Postgraduate Programmes

Course Structure and Syllabi

For the specializations of

(1) MACHINE LEARNING IN MATERIALS ENGINEERING

(2) MATERIALS SCIENCE AND ENGINEERING



Department of Metallurgy and Materials engineering

Indian Institute of Engineering Science and Technology (IIEST), Shibpur Botanic Garden, Howrah

Table of Contents

	Page					
Course Structure for the specialization of	3					
Machine Learning in Materials Engineering						
Materials Science and Engineering	5					
1st semester syllabus for core subject for both the specialization of "Machine Learning in Materials Engineering", and "Materials Science and Engineering"	6					
1st semester PSE syllabus for "Machine Learning in Materials"						
1st semester PSE syllabus for "Materials Science and Engineering"						
1st semester syllabus for Open Elective	20					
1 st semester practical syllabus for both the specialization of "Machine Learning in Materials Engineering", and "Materials Science and Engineering"						
2 nd semester syllabus for core subject for both the specialization of "Machine Learning in Materials Engineering", and "Materials Science and Engineering"						
2 nd semester PSE syllabus for the specialization of "Machine Learning in Materials"						
2 nd semester PSE syllabus for the specialization of "Materials Science and Engineering"						
2 nd semester syllabus for Open Elective	39					

COURSE STRUCTURE FOR M. TECH. IN MACHINE LEARNING IN MATERIALS ENGINEERING

Firs	t Seme	<u>ester</u>							
Sl.			Course	Class	Load/V	Veek		Class	
No.	Type	Course Name	code	L	T	P	Credit	load/ week	Marks
1	PC	Materials Technology	MM5101N	3	0	0	3	3	100
2	PC	Advanced Characterization of Materials	MM5102N	3	0	0	3	3	100
3	PC	Advanced Thermodynamics and Kinetics	MM5103N	3	0	0	3	3	100
4	PSE	Machine Learning in Materials Discovery/Atomistic Simulation of Materials	MM5123N/ MM5124N	3	0	0	3	3	100
5	OE	Mechanical Behaviour of Engineering Materials/Selection of Engineering Materials	MM5161N/ MM5162N	3	0	0	3	3	100
		Theory Sub-total		15	0	0	15	15	500
6	PC	Materials Technology Lab.	MM5171N	0	0	3	2	3	50
7	PC	Materials Characterization Lab.	MM5172N	0	0	3	2	3	50
8	PC	Machine Learning in Materials Lab	MM5173N	0	0	3	2	3	50
		Practical Sub-total		0	0	9	6	9	150
		First Semester Total		15	0	9	21	24	650

Seco	ond Se	mester							
Sl.			Course	Class	Load/V	Veek		Class	
No.	Type	Course Name	code	L	T	P	Credit	load/ week	Marks
1	PC	Manufacturing Processes	MM5201N	3	0	0	3	3	100
2	PC	Mechanical Behaviour of Materials	MM5202N	3	0	0	3	3	100
3	PC	Multiscale Material Modeling	MM5203N	3	0	0	3	3	100
4	PSE	Deep learning for materials engineering/Microstructure modelling for metallic systems	MM5224N/ MM5225N	3	0	0	3	3	100
5	OE	Nanostructures and nanomaterials/Biomedical Materials and Devices	MM5261N/ MM5262N	3	0	0	3	3	100
		Theory Sub-total		15	0	0	15	15	500
6	P	M.Tech. Thesis Part-I (Term-paper)	MM5291N	0	0	3	2	3	50
7	О	Seminar/Viva Voce	MM5292N	0	0	3	2	3	50
		Practical Sub-total		0	0	6	4	6	100
		Second Semester Total		15	0	6	19	21	600

COURSE STRUCTURE FOR M. TECH. IN MATERIALS SCIENCE AND ENGINEERING

First Semester

Sl. No.	Type	Course Name	Course code	Class Load/Week L T P		Credi t	Class load/ week	Mark s	
1	PC	Materials Technology	MM5101N	3	0	0	3	3	100
2	PC	Advanced Characterization of Materials	MM5102N	3	0	0	3	3	100
3	PC	Advanced Thermodynamics and Kinetics	MM5103N	3	0	0	3	3	100
4	PSE	Functional Materials/Composite Materials	MM5121N/ MM5122N	3	0	0	3	3	100
5	OE	Mechanical Behaviour of Engineering Materials/Selection of Engineering Materials	MM5161N/ MM5162N	3	0	0	3	3	100
		Theory Sub-total		15	0	0	15	15	500
6	PC	Materials Technology Lab.	MM5171N	0	0	3	2	3	50
7	PC	Materials Characterization Lab.	MM5172N	0	0	3	2	3	50
8	PC	Machine Learning in Materials Lab	MM5173N	0	0	3	2	3	50
		Practical Sub-total		0	0	9	6	9	150
		First Semester Total		15	0	9	21	24	650

Seco	nd Se	mester							
Sl. No.	Туре	Course Name	Course Class Load/Week				Credi t	Class load/	Mark s
140.			couc	L	T	P		week	3
1	PC	Manufacturing Processes	MM5201N	3	0	0	3	3	100
2	PC	Mechanical Behaviour of Materials	MM5202N	3	0	0	3	3	100
3	PC	Multiscale Material Modeling	MM5203N	3	0	0	3	3	100
4	PSE	Design and selection of Materials/Surface treatment and Modifications	MM5221N/ MM5223N	3	0	0	3	3	100
5	OE	Nanostructures and nanomaterials/Biomedical Materials and Devices	MM5261N/ MM5262N	3	0	0	3	3	100
		Theory Sub-total		15	0	0	15	15	500
6	P	M.Tech. Thesis Part-I (Term-paper)	MM5291N	0	0	3	2	3	50
7	О	Seminar/Viva Voce	MM5292N	0	0	3	2	3	50
		Practical Sub-total		0	0	6	4	6	100
		Second Semester Total		15	0	6	19	21	600

Syllabus: <u>First Semester</u>

Core Subject (Machine Learning in Materials Engineering & Materials Science and Engineering)

Course Code	MM5101N	Course	Materials	Course	PC	L	T	P
Course Code	WIWISTOTIN	Name	Technology	Category	PC	3	0	0

Pre-requisite Courses	NIL	Co-requisite Courses	NIL	Progressive Courses	Materials Technology Lab.
Course Offering Do	Course Offering Department		laterials	Data Book / Codes/Standards	NIL

Course	To gain an in-depth understanding of the structure, classification, and behavior of			
Objective	engineering materials by exploring crystallography, phase diagrams, solidification,			
	diffusion, and solid-state transformations, enabling them to analyze microstructural			
	evolution and apply materials principles to the design, processing, and performance			
	optimization of advanced engineering materials.			

Module	Syllabus	Duratio n (h)	Module outcome
Module-I	Engineering Materials: Classification and Structure Classification of engineering materials; Elements of crystallography: Atomic packing, Stacking sequence; Bravais lattice & Miller indices; Crystal imperfections.	5	Able to classify engineering materials, interpret crystal structures using Bravais lattices and Miller indices, analyze atomic packing, and identify crystal imperfections and their effects on material properties.
Module-II	Phase diagram and Transformation Phase rule; Types and construction of phase diagrams; Free energy-composition diagrams; Lever Rule; Isomorphous and phase diagrams with invariant reactions; Introduction to ternary system.	6	Interpret and construct phase diagrams, apply phase and lever rules, analyze free energy-composition curves, and understand invariant reactions and ternary systems to predict phase stability and transformations in multicomponent materials.
Module - III	Steel and Cast Iron Fe-C system; Steel and castiron microstructures with phase relations.	5	Understand the Fe-C phase diagram, analyze steel and cast-iron microstructures based on composition and thermal history to predict phase transformations and properties.
Module -1V	Solidification Homogeneous and Heterogeneous nucleation, and growth; Planar, Columnar	6	Analyze nucleation types, solidification growth modes, solute segregation, and casting defects to understand and control microstructure evolution during solidification.

	and dendritic solidification; Segregations; Casting defects.		
Module-V	Diffusion Diffusion laws; Kirkendall effect; activation energy; Diffusion mechanisms; uphill diffusion etc.	6	Apply diffusion laws and mechanisms, interpret the Kirkendall effect, calculate activation energy, and analyze phenomena like uphill diffusion to understand mass transport and its impact on microstructural evolution in materials.
Module -VI	Solid-state phase transformation Thermodynamics and Kinetics of nucleation and growth; Mechanisms; T-T-T and C-C-T diagrams.	6	Analyze the thermodynamics and kinetics of nucleation and growth, understand transformation mechanisms, and interpret T-T-T and C-C-T diagrams to predict microstructural evolution during solid-state phase transformations.
Module - VII	Diffusional less transformation processes Polymorphic transformation; Pearlite, bainite and martensite transformations; Massive and order-disorder transformation; Precipitation; Recrystallization	8	Understand and analyze diffusional and diffusionless transformations, including polymorphic changes, pearlite, bainite, martensite, massive and order-disorder transformations, as well as precipitation and recrystallization, to evaluate microstructural evolution and material properties in solid-state phase transformations.
	Total	42	

Course	Upon successful completion, students will:
Outcome	CO1: Recognize and categorize engineering materials based on their structural attributes,
	properties, and applications.
	CO2: Describe the connection between material microstructures and their mechanical
	behaviors.
	CO3: Evaluate properties such as strength, hardness, toughness, and corrosion resistance
	utilizing standardized testing procedures.

