vacuum bag moulding - Properties of composites: Mechanical, Electrical, Thermal properties-Biological materials.

TEXT BOOKS/REFERENCES:

1. J.A. Brydson, *Plastics Materials*, Seventh Edition, Butterworth-Heinemann, Oxford, 1999.
2. M. Morton, *Rubber Technology*, Third Edition, Kluwer Academic Publishers, Dordrecht, Netherlands, 1999.
3. Chanda and S.K. Roy, *Plastics Technology Handbook*, CRC Press, Atlanta, 2007.
4. J.S. Dick, *Rubber Technology*, Hanser, Munich, 2001.
5. Jozef. Bicerano, *Prediction of Polymer Properties*, Second Edition, Marcel Dekker Inc. New York, 1995.

MS615	TRANSPORT PROCESSES IN MATERIALS ENGINEERING	4-0-0-4
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Basics of fluid flow, heat and mass transfer; Derivation of mass, momentum and energy transport equations through shell balance approach and their solutions; Laminar and turbulent flows – pumping requirements; Momentum transport in polymeric liquids and liquid metals; Momentum exchange between two immiscible fluid layers; Energy transport – heat conduction in solids, cooling of solids under natural and forced convection – temperature profile, heat conduction in melting solids – polymers and metals; Mass Transport – Binary diffusion vs. multi-component diffusion, Diffusion with reaction – Application to metal oxidation, Metal oxide complex formation at high temperature, Agglomeration in metal oxides and its control.

TEXT BOOKS/ REFERENCES:

1. D.R. Gaskell, *Introduction to Transport Phenomena in Materials Processing*, Wiley Publishing 1996.
2. R.B. Bird, W.E. Stewart and E.N. Lightfoot, *Transport Phenomena*, Second Edition, John Wiley & Sons Inc., 2002.
3. D.R. Poirier and G.H. Geiger, *Transport Phenomena in Materials Processing*, Wiley, 2010.
4. A.K. Mohanty, *Rate Processes in Metallurgy*, Third Edition, PHI Learning, 2009.

MS621	MATERIALS SYNTHESIS LAB – I	0-0-1-1
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Synthetic techniques for materials such as Ball Milling, Crystal Growth, Hydrothermal Synthesis, Sol-Gel Synthesis, Bulk Polymerization, Electrodeposition, Solution-phase Synthesis of Quantum Dots, Self-Assembled Monolayers, Hummers Method of Synthesis of Graphene Oxide, Casting of Thick Films, Spray Pyrolysis of Thin Films

MS622	MATERIALS SYNTHESIS LAB – II	0-0-1-1
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The lab will focus on characterization of materials with focus on interpretation. Techniques such as the ones listed below will be covered:

Structural and Composition Analysis:

Uv-visible Spectroscopy, Infrared Spectroscopy, Raman Spectroscopy, X-ray Photoelectron Spectroscopy, Atomic Absorption Spectroscopy, Mass Spectrometry

Separation and Size:

Thin Layer Chromatography, Gas Chromatography, Dynamic Light Scattering

Crystallinity:

X-ray Diffraction, Selected Area Electron Diffraction

Morphology:

Optical Microscopy, Scanning Electron Microscopy, Transmission Electron Microscopy, Atomic Force Microscopy

Surface Properties:

Contact Angle and Surface Tension, Surface Composition - FTIR-ATR

Thermal Properties:

Phase Diagram of a Binary Eutectic Alloy, Thermogravimetry analysis, Differential Scanning Calorimetry

MS623	MATERIALS PERFORMANCE ANALYSIS LAB	0-0-1-1
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Hardness Test, Impact Test, Tensile/Compression Test, Three-Point Bending Analysis, Uv-visible Spectroscopy - Transparency of a Thin Film, Photocatalytic Degradation of a Volatile Organic

Compound, Electrical Conductivity - Ac and Dc, Magnetoresistance, Charge-Discharge of Batteries, Charge-Discharge Behavior of Capacitor, Hall Effect Measurement, I-V Characteristics of a Solar Cell, Energy Storage in a Phase Change Material; dielectric constant, thermal conductivity and EMI measurement

EN600

TECHNICAL WRITING

P/F

Technical terms, Definitions - extended definitions; grammar checks: error detection, punctuation, spelling and number rules; tone and style; pre-writing techniques; online and offline library resources; citing references; plagiarism; graphical representation; documentation styles; instruction manuals; information brochures; research papers, proposals & reports (dissertation, project reports etc.), oral presentations.