	Materials Science and Engineering: W.F. Smith, J. Hashemi and R Prakash, McGraw Hill
Learning	The Science and Engineering of Materials, D.R. Asheland, Springer Science
Resources	Fundamentals of Materials Science and Engineering : W.D. Callister, Jr, John Wiley & Sons, Inc.
	Science and Engineering - A First Course, V. Raghavan, PHI

Course Code	MM5102N	Course	Advanced Characterization	Course	PC	L	T	P
Course Code	WIWI5102N	Name	of Materials	Category	PC	3	0	0

Pre-requisite Courses	NIL	Co-requisite Courses	NIL	Progressive Courses	NIL
Course Offering l	Department	Metallurgy and Materials Engineering		Data Book / Codes/Standards	NIL

Course	☐ To provide a thorough understanding of advanced characterization techniques for				
Objective	materials at micro- and nano-scales.				
	☐ To develop the ability to select and apply appropriate characterization tools for				
	analyzing structure, morphology, composition, and properties.				
	☐ To prepare students for research and industrial problem-solving using modern materials				
	characterization methods.				

Module	Syllabus	Duration (h)		
I	Introduction to Advanced material characterization techniques	02		
II	x-ray diffraction pattern analysis: Determination of crystal structure, crystal size, lattice parameter, quantitative phase analysis and defect analysis.	08		
III	Advanced optical Microscopy: Interference, Phase contrast, polarized light and near field scanning optical microscopy			
1V	Electron Microscopes: Scanning Electron Microscopes and Transmission Electron microscopes, Electron diffraction and diffraction pattern analysis	10		
V	Scanning probe Microscope : Scanning tunneling microscope, Atomic force microscope, Magnetic force microscope			
VI	Spectroscopy: Principle and application of Energy dispersive spectroscopy, Auger electron spectroscopy, X ray photo electron spectroscopy, x-ray fluorescence spectroscopy, Raman spectroscopy. Fourirer transform Infrared spectroscopy	08		
VII	Thermal Characterization techniques: DSC, DTA-TGA, principles and applications	05		
	Total contact hours	42		

Course	At the end of this course, students will be able to:					
Outcome	 Understand the principles and working mechanisms of various advanced 					
	characterization techniques.					
	Interpret experimental data obtained from XRD, microscopy, and spectroscopic					
	characterization techniques.					
	 Select appropriate techniques for specific materials analysis problems. 					
	• Critically analyze microstructural, compositional, and surface properties of materials.					

	B.D Cullity: Elements of x- ray diffraction
Learning	Yang Leng: Materials Characterization: Introduction to Microscopic and Spectroscopic
Resources	Methods
	David B Williams, C. Barry Carter: Transmission Electron Microscopy

Course	MM5103N	Course	ourse Advanced Thermodynamic	Course	Course	L	T	P
Code	MINISTUSIN	Name	s and Kinetics	Category	PC	3	0	0

Pre-requisite Courses	Nil	Co-requisite Courses	Nil	Progressive Courses	
Course Offering Department		Metallurgy and Materials Engineering		Data Book / Codes/Standards	

Course Objective

- 1. **Deepen understanding of classical and statistical thermodynamics** as applied to materials and chemical systems.
- 2. **Explore advanced thermodynamic models** for multicomponent, multiphase systems, including solutions and phase equilibria.
- 3. **Develop knowledge of kinetics** including rate theories, diffusion, and phase transformation mechanisms.
- 4. **Apply thermodynamic and kinetic principles** to real-world processes such as alloy solidification, corrosion, catalysis, and materials degradation.
- 5. **Enhance critical thinking skills** for interpreting complex phase diagrams and reaction mechanisms.

Module	Syllabus	Duration (class-hour)	Module Outcome
I	Review of Classical Thermodynamics: Laws of thermodynamics (Zeroth, first, second and third), Thermodynamic potentials: Basics and appllications (U, H, A, G), Maxwell's relations and their applications, Stability criteria and phase equilibrium	08	Understanding the need and challenges of thermodynamics for materials engineering applications.
П	Basics of Statistical Thermodynamics: Microstates, macrostates, and partition functions, Maxwell-Boltzmann, Fermi-Dirac, and Bose-Einstein statistics, Connection between statistical and classical thermodynamics, Configurational entropy and mixing.	08	Basics of statistical mechanics and its application for derivation of thermodynamic parameters.
III	Thermodynamics of Solutions and Phases: Ideal, regular, and real solutions, Partial molar quantities and chemical potential, Activity, fugacity, and excess properties, Gibbs phase rule and phase equilibria.	06	Understanding about the thermodynamics of solutions and its applications for the materials design.
IV	Diffusion and Mass Transport: Fick's laws and atomic mechanisms of diffusion, Diffusion in solids, liquids, and gases, Interdiffusion, Darken's equations, Kirkendall effect and tracer diffusion.	06	Understanding about the diffusion phenomena and its basics.
V	Reaction Kinetics and Mechanisms: Rate laws and reaction order, Arrhenius equation and activation energy, Transition state theory and reaction coordinate diagrams, Catalysis and surface reactions.	06	Application of kinetics for the chemical reactions and catalytic phenomena.

VI	film growth Total contact hours	42	principles to industrial relevant phenomena.
	Applications and Case Studies: Thermo-kinetics in alloy design, Corrosion and oxidation and thin	07	Application of thermodynamic and kinetic

Course	Explain advanced thermodynamic concepts, including chemical potential,
Outcome	Gibbs energy minimization, and entropy production.
	2. Analyze multicomponent phase equilibria using analytical methods.
	3. Apply kinetic theories (e.g., transition state theory and diffusion mechanisms)
	to describe reaction rates and phase changes.
	4. Conduct and critique thermodynamic and kinetic analyses in academic or
	industrial research contexts.
Learning	1. Statistical mechanics: A survival guide, A. M. Glazer and J. S. Wark, Oxford
Resources	University Press.
	2. Textbook of Materials and Metallurgical Thermodynamics, Ahindra Ghosh,
	PHI Eastern Economy edition.
	3. Introduction to the Thermodynamics of Materials, David R. Gaskell, Taylor
	and Francis Learning Resources
	4. A Textbook of Metallurgical Kinetics, Sudipto Ghosh and Ahindra Ghosh, PH

PSE: Machine Learning in Materials Engineering

Course		Course	Machine Learning in Course		L	T	P		
Code	MM5123N	Name	Materials Discovery	Category	PSE	3	0	0	

Pre-requisite Courses	Nil	Co-requisite Courses Nil		Progressive Courses	
Course Offering	g Department	Metallurgy and Materials Engineering		Data Book / Codes/Standards	

Course Objectives

- To provide students with a foundational understanding of machine learning principles, algorithms, and workflows, with a focus on supervised, unsupervised, and reinforcement learning.
- To foster the ability to integrate knowledge of materials science with data science to solve complex industrial challenges innovatively and efficiently.

Module	Syllabus	Duration	Module Outcome
		(class-	
Т	Mathematical Foundations for Machine	hour)	The Students will be able to
I	Mathematical Foundations for Machine Learning: Vectors, matrices, and tensors, Matrix operations: addition, multiplication, transpose, inverse; Eigenvalues and eigenvectors, Singular Value Decomposition (SVD), Vector spaces, span, linear independence, Orthogonality and projections. Partial derivatives and multivariable calculus, Chain rule and the gradient descent algorithm; Optimization methods: gradient ascent/descent, Taylor series and approximations; Probability theory basics (conditional probability, Bayes' theorem), Random variables and distributions (Normal, Binomial, Poisson, etc.), Expectation, variance, and covariance, Maximum likelihood estimation (MLE), Hypothesis testing, Confidence intervals and p-values;	7	The Students will be able to demonstrate foundational knowledge in linear algebra, calculus, probability theory, and optimization as they pertain to machine learning algorithms.
II	Machine Learning Fundamentals: Linear	4	The Students will be able to
	regression and classification algorithms, Feature extraction, Evaluation metrics for machine learning models (accuracy, precision, recall, F1 score, etc.)		explain the foundational principles of machine learning, including supervised, unsupervised, and reinforcement learning paradigms.
III	Supervised Learning for Property	7	The Students will be able to
	Prediction: Predicting material properties		implement and utilize common
	using regression models (e.g., elastic moduli,		supervised learning algorithms
	band gaps, melting points), Case study:		(e.g., Linear Regression,