TEXT BOOKS/REFERENCES

1. Hirsch, Herbert L., *Essential Communication Strategies for Scientists, Engineers and Technology Professionals*, Second Edition, Wiley-IEEE Press, New York, 2000
2. Paul V. Anderson, *Technical Communication: A Reader-Centred Approach*, Sixth Edition. Cengage Learning India Pvt. Ltd., New Delhi, 2010.
3. William Jr., E.B. White, and Roger Angell, *The Elements of Style*, Fourth Edition, Longman, 1999.

MS701

POLYMER PROCESSING

3-0-0-3

Physical Basis of Polymer Processing- Mixing- Types of mixing process. Extrusion-Features of a Single Screw Extruder, Analysis of Flow, Aspects of Screw Design, Operating Point. Twin Screw Extrusion-Processes - Pipe, Profile, Blown Film, Wire and Cable coating, Fibre, Film and sheet extrusion, Co extrusion-Melt Fracture-Sharkskin-Die swell. Injection Moulding-Principles-Moulding Cycle-Reciprocating Screw Injection Moulding Machine-Types of Clamping Units-PVT diagram-Aspects of Product Quality-Hot Runner Moulding-Gas Assisted Injection Moulding. Blow Moulding-Principles-Injection Blow Moulding-Extrusion Blow Moulding-Stretch Blow Moulding-Trouble shooting-Thermoforming-Vacuum Forming-Pressure Forming-Material Stress and Orientation-Applications in Packaging. Compression and Transfer Moulding-Thermosetting Compounds-Flash, Semi Positive, Positive Type Moulds-Types of Moulding Machines-Transfer Moulding-Trouble shooting-Comparison. Fibre Reinforced Plastics-Materials-Lay up processes-SMC, DMC-Resin Transfer Moulding- Pultrusion, Bag Moulding Processes-Filament Winding-Process Variants-Newer developments using thermosets.Polymers in Rubbery State- Calendering Process-Types of Calendars, Roll Deflection, Roll Cambering-Rotational Moulding-Types of Machines, Moulds, Materials. Joining and Machining of Plastics-Welding of Plastics-Ultrasonic, Induction, Hotplate, High Frequency-Solvent Cementing-Adhesive Bonding.

Introduction – Rheological parameters stress, strain and rate of deformation - Newtonian and Non Newtonian fluids – time dependent fluids – isothermal viscous flow in tubes – Entrance and exit effects - elastic effects in polymer melt flow - die- swell and melt fracture – Weissenberg effect - Extensional Viscosity. Measurement of rheological properties – capillary rheometers – melt flow indexer – cone and plate viscometer – torque rheometers – Mooney viscometer.– Applications of rheology to polymer processing [injection moulding, extrusion, blow moulding, two roll mill - calender] . Mechanical models – Maxwell element – Voigt Kelvin element – Boltzmann and time temperature superposition principles – WLF equation.

TEXT BOOKS/REFERENCES:

1. D. H. Morton – Jones, *Polymer Processing*, Chapman and Hall, New York, 1996.

2. Michael L Berins (ed), *Plastics Engineering Handbook Society of Plastics Industry*, Kluwer Academic Publishers, 2000.
3. B. R. Gupta, *Applied Rheology in Polymer Processing*, Asian Books Pvt Ltd, New Delhi, 2005
4. R. J. Crawford, *Plastics Engineering*, Butterworth-Heinemann, Oxford, 1998
5. D.V. Rosato and Rosato, *Injection Molding Handbook Complete Molding Operation, Technology, Performance and Economics*, CBS Publishers New Delhi, 1987.
6. Chris Rauwendaal, *Polymer Extrusion*, Hanser, 2001.
7. A. Brydson, *Flow Properties of Polymer Melts*, Illife Books, London, 1978.
8. John M. Dealy and Kurt F. Wissburn, *Melt Rheology and its Role in Plastics Processing*, Chapman, London, 1995.