	mundicting the electronic array artist of		Cumpart Vactor Machines
	predicting the electronic properties of		Support Vector Machines,
	materials, Techniques: Random Forest,		Decision Trees, Random
	Support Vector Machines, k-Nearest		Forests, Neural Networks,
	Neighbors, and Gradient Boosting.		Graph Neural Networks) for
			both regression and
			classification tasks.
IV	Deep Learning in Materials Discovery:	6	The Students will be able to
	Neural networks and their application in		utilize common deep learning
	materials science, Convolutional Neural		architectures such as
	Networks (CNNs) for image-based data,		Convolutional Neural
	Recurrent Neural Networks (RNNs) for		Networks (CNNs), Recurrent
	sequence prediction (e.g., material design		Neural Networks (RNNs),
	through molecular structure), Transfer learning		Graph Neural Networks
	in material property prediction.		(GNNs), and Transformer
			networks for materials-related
			tasks.
V	Unsupervised Learning and Clustering:	6	The Students will be able to
	Clustering techniques (e.g., k-means,		implement unsupervised
	hierarchical clustering) for materials discovery,		learning algorithms using
	Dimensionality reduction (e.g., PCA, t-SNE)		popular programming
	for high-dimensional materials data,		languages (e.g., Python) and
	Identifying trends in materials datasets: finding		libraries (e.g., scikit-learn,
	novel materials based on clustering.		SciPy).
	no ver materials cuses on erastering.		
VI	Materials Genome Initiative and High-	6	The Students will be able to
	Throughput Screening: The Materials		navigate and leverage
	Genome Initiative (MGI): an overview and		prominent materials databases
	its impact on materials discovery, High-		for accessing existing
	throughput computational screening and		materials data and properties
	Machine Learning-based optimization.		
VII	Reinforcement Learning for Materials	6	The Students will be able to
	Discovery: Introduction to reinforcement		explain the core components
	learning (RL) and its application in materials		of an RL problem: agents,
	science, RL for material design: agent-based		environments, states, actions,
	modeling and reward structures, Case study:		rewards, and policies,
	RL in the discovery of alloys and polymers.		specifically as they apply to
	F 2.3 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2		materials design and discovery
			materials design and discovery

Course	The Students will be able to					
Outcome	1. Explain the core concepts of supervised, unsupervised, and reinforcement learning relevant to metallurgical processes and materials.					
	2. Identify and articulate specific challenges and opportunities for applying machine learning within the metallurgical industry (e.g., complex process parameters, material property variations, data sparsity, sensor noise).					
	3. Apply techniques for data cleaning, handling missing values, outlier detection, and data integration specific to metallurgical datasets.4. Apply machine learning techniques for predicting structure-property relationships in alloys, ceramics, and composites					

Learning	"Machine Learning for Materials Scientists: An Introduction to the Application of
Resources	Machine Learning Algorithms in Materials Science" by James A. Pask, Malgorzata
	K. S. K. and Shreyas Shinde

Learning Resources	"Machine Learning for Materials Scientists: An Introduction to the Application of Machine Learning Algorithms in Materials Science" by James A. Pask, Malgorzata K.
	S. K. and Shreyas Shinde.

Cour		Course	Atomistic Simulation	Солича		L	T	P
se Code	MM5124N	Name	of Materials	Course Category	PSE	3	0	0

Pre-requisite Courses	Nil	Co-requisite Courses		Progressive Courses	
Course Offering	g Department Metallurgy and Materi Engineering			Data Book / Codes/Standards	

Course Objectives

- Provide the theoretical foundations of molecular dynamics (MD), Density Functional Theory (DFT) and Monte Carlo (MC) simulations, including their statistical mechanical basis.
- Provide understanding how atomistic simulations complement experimental observations and higher-scale computational methods in materials research

Module	Syllabus	Duration (class- hour)	Module Outcome
I	Mathematical Background for Atomistic Simulation of Materials: Ordinary Differential Equations (ODEs), Partial Differential Equations (PDEs), Probability distributions (Gaussian, Poisson, etc.), Random variables and expectation values, The concept of ensembles in statistical mechanics (micro-canonical, canonical, grand canonical); Partition function and its connection to thermodynamic quantities, Relation between macroscopic observables and microscopic states; Bose-Einstein and Fermi-Dirac statistics; Quantum gases and their equations of state; Bose- Einstein condensation, Fermi surfaces, Time- dependent and time-independent Schrödinger equation, Perturbation theory (time-independent and time-dependent), Interaction picture and path integrals Introduction to Atomistic Simulation Methods Overview of Atomistic Simulation: Introduction to the field, significance in materials science, and	8	Students will be able to formulate and analyze the mathematical equations underlying classical molecular dynamics (Newton's laws of motion) and Quantum Chemical Calculations. Students will be able to know atomistic simulation techniques and their roles in
III	applications in industry and research. Material Properties and Modeling: Connection between atomistic models and macroscopic material properties. Overview of Computational Tools: Introduction to software packages. Classical Simulation Techniques Molecular Dynamics (MD): Principles of MD simulations: Newton's equations of motion, time	10	Students will be able to set up, run, and analyze basic molecular dynamics (MD)
	integration, and boundary conditions. Interatomic potentials (Lennard-Jones, embedded atom model (EAM), etc.). Thermodynamic properties from MD simulations (temperature, pressure, heat capacity).		and/or Monte Carlo (MC) simulations using an industry-standard atomistic simulation software package,

	Applications of MD: Diffusion, phase transitions, defect formation, etc. Monte Carlo (MC) Simulations: Introduction to probabilistic methods and the Monte Carlo approach. Applications in simulating equilibrium states, thermodynamic properties, and material behavior.		and interpret the resulting material properties and atomic behaviors.
IV	Quantum Mechanical Simulations Density Functional Theory (DFT): Basic principles and the Hohenberg-Kohn theorems. Kohn-Sham equations and self-consistent field methods. Applications in calculating electronic structure, total energy, and forces. Exchange- Correlation Functionals:LDA, GGA, and hybrid functionals.Plane-Wave and Pseudopotential Methods: Use of plane waves and pseudopotentials in solving DFT equations.Quantum simulations using codes like VASP and Quantum ESPRESSO. Applications of DFT: Structural optimization, band structure calculations, and defect studies.	8	Students will be able to set up and perform Density Functional Theory (DFT) calculations using a widely- used computational package to predict fundamental electronic and structural properties of materials (e.g., band structure, density of states, equilibrium lattice parameters), and critically interpret the results.
V	Simulation of Material Properties : Calculation of stress-strain relationships. Defects and Dislocations: Study of point defects, dislocations, and grain boundaries in materials. Impact of defects on mechanical properties. Phase Transitions and Material Behavior: Simulation of phase changes, crystallization, melting, and amorphization. Nucleation and growth mechanisms in materials.	10	Students will be able to perform atomistic simulations to predict and analyze the elastic constants, physical and mechanical properties of materials.

- The Students will be able to
- Design and set up simulation cells, including defining atomic positions, boundary conditions, and initial velocities/temperatures.
- Calculate and interpret various material properties from simulation trajectories, such as radial distribution functions, diffusion coefficients, elastic constants, thermal conductivity, and phase transitions.
- Simulate phenomena such as diffusion, phase transformations, defect interactions, mechanical deformation, and thermal transport at the atomic level.
- Predict material properties that are challenging or expensive to obtain experimentally

Learning Resources

- 1. "Atomistic Simulations of Materials" by Zhiqiang Wang
- 2. "Molecular Dynamics Simulation of Nanostructured Materials: An Understanding of

Mechanical Behavior" By Snehanshu Pal, Bankim Chandra Ray

3. "Molecular Dynamics for Materials Modeling: A Practical Approach Using LAMMPS Platform" By Snehanshu Pal, K. Vijay Reddy

PSE: Materials Science and Engineering

Course	MM5121N	Course	Course Functional Cours		Course	PSE	L	Т	P
Code	Code		Mat	erials	Category	IBL	3	0	0
				1					
Pre-requisite Courses	Physics of Materials	_	Co-requisite Courses Thermodynamics		Progressi Courses				
Course Offeri	ng Department	Me	Metallurgy and Materials Engineering		Data Boo Codes/Stand				

Course	The course objectives include understanding fundamental concepts of different classes of
Objective	functional materials. Understanding different synthesis approaches and characterization
	techniques. Exploring the diverse applications of functional materials.

Module	Syllabus	Duration (class-hour)
I	Overview of functional Materials, structure properties and their classification.	02
II	Ferroelectric, Piezoelectric and Piezoelectric Materials: Perovskite structure and spontaneous polarization, relationship of ferroelectrics and piezoelectric to crystal symmetry, Devices based on piezoelectric property, Piezoelectric composites, pyroelectric materials and devices	10
III	Shape Memory Alloys: Structural Thermo-elastic Phase Transition in Shape Memory Alloys, Dependency Between Microstructure and Elastic Behavior of SMA, Discontinuous Change of Physical Properties— Martensitic Phase Transition, Different Approaches to Describe the Shape- Memory Effect,	08
IV	Quantitative Models for Shape Memory Alloys Magnetorheological and Electrorheological Fluids: Viscoelastic Properties and Basic Rheology, Some Rheological Models, Understanding the Microscopic Structure of ERF and MRF, ER- and MR-effect Explained by the Interaction of Induced Dipoles, Applications—Switchable Fluid Acting as a Valve	08
V	Nanostructured functional materials: Semiconducting oxide films, Metallic nanoparticles, Carbon-based nanostructured materials for energy storage and conversion	06
VI	Functionally graded materials and their applications.	06
	Total contact hours	42

Course Outcome	 After the completion of the course the students will be able will be able to apply their knowledge to solve problems related to functional materials, including designing, synthesis and characterization of functional materials for devices. Students will also develop critical thinking skills to evaluate and understand the scientific literature related to nanomaterials.
Learning	➤ The Physics of Multifunctional Materials Concepts, Materials, Applications,
Resources	Martin Gurka

Course Code	MM5122N	Course Name	Composite Materials	Course Category	PSE	L 3	T 0	P 0
Pre- requisite Courses	NIL		requisite Courses	NIL	Progressive Courses		NIL	v
Course Department	_		Metallurgy and Materials Data Book / Codes / Standards				NI	L

Course Objective

The objective is to equip students with the advanced knowledge of fundamentals of composite materials, design and analysis, innovation and newer applications, problem-solving and project development. They can work in industries that develop and apply composite materials, such as aerospace, automotive, or energy and apply knowledge to consulting or entrepreneurial ventures related to composite materials. In summary, this course aims to produce highly skilled professionals who can contribute to the advancement of composite materials and their applications in various industries.

Module	Syllabus	Duration (h)	Module Outcome
I	Introduction Definition of composite material, Classification of composite materials, Reinforcements and matrices, Types of reinforcements, Types of matrices, Types of composites, Dispersion strengthened, particle reinforced and fiber reinforced composites, applications.	04	Understanding the basics of composite materials
II	Design of Composites In-situ and ex-situ composites; Interfaces between reinforcements and matrices in composites; Bonding Mechanisms, Bond Strength, Interfacial Toughness.	04	Understanding the design and bonding mechanisms of composite materials
III	Manufacturing Methods Polymer Matrix Composites: Polymer Matrices, Processing Techniques, Glass Reinforced Plastics, Carbon Fiber Composites; Metal Matrix Composites; Metal Matrices, Processing Techniques, Interfacial Controls, Discontinuously Reinforced Composites, Fiber Composites; Ceramic Matrix Composites: Ceramic Matrices, Processing Techniques, Alumina Matrix Composites, Glass Matrix Composites.	08	Understanding the manufacturing methods of various composites
IV	Mechanical Properties Strengthening mechanisms, Properties of composites: Elastic Properties, Strength and toughness, Geometrical aspects – volume and weight fraction. Unidirectional continuous fibre, discontinuous fibers, Short fiber systems, woven reinforcements – Mechanical Testing: Determination of stiffness and strengths of unidirectional composites; tension, compression, flexure and shear.	08	Understanding the mechanical properties of composite materials
V	Laminates Plate Stiffness and Compliance, Assumptions, Strains, Stress Resultants, Plate Stiffness and Compliance, Computation of Stresses, Types of Laminates -, Symmetric Laminates, Antisymmetric Laminate, Balanced Laminate, Quasi-isotropic Laminates, Cross-ply Laminate, Angle-ply Laminate. Orthotropic Laminate, Laminate Moduli, Hygrothermal Stresses	08	Understanding the different laminates and their stress-strain behaviour
VI	Joining Methods and Failure Theories Joining — adhesive and mechanically fastened joints, advantages and disadvantages. Typical bond strengths and test procedures.	06	Understanding the joining methods and failure theories of composite joints

VII	Recent Developments Self-healing (Repairing) composites, Nano-composites, Bio-composites and their usefulness.	04	Understanding the recent developments in composites
	Total contact hours	42	

Course	Upon completing a course in Composite Materials, students are expected to apply knowledge to
Outcome	design, analyse and develop innovative solutions to complex problems to achieve common goals
	related to composite materials. The learners will be well-equipped to pursue careers in research,
	industry, or academia, and make significant contributions to the field of composite materials.

		,							
	1. F. L. Mathews and R. D. Rawlings: Composite Materials: Engineering and Woodhead Publishing Limited.								
Laguning									
Learning Resources	2.	K. K. Chawla: Composite Materials: Science and Engineering, Springer.							
	3.	T. W. Clyne and D. Hull: An Introduction to Composite Materials, Cambridge University							
		Press.							

Open Elective

Course	MM5161N	Course	Mechanical Behaviour of	Course	OE	L	Т	P	
Code	MM2101N	Name	Engineering Materials	Category	UE	3	0	0	

Pre-requisite Courses	NIL	Co-requisite Courses	NIL	Progressive Courses	NIL
Course Offering Department		٠.	y and Materials ineering	Data Book / Codes/Standards	NIL

Course Objective

To develop an in-depth understanding of the mechanical properties, deformation behavior, and failure mechanisms of engineering materials, enabling students to analyze the influence of microstructure, loading conditions, and environmental factors on strength, toughness, fatigue, and fracture for advanced material design and application.

Module	Syllabus	Duration (h)	Module Outcome
I	Introduction to deformation and failure Concept of stresses and strains; Engineering and true stresses and strains; Different types of loading and temperatures encountered in engineering applications; Mechanical behaviour and failure of metals, alloys, ceramics, polymer and composites materials.	4	Understand stress-strain behavior under various loading, temperature and application conditions, and evaluate the mechanical response and failure mechanisms of various engineering materials.
II	Elastic deformation State of stress and strain; Principal stress and strain; elastic stress-strain relation; Elastic behaviour of engineering materials.	6	Analyze elastic deformation in engineering materials by understanding stress and strain states, principal stresses and strains, and elastic stress-strain relationships to evaluate material response under elastic loading conditions.
III	Plastic deformation Plastic stress-strain relation; Hydrostatic and deviatoric stress; Octahedral stress; Effective stress and strain; Yield criteria; Mohr circle.	6	Explain plastic stress-strain behavior, distinguish hydrostatic and deviatoric stress components, interpret octahedral and effective stress-strain, apply yield criteria, and construct Mohr's circle to understand material response under complex loading conditions.
IV	Mechanisms of plastic deformation Crystal defects; Dislocation; Geometrical and statistical dislocations; Dislocation multiplication; Dislocation reactions; Slip and twinning; Critical resolved shear stress; Strain hardening; Hall-Petch relationship.	6	Explain the mechanisms of plastic deformation by analyzing crystal defects, dislocation behavior, slip and twinning, strain hardening, and the Hall-Petch relationship to understand how microstructural features influence the strength and deformation of engineering materials.
V	Fatigue Types of dynamic loading; S-N curves; Classification of fatigue; Fatigue of engineering materials; Mechanisms of	6	Understand types of dynamic loading, interpret S-N curves, classify fatigue, understand fatigue behavior in engineering materials, and apply

	fatigue failure; Fatigue life prediction		failure mechanisms to predict fatigue life and enhance material performance under cyclic loading conditions.
VI	Creep Time dependent deformation; Different stages of creep; Creep and stress rupture; Creep mechanisms and maps; Design of materials for high temperature applications	6	Explain time-dependent deformation, stages of creep, stress rupture behavior, underlying creep mechanisms and maps, and apply this knowledge to select and design materials suitable for high-temperature applications.
VII	Fracture Fracture in engineering materials; Modes and mechanisms of fractures; Linear elastic fracture mechanisms; Elastic-plastic fracture mechanisms; Measurement of fracture toughness.	8	Analyze fracture behavior in engineering materials, including fracture modes and mechanisms, apply linear elastic and elastic-plastic fracture mechanics principles, and evaluate fracture toughness to assess material reliability and failure resistance.
	Total	42	

Upon successful completion, students will:

CO1: Understand stress-strain behavior under various loading and temperature conditions, and evaluate elastic and plastic deformation of different engineering materials.

CO2: Analyse plastic deformation mechanisms including dislocation dynamics, strain hardening, and yield criteria, and assess their influence on material strength and ductility.

CO3: Understand fatigue, creep, and fracture mechanisms in engineering materials, and apply this knowledge to predict material performance and failure under long-term or cyclic loading in critical applications.

	Dieter, G.E. (1988) <i>Mechanical Metallurgy</i> . 3rd edn. London: McGraw-Hill.						
	Hertzberg, R.W., Vinci, R.P. and Hertzberg, J.L. (2020) <i>Deformation and Fracture</i>						
	Mechanics of Engineering Materials. 6th edn. Hoboken, NJ: Wiley.						
	Hosford, W.F. (2010) <i>Mechanical Behavior of Materials</i> . 2nd edn. Cambridge: Cambridge						
	University Press.						
Learning	Meyers, M.A. and Chawla, K.K. (2009) <i>Mechanical Behavior of Materials</i> . 2nd edn.						
Resources	Cambridge: Cambridge University Press.						
	Hosford, W.F. (2010) <i>Mechanical Behavior of Materials</i> . 2nd edn. Cambridge: Cambridge						
	University Press.						
	Suresh, S. (1998) <i>Fatigue of Materials</i> . 2nd edn. Cambridge: Cambridge University Press.						
	Dyson, B.F. and McLean, M. (2003) Creep Deformation and Fracture. Warrendale, PA:						
	ASM International						

Course	MM5162N	Course Selection of	Course	OE	L	T	P	
Code	WIWISTOZIN	Name	Engineering Materials	Category	OE	3	0	0

Pre-requisite Courses	NIL	Co-requisite Courses	NIL	Progressive Courses	NIL
Course Offering Department		Metallurgy and Materials Engineering		Data Book / Codes/Standards	NIL

Course
Objective
The main objective of the course is to allow students to develop a systematic procedure for selecting materials for structural, thermal, electrical and magnetic applications

Module	Syllabus	Duration (class- hour)	Duration (h)
I	Classification of materials and introduction to material property charts	3	Students will be able to classify materials, and have preliminary understanding of material property charts
II	Design-linked strategy of selecting materials and processes	3	Students will be able to understand the strategies for selecting materials and processes
III	Review of Mechanical properties of materials: concepts of stress and strain, stress versus strain curve of elastoplastic materials,	6	Students will review mechanical properties of materials associated with elastoplastic deformation
IV	Structural or Load-bearing materials: Stiffness-limited design, Strength-limited design, Material indices for yield-limited design	6	Students will be able to derive material indices associated with different mechanical responses.
V	Thermal materials: Review of thermal properties of materials, Thermal property charts, Case studies of material selection based on thermal properties	6	Students will review thermal properties and will be able to select materials based on thermal requirements of the product/application.
VI	Electrical materials: Review of electrical properties, Charts for electrical properties, Case studies of selection of materials using electrical properties	6	Students will review electrical properties and will be able to select materials based on electrical requirements of the product/application.
VII	Magnetic materials: Review of magnetic properties, Charts for magnetic properties, Case studies of materials selection for magnetic design	6	Students will review magnetic properties and will be able to select materials based on magnetic requirements of the product/application.