MS702

ELECTROCHEMISTRY AND CORROSION

3-0-0-3

Fundamentals of Electrochemistry: Arrhenius theory of dissociation, Solvation, Mobility, Transport Number; Ionics: Guoy-Chapman and Debye-Huckel theories of ion-ion interaction; Electrified Interface: Structure of electrode-electrolyte interface – Non-Faradaic processes, Thermodynamic activity, Electrochemical potential and Nernst Equation; Mass Transfer in Electrolytes – Convection, Diffusion, and Migration; Electrode Kinetics – Butler-Volmer Equation, Tafel Equation, Polarization of Electrodes – Activation and Concentration polarization, Reaction Mechanisms in Electrochemistry – Rate Laws; Electroanalytical Techniques: Conductometric and Potentiometric Titrations, Potential Step Methods – Chronoamperometry, Potential Sweep Methods – Linear Sweep Voltammetry and Cyclic Voltammetry: Reversible, Quasireversible, and Irreversible Systems; Pulse Voltammetry – Normal Pulse, Differential Pulse, and Square Wave Voltammetry; Electrochemical Impedance Analysis; Selected Applications such as Electrodeposition of Alloys, Corrosion, Batteries, Fuel Cells, and Electrochemical Sensors; Corrosion - Introduction - Types of corrosion – Chemical and Electrochemical corrosion; Factors influencing the rate of corrosion - Nature of the metal and Nature of the environment - Corrosion control methods – including cathodic protection, coatings, inhibitors, passivators; Influence of material's chemical composition and microstructure on corrosion behavior; introduction to tribology

TEXT BOOKS/REFERENCES:

1. J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Volumes 1, 2A, and 2B, Second Edition, Kluwer Academic Publishers, NY, 2000
2. A. J. Bard and L. R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, Second Edition, John Wiley and Sons, NY, 2001
3. V. S. Bagotsky, *Fundamentals of Electrochemistry*, Second Edition, Wiley-Interscience, 2006
4. Mars G. Fontana, *Corrosion Engineering*, Third Edition, Tata McGraw Hill Education Private Limited, 1986

MS703

CATALYTIC CHEMISTRY

3-0-0-3

Catalysis – introduction, Catalyst and catalysis, positive and negative catalysis, Type of catalysis, Characteristics of catalytic reactions, promoters, Catalytic poisoning, Catalysis in gas phase – examples, Catalysis in solution phase – Homogeneous catalysis – acid base catalysis, oxidation reactions, heterogeneous catalysis – introduction, organometallic catalysis, metallocenes, Ziegler Natta catalyst, phase transfer catalysts and various industrially employed reactions; Enzyme catalysis –introduction, classification, mechanism of enzyme catalysis, characteristics of enzyme catalysis, metalloenzymes, solid support, application of catalysis in industries (including auto-exhaust catalysis); Catalysis by zeolites – introduction, classifications, synthesis, examples of various reactions and functional modification on zeolite surface.

TEXT BOOKS/REFERENCES:

1. Bruce C. Gates, *Catalytic Chemistry*, John Wiley and Sons USA, 1992.
2. R. Gopalan and V. Ramalingam, *Concise Coordination Chemistry*, Sangam Books Ltd., 2001.
3. B. R. Puri, L. R. Sharma, and M. S. Pathania, *Principles of Physical chemistry*, Vishal Publishing Company, 2008.
4. James E. House, *Principles of Chemical Kinetics*, Academic Press, 2007.
5. B. Viswanathan, S. Sivashanker and A. V. Ramaswamy, *Catalysis: Principles and Applications*, CRC Press, 2006.