Course
Outcome

CO1: On completion of the course, the students should gain an understanding of material selection as an integral part of the design process

CO2: On completion of the course, the students should be able to interpret material property charts and use appropriate material indices based on the requirement of design

CO3: On completion of the course, the students should be able to select appropriate materials
for applications that involve mechanical deformation or are subject to temperature
fields/electrical fields/magnetic fields.

	Materials: Engineering, Science, Processing and Design , Michael Ashby, Hugh Shercliff, and David Cebon, Butterworth-Heinemann, 4 th edition
Learning Resources	Materials Selection in Mechanical Design , Michael F. Ashby, Butterwoth-Heinemann, 6 th edition
	Materials Science and Engineering: An Introduction, William D. Callister Jr. and David G. Rethwisch, Wiley, 10 th edition

Practical Subject (Machine Learning in Materials Engineering & Materials Science and Engineering)

Course		Course	Materials	Course	D.C.	L	T	P
Code	MM5171N	Name	Technology Lab.	Category	PC	0	0	3

Pre-requisite Courses	NIL	Co-requisite Courses	Nil	Progressive Courses	MM5101N
Course Offering D	epartment	Metallurgy Materials Engir		Data Book / Codes/Standards	ASTM E407-23, E384-23, E8M-23, E23-18

Course	To develop practical skills in metallographic sample preparation, microstructural
Objective	characterization, mechanical testing, and fracture analysis to evaluate the structure-
	property relationship of ferrous and non-ferrous engineering materials using standard
	laboratory techniques.

Lab.	Syllabus	Duratio n (h)	Lab. Outcome
I	Metallographic Sample preparation -I: Sectioning, Mounting, Grinding, and Polishing.	3	Prepare metallographic samples using sectioning, mounting, grinding, and polishing to obtain smooth, defect-free surfaces for microstructural analysis.
II	Metallographic Sample preparation -II: Fine polishing, Electropolishing, and Etching	3	Apply various polishing and etching techniques to reveal microstructural features essential for accurate metallographic analysis of engineering materials.
III	Optical Microscope and microstructural characterization	3	Use optical microscopy to examine microstructures and identify phases, grain boundaries, and features relevant to material properties and processing.
IV	Macro- and micro- structure of cast alloys	3	Examine and interpret the macro- and microstructural features of cast alloys to understand solidification patterns, phase distribution, and structural integrity.
V	Microstructure of ferrous materials	3	Identify and interpret the microstructural features of ferrous materials, including phases and phase transformations, to understand their influence on mechanical properties and processing behavior.
VI	Microstructures of non- ferrous materials	3	Interpret microstructures of non-ferrous materials to assess their composition, phases, and processing history using standard metallographic and microscopy techniques.
VII	Image Analyses: Measurement of Grain size and Phase content	3	Perform image analysis to accurately measure grain size and phase content, enabling quantitative evaluation of microstructural characteristics in engineering materials.
VIII	Hardness Test-I:	3	Conduct Rockwell and Brinell tests to assess

	Rockwell and Brinell		material hardness and select appropriate indenter, load, and scale.
IX	Hardness Test-I: Vickers	3	Perform the Vickers hardness test and interpret the results to evaluate material hardness and understand its correlation with microstructure and mechanical properties.
X	Microhardness Test	3	Conduct Vickers microhardness testing to evaluate phase-specific hardness variations in multiphase materials
XI	Tensile Test	3	Perform tensile tests on materials like mild steel and copper, and interpret stress-strain data to determine yield strength, tensile strength, elongation, and strain hardening exponent.
XII	Impact Test	3	Analyze the influence of heat treatment and steel composition on Charpy impact toughness to understand the ductile-to-brittle transition temperature
XIII	Analyses of Fractured surfaces	3	Interpret SEM fracture surfaces to distinguish ductile and brittle modes and relate features to failure mechanisms.
XIV	Test and Viva Assess practical understanding of characterization techniques and mechanimethods through structured oral examination.		
	Total contact hours	42	

On completion of the course, the students should be able to

CO1: Develop practical skills in metallographic sample preparation and use optical microscopy with image analysis to evaluate grain size, phase distribution, and microstructural features in ferrous and non-ferrous alloys.

CO2: Conduct mechanical tests including hardness, tensile, and impact testing, and interpret fractured surfaces to understand material behavior and failure mechanisms.

CO3: Demonstrate critical thinking, collaborative laboratory work, and effectively communicate findings through technical reports.

Learning Resources

ASTM International (2023) *Annual Book of ASTM Standards: Metals Test Methods and Analytical Procedures*. West Conshohocken, PA: ASTM International.

Vander Voort, G.F. (ed.) (2004) *Metallography and Microstructures*. ASM Handbook, Vol. 9. Materials Park, OH: ASM International.

In-house Laboratory Manuals

Virtual Labs (NPTEL/VTU Virtual Lab)

Course	A CAREAGON	Course	Material	Course	D.C.	L	T	P	
Code	MM5172N	Name	Characterization Lab.	Category	PC	0	0	2	
Course Offering		Metallurg	etallurgy and Materials		Requisite Courses			Nil	
		Engineer	ing	кеци	isue Courses		IVI	ı	

	• To provide hands-on experience with advanced material characterization equipment and
Course	techniques.
Objective	• To teach experimental design, data acquisition, and interpretation related to material
	structure, composition, and morphology.
	• To bridge the gap between theoretical knowledge and real-world applications of
	characterization tools.

Module	Syllabus	Duration (h)
I & II	X-ray diffraction pattern analysis: Crystal structure, size and precise lattice parameter determination.	06
III & IV	Optical microscopy: Sample preparation and microstructural characterization.	09
V & VI	Electron Microscopes: Scanning Electron Microscopes and Transmission Electron microscopes, Image and diffraction pattern analysis	09
VII & VIII	Scanning probe Microscope: Scanning tunnelling microscope, Atomic force microscope, Magnetic force microscope demonstration	09
IX & X	Thermal Characterization techniques: DSC, DTA-TGA demonstration and analysis	06
XI	Test and Viva	3
	Total contact hours	42

	At the end of this course, students will be able to:						
Course	Basic knowledge about operating key characterization instruments like						
Outcome	XRD, SEM, AFM, and spectrometers.						
	Prepare samples and perform measurements.						
	Analyze and interpret real experimental data.						
	Choose suitable characterization methods for various material systems.						

Learning	B.D Cullity: Elements of x- ray diffraction Yang Leng: Materials Characterization: Introduction to Microscopic and Spectroscopic
Resources	Methods David B Williams, C. Barry Carter, Transmission Electron Microscopy

Course	MM5173N	Course	Mini Project/Machine	Course	PC	L	T	P
Code		Name	Learning in Materials Lab	Category		0	0	2
Course Offering		Metallurgy and Materials		Requisite Courses		NIL		
Department		Engineer	Engineering		Course	23	111.	L

	1.	Students will learn data preprocessing and feature engineering specific to materials				
Course		datasets (e.g., crystallographic, spectroscopic, mechanical properties).				
Objective	2.	Students will learn to use ML algorithms to predict material properties, discover new				
		materials, and optimize processing parameters.				
	3.	Students will learn to use tools and programming environments (e.g., Python, scikit-				
		learn, TensorFlow, Matminer) commonly used in materials informatics.				

Module	Syllabus					
I & II	& II Setting up a Python environment (Anaconda/Google Colab), Writing basic Python scripts, Loading and visualizing materials datasets using Pandas and Matplotlib.					
III & IV	& IV Work with materials databases (e.g., Materials Project), Perform data cleaning and visualize distributions of key material properties, Identify key features affecting material properties (e.g., composition, structure)					
V & VI	V & VI Predict material properties (e.g., hardness, conductivity) from composition and structure, Implement and compare models for prediction using scikit-learn, Hyperparameter tuning and cross-validation.					
VII & VIII	Use SVM to classify materials based on performance (e.g., brittle vs. ductile materials).	06				
IX & X	Build a simple neural network for regression or classification (e.g., predicting material properties from structure/composition).					
	Total contact hours	30				

	1.	Students will be able to Apply machine learning algorithms to analyze and interpret materials science data sets.
	2.	Develop predictive models for material properties using supervised learning techniques.
	3.	Implement unsupervised learning methods (e.g., clustering, dimensionality reduction) to
Course		explore and classify materials data.
Outcome	4.	Use open-source ML libraries (e.g., Scikit-learn, Matplotlib, Pandas, Matminer) to build
		reproducible data-driven workflows.
	5.	Evaluate model performance using appropriate metrics and improve models through
		hyperparameter tuning and feature selection.

Syllabus: Second Semester
Core Subject (Machine Learning in Materials Engineering & Materials Science and Engineering)

	Course Code	MM5201N	OlN Course Manufacturing Processes		0	Course	PC	L	T	P
	Code		Name	FI	ocesses	Category		3	0	0
Ī						_				

Pre-requisite Courses	NIL	Co-requisite Courses	NIL	Progressive Courses	NIL
Course Offering Department		Metallurgy and Enginee		Data Book / Codes/Standards	NIL

Course	Equip students with a deep understanding of scientific principles in manufacturing				
Objective	processes relevant to metallurgy and materials engineering, enabling analysis of				
	material-process interactions. Introduce advanced technologies like Semi-conductor				
	manufacturing and additive manufacturing, focusing on their applications.				

Module	Syllabus	Duration (class-hour)				
I	Overview of manufacturing science, materials behaviour, processing- structure-property relationships, classification of manufacturing processes					
II	Principles of casting, solidification mechanisms, casting processes (sand, die, investment), defects and quality control	6				
III	Plastic deformation, bulk forming (rolling, forging, extrusion), sheet metal forming,	8				
IV	Powder metallurgy processes: Metal powder production & characterization, powder blending, powder compaction, sintering, applications	4				
V	Joining Process: Arc Welding, Resistance welding, High energy beam welding, solid state welding, brazing, adhesive bonding	8				
VI	VI Semiconductor manufacturing: Crystal growth and wafer preparation, Ion Implantation, Photolithography, Thin Film Deposition, Etching, Metallization, Packaging					
VII	Additive manufacturing: Fundamentals of additive manufacturing VAT photopolymerization, Material Jetting, Material extrusion, direct energy deposition	4				

Course	Students will learn and analyze the scientific principles and material-process						
Outcome	interactions in manufacturing processes like casting, forming, powder metallurgy,						
	and additive manufacturing, evaluating and designing processes for specific						
	applications. They will apply advanced techniques, such as additive manufacturing,						
	to address modern engineering challenges, optimizing performance, cost, and						
	sustainability.						

Learning Resources	 Materials Processing and Manufacturing Science, Authors: Rajiv Asthana, Ashok Kumar, Narendra B. Dahotre Manufacturing Technology: Materials, Processes, and Equipment Authors: Helmi A. Youssef, Hassan A. El-Hofy, Mahmoud H. Ahmed
-----------------------	--

Course	MM5202N	Course	Mechanical Behaviour	Course	DC	L	Т	P
Code	1/11/15/20/21/	Name	of Materials	Category	PC	3	0	0

Pre-requisite Courses	NIL	Co-requisite Courses	NIL	Progressive Courses	NIL
Course Offering Department		Metallurgy and Materials Engineering		Data Book / Codes/Standards	NIL

Course Objective 1. Analyze the elastic and plastic response of materials using fundamental elasticity and plasticity theories 2. Explain the microstructural basis of plasticity utilising the concepts of resolved shear stress in single crystals and the role of defects in crystalline materials 3. Evaluate and analyze the role of Strengthening Mechanisms, including strain hardening, grain boundary effects (Hall-Petch), solid solution strengthening, and second-phase/precipitation hardening. 4. Analyze fracture behaviour in materials in light of fracture mechanics and toughening mechanisms

Module	Syllabus	Duration (h)
I	Review of Basic Mathematics Vectors and tensors, dot and cross products; rotation of vectors and tensors; calculation of eigenvalues and eigenvectors; introduction to programming using MATLAB	04
II	Theory of Elasticity Definition of stress and strain in 2-dimensions and in 3-dimensions; Mohr's circle of stress in two-dimensions; hydrostatic and deviatoric components of stress and strain; conversion of stresses to strains and vice-versa in elastic regime; Definition of elastic stiffness tensor for anisotropic materials; Micromechanics of linear elastic composites	08
III	Theory of Plasticity Yield criteria in metals, ceramics and polymers; yield locus in 2D and in 3D; Octahedral stresses and strains; Levi-Mises and Prandtl-Reuss equations; yielding of anisotropic materials;	08
IV	Microstructural Aspects of Plasticity Plasticity in single crystals; calculation of critical resolved shear stress; use of stereographic projection; Dislocations, interaction of dislocations; Twins; Stacking Faults	08
V	Strengthening Mechanisms Strain hardening, grain boundary strengthening, solid solution strengthening, second phase strengthening	04
VI	Fracture Fracture mechanisms, linear elastic fracture mechanics, toughening mechanisms	08
	Total contact hours	40

	1.	Apply Mathematical Frameworks employing computational tools like MATLAB for
		analyzing material behaviours
Course	2.	Analyze and study material behaviour applying the theory of elasticity and plasticity
Outcome		under practical applications.
Outcome	3.	Design microstructure and materials to improve mechanical properties utilising the
		knowledge of various strengthening mechanisms
	4.	Analyze failures in materials across length scales

Learning Resources Mechanical Behaviour of Materials, T. H. Courtney, Waveland Press Deformation and Fracture Mechanics of Engineering Materials: R.W. Hertzberg, John Wiley and Sons Mechanical Metallurgy, G.E. Dieter, McGraw-Hill Mechanical Behavior of Materials: M.A. Meyers, K K. Chawla, Cambridge Press Physical Properties of Crystals: Their Representation by Tensors and Matrices, J. Nye, Clarendon Press Getting Started with MATLAB, R. Pratap, Oxford University Press

Course	MM5203N	Course	Multiscale Materials	Course	PC	L	T	P
Code	IVIIVI32U3IN	Name	Modelling	Category	PC	3	0	0

Pre-requisite Courses	Nil	Co-requisite Courses	Nil	Progressive Courses	Nil
Course Offering Department		Metallurgy and Materials Engineering		Data Book / Codes/Standards	

Course Objective

- 1. **Understand the fundamentals** of materials modeling across different length and time scales (from electronic to continuum).
- 2. **Explore computational techniques** such as ab initio (first principles), molecular dynamics (MD), Monte Carlo (MC), and finite element methods.
- 3. **Develop skills in coupling methods** that integrate different scale models (e.g., quantum-atomistic, atomistic-mesoscopic).
- 4. **Apply multiscale modeling tools** to analyze mechanical, thermal, electrical, and optical properties of materials.
- 5. **Interpret simulation results** and correlate them with experimental data.

Module	Syllabus	Duration	
Wioduic	Synabus	(class-hour)	
I	Mathematical description of physical phenomena-basics of partial differential equations, statistical techniques and numerical analysis. Basics of optimization schemes: Simplex method, Steepest-descent Method, Conjugate Gradient Method, Newton-Raphson Method and Genetic Algorithm based schemes.	06	Basics of mathematical tool as applicable to the materials modelling.
П	Schemes of modelling- empirical, phenomenological and mechanistic approach of modelling. Deterministic, stochastic and probabilistic modelling approach of materials modelling.	06	Hierarchy of mathematical modelling and simulations for the problem formulation.
III	Quantum mechanics-based materials modelling approach – Applications of Density Functional Theory in materials modelling. Issue of convergence in Density Functional Theory calculations.	03	Basics of the quantum mechanics-based materials modelling.
IV	Atomistic modelling approaches. Classical interatomic potentials and their application for simulation of materials. Basics of Molecular Dynamics and Monte Carlo approach.	02	Understanding of atomistic modelling approach and its applications in materials engineering.
V	Mesoscale approach for materials modelling-Basics of Finite Difference and Finite Element Method. Application of Finite Element Method for studying multi-physics phenomena. Cellular Automata and its application in Materials Engineering.	03	Understanding about mesoscale materials modelling approach and their application for modelling the microstructural phenomena.

VI	Coupling of scales for development of multiscale materials models for structure-property correlation in materials science and manufacturing. Uncertainty quantification in multiscale modelling-traditional and Bayesian approaches.	05	Basics of the bridging between various modelling schemes at range of spatiotemporal scale and error propagation schemes.
VII	Case-studies: 1. Integrated Computational Materials Engineering (ICME) approach for studying plasticity in materials. 2. Multiscale modelling of design of high temperature material for turbine applications.	05	Application of various modelling and simulation schemes for the industrial relevant applications.

- 1. **Explain key concepts** of different modeling approaches and their applicable scales (e.g., DFT at quantum scale, MD at atomistic scale).
- 2. **Select appropriate models** and techniques for analyzing a given materials problem across multiple scales.
- 3. **Analyze and interpret simulation data**, identifying limitations and sources of error across scales.
- 4. **Implement coupling strategies** to link models at different scales (e.g., quantum-to-continuum approaches).
- 5. **Demonstrate problem-solving ability** in case studies involving real-world material systems (e.g., metals, polymers, composites).