MS704**CARBON NANOMATERIALS****3-0-0-3**

Graphene: Synthesis, Properties, and Applications; Fullerene C60 Architectures in Materials Science; Graphite Whiskers, Cones, and Polyhedral Crystals; Epitaxial Graphene and Carbon Nanotubes on Silicon Carbide; Cooperative Interaction - Crystallization, and Properties of Polymer–Carbon Nanotube Nanocomposites; Carbon Nanotube Biosensors; Carbon Nanostructures in Biomedical Applications, Field Emission from Carbon Nanotubes; Nanocrystalline Diamond; Carbon Onions; Carbide-Derived Carbons; Templated and Ordered Mesoporous Carbons; Oxidation and Purification of Carbon Nanostructures; Hydrothermal Synthesis of Nano-Carbons; Carbon Nanomaterials for Water Desalination by Capacitive Deionization; Carbon Nanotubes for Photoinduced Energy Conversion Applications;

TEXT BOOKS/REFERENCES:

1. Yury Gogotsi and Volker Presser, *Carbon Nanomaterials*, Second Edition, CRC Press, 2013.
2. Francis and Karl M. Kadish, *Handbook of Carbon Nanomaterials*, Vol.1&2, World Scientific, 2011.

MS705**INTERFACIAL SCIENCE AND ENGINEERING****3-0-0-3**

Introduction to Surfaces, Interfaces, and Colloids; Surface and Interface – Molecular Origin, the work of cohesion and adhesion, Surfactants structure, types Interaction forces and potential, chemical and physical interaction, classification of physical forces. Van der Waals force, interaction between surface and particles - Electrostatic forces and electric double layer; DLVO theory, Hamaker constant, Boltzmann distribution, Debye length, specific ion adsorption, ion adsorption, Stern layer, Electrostatic, steric and electrosteric stabilization, zeta potential, surface tension, wetting and spreading, Young's equation, contact angle - Solid surfaces - surface mobility, characteristics, formation; Adsorption, energy consideration of physical adsorption vs. chemisorptions, Gibbs surface excess, Gibbs adsorption equation, Langmuir isotherm, BET isotherm, adsorption at solid-liquid interfaces - Stability of colloids – Emulsions, formation and stability, HLB number, PIT (phase inversion temperature) Foams, Aerosols, Microemulsions, Vesicles, Micelles and Membranes - Applications of various colloidal systems

TEXT BOOKS/REFERENCES:

1. D. Myers, *Surfaces, Interfaces, and Colloids: Principles and Applications*, Second Edition, Wiley-VCH, 1999.
2. T. Cosgrove, *Colloid Science: Principles, Methods and Applications*, Second Edition, Wiley-Blackwell, 2010.
3. P.C. Hiemenz and R. Rajagopalan (Editors), *Principles of Colloid and Surface Chemistry*, Third Edition, Academic Press, New York, 1997.

Waste – energy content, waste classification, waste composition, and waste segregation; Introduction to gasification, pyrolysis and combustion technology(s); Pyrolysis of waste to liquid fuels – Thermal, catalytic / thermal, catalyst and reactor choice for pyrolysis; Gasification to Liquid fuels via synthesis gas route – Petrol and Diesel production, Processes for waste to value-added chemicals via synthesis gas– Hydrogen production, methanol production, ethanol production – Design and catalyst choice for various technologies; Gasification to Electricity – A Case study; Biomass – Classification and Composition; Biomass pyrolysis and gasification to engine grade fuels – catalyst and equipment design.

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2. Marc J. Rogoff and Francois Screve, *Waste to Energy: Technologies and Project Implementation*, Second Edition, Elsevier Inc., 2011.
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Solar energy: Solar radiation, its measurements and analysis. Solar angles, day length, angle of incidence on tilted surface, Sun path diagrams, Shadow determination. Extraterrestrial characteristics, Effect of earth atmosphere, measurement & estimation on horizontal and tilted surfaces. Solar cell physics: p-n junction, homo and hetero junctions, Metal-semiconductor interface, Dark and illumination characteristics, Figure of merits of solar cell, Efficiency limits, Variation of efficiency with band-gap and temperature, efficiency measurements, high efficiency cells, Tandem structure. Solar cell fabrication technology: Preparation of metallurgical, Electronic and Solar grade Silicon, Production of Single Crystal 'Si', Chocharski (CZ) and Float Zone (FZ) method for preparation of silicon, procedure of masking, photolithography and etching, Design of a complete silicon, GaAs, InP solar cell. High efficiency III-V, II-VI multijunction solar cell, a-Si-H based solar cells, Quantum well solar cell, Thermophotovoltaics. Nanosolar cells. Solar photovoltaic system design: Solar cell arrays, system analysis and performance prediction, shadow analysis, reliability, solar cell array design concepts, PV system design, Design process and optimization, Detailed array design, storage autonomy, Voltage regulation, maximum tracking, Power electronic converters for interfacing with load and grid, use of computers in array design, Quick sizing method, Array protection and troubleshooting; Solar Photovoltaic applications – detailed design and economics; Solar Thermal systems: Solar thermal collectors, flat plate collectors, concentrating collectors, solar heating of buildings, solar still, solar water heaters, solar driers; conversion of heat energy in to mechanical energy, solar thermal power generation systems.

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1. J. W. Twidell and A.D. Weir, *Renewable Energy Resources*, Second Edition, Taylor & Francis, New York, 2005.
2. H.P. Garg and J. Prakash, *Solar Energy: Fundamentals & Applications*, Tata McGraw Hill, New Delhi, 1997.
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1. Tetsuya Osaka and Madhav Datta, *Energy Storage Systems in Electronics*, CRC Press, 2000.
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3. Andreas Züttel, Andreas Borgschulte and Louis Schlapbach, *Hydrogen as a Future Energy Carrier*, Wiley-VCH, 2008.
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Definitions, Scope; Approaches for Molecular Simulation; Statistics – Estimating Macroscopic Properties from Molecular Simulations; Quantum Mechanics, Symmetry and Group Theory – Representing Molecules and Molecular Interactions; Molecular Orbital Theory; Hartree-Fock Approach; Density Functional Theory; Molecular Mechanics – Energy and Forces for Molecular Interactions; Constraints; Periodic Boundaries and Neighbor Lists; Introduction to Monte Carlo (MC) Simulations and Molecular Dynamics (MD); Minimization of functions – Advanced Energy Minimization Techniques

Introduction to Unix; Software for Molecular Modeling (any two): GROMACS, ABINIT, ADUN, CP2K, CHARMM, DALTON, NAMD, LAMMPS, SPARTAN, TINKER; Programming Exercises (any five): Evaluation of Pi (MC), Pair-correlation functions, Integration using MC, MD of a simple fluid, MD of an excluded-volume polymer chain, 3D Visualization of Molecules, Model Building, Energy Minimization, Dynamics, Surface Properties, Thermodynamic Properties, Electronic Structure Calculations, Electronic Transport Properties; Case Studies

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1. K. I. Ramachandran, D. Gopakumar and K. Namboori, *Computational Chemistry and Molecular Modeling: Principles and Applications*, Springer, 2008.
2. T. Schlick, *Molecular Modeling and Simulation: An Interdisciplinary Guide*, Springer, 2002.
3. D. Frenkel and B. Smit, *Understanding Molecular Simulations: From Algorithms to Applications*, Second Edition, Academic Press, 2002.
4. M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, Clarendon Press, 1987.
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Philosophy of Sustainability: Fundamental causes of unsustainability, justice and sustainability ethics, societal and personal goals. Principles of Sustainable Design: The design process, cyclical design, goal-based design, systems thinking, LCA, EIA, resource management, socio-economic considerations. Case studies: Building, Water, Agriculture, Energy, Transportation, Industrial symbiosis.

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4. B. B. Marriott, *Environmental Impact Assessment: A Practical Guide*, McGraw-Hill, New York, 1997.