Learning Resources

- 1. Multiscale materials modelling: Fundamentals and applications, Z. Xiao Guo, CRC press.
- 2. Multiscale Modelling: A Bayesian Perspective, Springer.
- 3. Integrated Computational Materials Engineering (ICME) for Metals: Using multiscale modelling to invigorate engineering design with science, M.E. Horstemeyer, Wiley.
- 4. Molecular Modelling: Principles and Applications, Andrew R. Leach, Pearson

PSE: Machine Learning in Materials Engineering

Course	obo ^r	MM5224N	Course	Deep learning	Course	PSE	L	Т	P
Course	Course Code	WIWI5224IN	Name	for materials engineering	Category	PSE	3	0	0

Pre-requisite Courses	NIL	Co-requisite Courses	NIL	Progressive Courses	NIL
Course Offering Department		Metallurgy and Materials Engineering		Data Book / Codes/Standards	NIL

Course Objective

- 1. Students will grasp the core concepts of deep learning, including neural networks, backpropagation, activation functions, and optimization techniques.
- 2. Students will implement machine learning and deep learning models to analyze experimental and computational materials datasets.
- 3. Students will use deep learning to discover and predict relationships between material structures, processing parameters, and resulting properties.
- 4. Students will employ deep learning frameworks for inverse design and property optimization in materials engineering.
- 5. Students will develop the ability to work in interdisciplinary teams, bridging materials science, computer science, and data analytics.

Module	Syllabus	Duration (h)
	Introduction to Deep Learning: Role of Data Science and Machine Learning	05
τ.	in MSE, Basics of Deep Learning: Neural Networks, Activation Functions, and	
I	Backpropagation, Introduction to Python for Deep Learning (libraries: Tensor	
	Flow, Keras, PyTorch).	
	Materials Data Representation: Types of Materials Data: Experimental Data,	05
	Simulation Data, Databases, Feature Engineering for Materials Science:	
II	Atomic Structures, Crystal Graphs, and Descriptors, Data Preprocessing:	
	Normalization, Scaling, and Encoding, Data Splitting, Cross-validation, and	
	Performance Metrics (Accuracy, Precision, F1-score)	
	Neural Networks and Architectures for Materials Science: Multi-layer	05
***	Perceptrons (MLP) for Materials Property Prediction, Convolutional Neural	
III	Networks (CNNs) for Image-based Materials Data (e.g., microscopy images),	
	Recurrent Neural Networks (RNNs) for Time-series Data (e.g., material	
	degradation over time), Transfer Learning and Fine-tuning for Materials Data	0.5
	Generative Models for Materials Design: Introduction to Generative Adversarial Networks (GANs), Variational Autoencoders (VAEs) for Material	05
IV	Generation,	
l v	Application of Generative Models for Predicting New Materials, Case Studies:	
	Designing Novel Alloys, Polymers, or Catalysts	
	Deep Learning for Microstructure and Process-Property Relations: Image	8
	Analysis of Microstructures: CNNs for Material Characterization, Predicting	O
V	Process-Property Relations (e.g., temperature, pressure effects), Multi-scale	
•	Modeling with Deep Learning, Case Study: Predicting the Effect of Processing	
	on Microstructure and Mechanical Properties	
	Transfer Learning in Materials Science: The theory of transfer learning:	4
VI	source and target domains. Types of transfer learning: inductive, trans-ductive,	
	and unsupervised. Domain adaptation and domain generalization.	
	Integration of Deep Learning with Quantum Mechanics and Molecular	4
VII	Simulations : Deep learning for electronic structure predictions (e.g., predicting	
V 11	HOMO-LUMO gaps, charge densities), Deep learning for electronic structure	
	calculations (energy, wave functions)	

VIII	AI-driven Materials Engineering in Industry : AI in manufacturing: additive manufacturing, casting, forging, Process optimization using AI: predictive modeling and process control, Industry 4.0 and smart factories in materials engineering	
	Total contact hours	40

- . Students will be able to describe the foundational principles of deep learning and their relevance to materials engineering problems.
- 2. Students will be able to preprocess, analyze, and visualize materials datasets for input into deep learning models.
- 3. Students will be able to design, train, and evaluate deep neural networks using libraries such as TensorFlow or PyTorch.
- 4. Students will be able to apply deep learning models to predict material properties, classify material phases, or simulate microstructural evolution.
- 5. Students will be able to develop and implement inverse design models for discovering materials with targeted properties.

Learning Resources

"Deep Learning" by Ian Good fellow, Yoshua Bengio, and Aaron Courville

"Neural Networks and Deep Learning: A Textbook" by Charu Aggarwal

"Materials Informatics: Data-Driven Discovery in Materials Science" by Rajiv S. Mishra and Akash M. Srivastava

"Machine Learning for Materials Informatics: Data-Driven Discovery in Materials Science" by S. S. Pandey, A. A. Hassan, and B. G. Sumpter

Course		Course Microstructure		Солича	Open	L	T	P	
Code	MM5225N	Name	Modelling for metallic system			Elective	3	0	0
		Metallur	Pro-ronnisho (nurs		ses	NI.	L		
Departm	Department 33 8		ing		170 704	mone com s		1,1	

	1.	Students will learn fundamental and practical understanding of microstructure evolution					
Course		in metallic systems through computational modeling techniques.					
Objective	2.	Students will learn to simulate and analyze microstructural changes—such as grain					
		growth, phase transformations, and precipitation—using theoretical concepts and					
		numerical methods					

Module	Syllabus	Duration (h)				
I	Thermodynamics of Phase Transformation: Solution thermodynamics, Introduction to CALPHAD thermodynamic modelling, Irreversible Thermodynamics					
II	Modeling of precipitation: Nucleation, Diffusion controlled growth, Sharp interface theory, Interface controlled growth, JMAK kinetics, Application in Multiparticle precipitation kinetics.	8				
III	Monte Carlo Potts Model: Hamiltoninan and dynamics, Ising model, Q-state Potts Model, Application in Grain growth and Recrystallisation	8				
IV	Phase-field Model: Concept of diffuse interface, Allen-Cahn equation, Multiphase-field model, Diffusion coupled phase-field model, Application in Solidification, Cahn-Hilliard Model for Phase Separation.	12				
V	Cellular Automata: Basic algorithm of Cellular Automata, Coupling of diffusion, Application in Phase Transformation.	6				
	Total contact hours					

	1.	Students will be able to apply theoretical models such as phase-field, Monte Carlo, and				
Course		cellular automata to simulate microstructural processes.				
Outcome	2.	Students will be able to use computational tools to model grain growth, recrystallization,				
		nd phase transformations in metals.				
	3.	Students will be able to design and optimize microstructures to achieve desired properties in engineering applications using modeling approaches				

Laguring	Computational Materials Engineering by Koenraad G. F. Janssens, Dierk Raabe, Ernst Kozeschnik, Mark A Miodownik, Britta Nestler; Elsevier.						
Learning Resources	Continuum Scale Simulation of Engineering Materials by Dierk Raabe, Franz Roters, Frederic Barlat, Long-Qing Chen; Wiley-VCH. Methods.						

PSE: Materials Science and Engineering

Course Code	MM5221N	Course Name	Sel	esign and lection of laterials	ection of Course		3	T 0	P 0
Pre-requisite Courses NIL		_	Co-requisite NIL		Progress Course			NIL	
Course Offering Department			Metallurgy and Materials Engineering		Data Book / Codes/Standards		NIL		

Course Objective	The main objective of the course is to allow students to develop a systematic procedure for selecting materials that best match the requirements of a product design.	
---------------------	---	--

Module	Syllabus	Duration (class- hour)				
I	Classification of materials and processes, Introduction to material property charts	3	Students will get a basic understanding of material property charts			
II	Design-linked strategy of selecting materials and processes	3	Students will understand the underlying mechanism for selecting materials and processes for different products/applications			
III	Review of Mechanical properties of materials: atomic/molecular origin of stiffness, yield criteria, strengthening mechanisms, fracture mechanics, fatigue	es of gin of associated with properties of materials es, fatigue				
IV	Selection of materials based on mechanical properties: Stiffness-limited design, Strength-limited design, Material indices for yield-limited design, Material property charts for toughness, Material property charts for fatigue, Fracture-limited design, Material property charts for friction and wear and associated case studies	9	Students will understand different material property charts associated with mechanical properties of materials.			
V	Selection of materials based on thermal properties: Review of thermal properties of materials, Thermal property charts, Case studies of design using thermal properties	3	Students will review concepts associated with thermal properties of materials. Students will be able to interpret thermal property charts			
VI	Selection of creep-resistant materials: Review of creep behaviour and deformation mechanism maps, Charts for creep behaviour, Case studies of design to cope with creep	6	Students will review high temperature deformation behaviour and understand material charts for creep			
VII	Selection of materials based on electrical properties: Review of electrical properties, Charts for electrical properties, Case studies of design using electrical properties	5	Students will review basic electrical properties and understand charts associated with electrical properties.			

	VIII	Selection of materials based on magnetic properties: Review of magnetic properties, Charts for magnetic properties, Case studies of materials selection for magnetic design	5	Students magnetic understand magnetic p	l charts	basic and ed with
ſ		Total contact hours	40			

CO1: On completion of the course, the students should gain an understanding of the concept of product design and how material selection is an integral part of the design process CO2: On completion of the course, the students should be able to interpret material property charts and use appropriate material indices based on the requirement of design CO3: On completion of the course, the students should be able to select appropriate materials for applications that involve mechanical deformation or are subject to temperature fields/electrical fields/magnetic fields.

Learning Resources

Materials: Engineering, Science, Processing and Design, Michael Ashby, Hugh Shercliff, and David Cebon, Butterworth-Heinemann, 4th edition **Materials Selection in Mechanical Design**, Michael F. Ashby, Butterwoth-Heinemann, 6th edition

Materials Science and Engineering: An Introduction, William D. Callister Jr. and David G. Rethwisch, Wiley, 10th edition

Course	MM5223N	Course	Surface Treatment	Course	PSE	L	Т	P
Code	WIWI5225IN	Name	and Modification	Category	FSE	3	0	0

Pre-requisite Courses	NIL	Co-requisite Courses	NIL	Progressive Courses	NIL
Course Offering	Department	Metallurgy and Materials Engineering		Data Book / Codes/Standards	NIL

Course
Objective

The students will learn the fundamental of surface treatment and modification techniques that enhance material performance. The students will understand possible techniques to improve properties such as wear resistance, corrosion resistance, and fatigue strength, enabling students to select appropriate processes for extending the life of engineering components in service.

Module	Syllabus	Duration (h)	Module Outcome
I	Introduction Conventional Surface Engineering, Types of Surface Modifications, Physical Modifications, Chemical Modifications, Applications of Surface Engineering towards Nanomaterials, Structure, Defects in solids, Bonds and Bands in Materials, Thermodynamics of Materials, Kinetics, Nucleation	06	Gain knowledge of surface engineering methods, material structures, thermodynamics, kinetics, and their applications
II	Vacuum Science and Technology Kinetic Theory of Gases, Gas Transport and Pumping, Vacuum Technology	06	Understand kinetic theory, gas transport mechanisms, and vacuum technologies for scientific and industrial applications.
III	Thin-film Evaporation Processes Physics and Chemistry of Evaporation, Film Thickness Uniformity, Evaporation Processes and Applications	06	Understand evaporation physics and chemistry, achieve uniform film thickness, and explore thinfilm applications and processes.
IV	Discharges, Plasma, and Ion-Surface Interactions Plasma Discharges and Arcs, Fundamentals of Plasma Physics, Reactions in Plasmas, Physics of Sputtering, Ion bombardment modification of growing films	06	Understand plasma physics, discharges, sputtering, and ion-surface interactions for thin-film growth and material modifications.
V	Chemical Vapor Deposition Reaction types, Thermodynamics of CVD, Gas transport, Film growth kinetics, Thermal CVD, Plasma-enhanced CVD	08	Understand CVD reaction types, thermodynamics, gas transport, and film growth kinetics in thermal and plasma-enhanced processes.
VI	Substrate Surface and Thin-film Nucleation Atomic view of substrate surface, Thermodynamic aspects of nucleation, Kinetic processes in nucleation and growth	08	Learn substrate structure, nucleation thermodynamics, and kinetics of thin-film growth.
		40	

	enhancing surface properties like hardness, corrosion and wear resistance, thereby improving the performance and durability of engineering materials.
Learning Resources	Materials Science of Thin Films by Milton Ohring Handbook of Surface Improvement and Modification Hardcover – Import, 1 March 2023 by George Wypych Chemical Modification of Solid Surfaces by the Use of Additives, by Ranjan Kumar

Mohapatra, Debadutta Das, Md. Azam

Students will be able to understand and analyse various surface treatment techniques,

select suitable methods for specific applications, and evaluate their effectiveness in

Course

Outcome

Open Elective

Course	MM5261N	Course	Nanostructures and	Course	OF	L	T	P	
Code	MM5261N	Name	Nanomaterials	Category	OE	3	0	0	

Pre-requisite Courses	Physics of Materials	Co-requisite Courses Thermodynamics		Progressive Courses	Nil
Course Offering	g Department	Metallurgy and Materials Engineering		Data Book / Codes/Standards	

Course Objective Course objectives include understanding fundamental nanoscience concepts, exploring synthesis methods, learning characterization techniques, and examining the diverse applications of nanomaterials.

Module	Syllabus	Duration (class-hour)	Module Outcome
I	Introduction to nanostructures and nanomaterials	02	The students will be get an historical overview about the evolution of nanostructures, nanomaterials and its importance for potential application in various advanced technologies.
II	Classification of nanomaterials. Effect of size on the properties of materials and nanomaterials. Microstructural features of nanomaterials. Characterization of nanostructures and nanomaterials.	08	The students will be able to understand and differentiate between nanostrucutures, nanomaterials and traditional materials. The students will also develop an understanding about the functionalities of this class of materials from the viewpoint of their crystal structure and size effects on the properties of the material.
III	Preparation of Nanomaterials by Physical Methods: Inert gas condensation, Arc discharge, Plasma arc technique, Laser ablation, Ball Milling, Chemical vapour deposition, Electro deposition	06	The students will be introduced to the different physical techniques for preparing nanomaterials. They will also learn to classify different top down and bottom up approaches
IV	Synthesis of Nanomaterials via chemical routes: Chemical precipitation and coprecipitation; Metal nanocrystals by reduction, Sol-gel synthesis; Solvothermal synthesis; Thermolysis, Microwave heating synthesis; Sono-chemical synthesis; Electrochemical synthesis; Photochemical synthesis, Synthesis in supercritical fluids	08	The students will be introduced to the different chemical techniques and other advanced processing techniques.
V	Properties of nanowires, quantum wells and quantum dots	06	The students will learn how quantum confinement affect material properties and impart unique functionalities.

VI	Carbon nanostructures: Synthesis and properties of fullerenes, carbon nanotubes, Graphene	08	This module will equip students with the knowledge and skills to understand, the structure property relations of carbon nanostructures. The module will also highlight the need for developing an economical technique for bulk production of different types of carbon nanostructures.
VII	Application of Nanostructures and nanomaterials	02	The student will become acquainted with the examples and methods of improving material properties, device performance across different fields
	Total contact hours	40	

Course	The student will be able to understand nano-length scales and the properties of size-
Outcome	dependent materials and also will be able to correlate properties of nanomaterials and
	nanostructures with their size, shape and surface characteristics.
	The course will offer a robust foundation for continued learning and involvement in
	nanoscience and nanotechnology, encompassing both research and development.

Learning	Nanostructures and nanomaterials: Synthesis, properties & applications by Guozhong Cao
Resources	Chemistry of nanomaterials: Synthesis, properties and applications by CNR Rao et.al.

Course Code	MM5262	Course Name	Materials and		OE	L 3	T 0	P 0	
Pre-requisite Courses	Physics Materia	_	Co-requisite Courses Thermodynamics		Progressive Courses		1	Vil	
Course Offerin	g Departme	mt Me	Metallurgy and Materials Engineering		C	Data Book odes/Stand			

Course Objective	To introduce the fundamental concepts of biomaterials, their properties, interactions			
	with biological systems, and the principles behind biomedical devices.			
	To provide knowledge on materials selection, design strategies, and fabrication			
	techniques for biomedical applications.			
	To develop an understanding of the regulatory, ethical, and clinical challenges			
	associated with biomedical materials and devices.			

Module	Syllabus	Duration (h)
I	Basics: Materials and Biology: Metal, Ceramic, Polymer, Composite; Bioresorbale and bioerodable materials	04
II	Biomaterials Surfaces: Physics; Surface Structure and Properties; Surface Energy; Adsorption, Segregation, and Reconstruction at Surfaces; Reactions at surfaces; Protein- Surface Interactions; Host Response to Biomaterials; Cell Adhesion Mechanisms; Coagulation Cascade	08
III	Testing of biomaterials: In vitro and in vivo assessment; evaluation of blood material interactions; Microscopic techniques; Spectorscopic Techniques	06
IV	Degradation of Materials: Degradation of polymers; Degradation effect on metals and ceramics	06
V	Materials in medicine, biology and artificial organs: Cardiovascular Medical Devices; Implantable Cardiac Assist Devices; Orthopedic Applications; Dental Implantation; Intraocular Lens Implants; Drug Delivery Systems; Biomedical Sensors and Biosensors	12
VI	Case studies: Fiber Optic Biosensors, Nanobarcodes; Drug Delivery: Controlled Release; Mechanical Pumps; Artificial Pancreas, Cartilage, Nerve Regeneration	06
	42	

Course	•	Understand the structure-property relationships of various biomaterials.
Outcome	•	Select appropriate materials for specific biomedical applications.
	•	Analyze the interaction of materials with tissues and biological fluids.
	•	Design and evaluate biomedical devices considering biocompatibility and mechanical
		performance.
	•	Familiarize themselves with clinical, ethical, and regulatory frameworks.

Learning Resources	Ratner, Buddy D., et al. Biomaterials Science: An Introduction to Materials in Medicine
	B.Basu, D.Katti and Ashok Kumar; Advanced Biomaterials: Fundamentals, Processing

and Applications; John Wiley & Sons, Inc., USA (ISBN: 978-0-470-19340-2), September, 2009.