M.Tech. in Computational Materials Engineering

॥ त्वं ज्ञानमयो विज्ञानमयोऽसि ॥

Introduction

Metallurgical and Materials Engineering is an interdisciplinary branch that deals with converting raw materials into a product by leveraging upon design, extraction, processing, and characterization of materials for aerospace, automotive, energy, electronics, and healthcare applications. The following are the focus areas of the Department: (a) Computational Materials Engineering, (b) Structural Materials, (c) Functional Materials, and (d) Process Metallurgy. Computational Materials Engineering provides an understanding of materials from atomistic to macro length scales and leads to smart and intelligent materials selection, alloy design, the discovery of unknown materials as well as improvement of metallurgical processes. The major focus of the Structural Materials area is to understand the processing-microstructure-property correlation for designing and processing materials with superior combinations of properties in the finished engineering products. Functional Materials possess one or more native properties that can be triggered by an external stimulus (electric/magnetic fields). Hence these materials are used for a plethora of functional devices ranging from energy harvesting, healthcare, and modern-day information technology. Process Metallurgy deals with mineral beneficiation and metal extraction.

The Department offers an M.Tech. program and an M.Tech.-Ph.D. dual degree program in Materials Engineering. Incoming students choose a specialization from the following four specializations at the beginning of their first semester: (a) Computational Materials Engineering, (b) Structural Materials, (c) Functional Materials, and (d) Process Metallurgy. The credits required for the M.Tech. degree are distributed among the program core, specialization core, specialization electives, program electives, open electives, project, and non-graded compulsory activities. The program core courses are common among all specializations and cover the core concepts within the discipline of Materials Engineering. The student will take the specialization core courses and the specialization elective courses offered in the chosen specialization and conduct a project within that specialization. The specialization core courses provide the essential background of the chosen specialization and prepare the students for the specialization electives as per their options exercised. The program elective courses in the program structure are designed to ensure sufficient breadth in Materials Engineering, and these courses must be chosen from the other specializations within the program. The open elective courses allow students to explore courses from any department. Previously, the course curriculum for the Structural Materials, and Process Metallurgy specializations was presented. Here, the course curriculum for Computational Materials Engineering is presented.

Objectives

- Provide rigorous academic and research training in advanced areas of Materials Engineering.
- Produce professionals with an in-depth understanding of Materials Engineering, capable of providing solutions to meet future materials challenges.
- Educate students to become academicians, scientists, innovators, and entrepreneurs.

Graduate attributes

- In-depth understanding of thermodynamic and kinetic principles of Materials.
- Knowledge to characterize features at various length scales using experimental and computational approaches.
- Comprehend and intelligently design structure, micro-structure property correlation.
- Skills to effectively communicate scientific findings to peers and the general public.
- Appreciation and adherence to professional ethics.
- Innovative skills to design and execute technical projects.

(a) Computational Materials Engineering

- Ability to use various computational techniques for studying materials behavior/properties starting from atomic to macro scale.
- Ability to employ various computational tools to understand process controlling parameters.
- Ability to apply emerging data analysis-based technologies for deeper understanding and innovation in materials design.

Learning Outcome

Ability to

- Apply thermodynamic and kinetic principles to understand and control materials processes and properties.
- Identify appropriate experimental techniques to characterize materials at various length scales.
- Define a research problem and devise an appropriate methodology for addressing the same.
- Identify normative commitments of technological knowledge, artifacts, and familiarity with the manifold responsibilities linked to their profession.
- Critically develop linguistic competence and subject competence in the genres of technical communication.

(a) Computational Materials Engineering

- Integrate computational techniques, combinatorial/high-throughput experiments, and advanced characterization to reduce the time scale of the development of engineered products.
- Apply artificial intelligence and data science techniques to design and innovation in materials engineering

Program structure with courses

Cat.	Course Number	Course Title	L-T-P-D	Credits		Cat.	Course Number	Course Title	L-T-P-D	Credits
I Semester						**II Semester**				
MC	MTL7XX0	Computational Thermodynamics and Kinetics of Materials	3-0-2-0	4		MC	MTL7XX0	Structure and Characterization of Materials	3-0-2-0	4
MC	MTL7XX0	Industry 4.0: Applications in Metallurgical and Materials Engineering	2-0-0-0	2		SC	MTL7XX0	Specialisation Core-2	2-0-0-0	2
SC	MTL7XX0	Specialisation Core - 1	3-0-2-0	4		SC	MTL7XX0	Specialisation Core-3	0-0-2-0	1
SE	MTL7XX0	Specialisation Elective-1	3-0-0-0	3		SE	MTL7XX0	Specialisation Elective-3	3-0-0-0	3
SE	MTL7XX0	Specialisation Elective-2	3-0-0-0	3		SE	MTL7XX0	Specialisation Elective-4	3-0-0-0	3
NH	HSN7XX0	Technical Communication	1-0-0-0	0		NH	HSN7XX0	Innovation and IP Management	1-0-0-0	0
Total				**16**		Total				**13**
III Semester						**IV Semester**				
SE	MTL7XX0	Specialisation Elective-5	3-0-0-0	3		OE		Open Elective-2	3-0-0-0	3
SE	MTL7XX0	Specialisation Elective-6	3-0-0-0	3		MP	MTD7XX0	Project (Stage-II)	0-0-0-11	11
OE		Open Elective-1	3-0-0-0	3		NH	HSN7XX0	Professional Ethics	1-0-0-0	0
MP	MTD7XX0	Project (Stage-I)	0-0-0-5	5						
NH	HSN7XX0	Systems Engineering and Project Management	1-0-0-0	0						
			Total	**14**					Total	**14**

Distribution of Credits (M.Tech.)

S.No.	*Category*	*Category Title*	*Total Credits*
1	MC	Program Core	10
2	SC	Specialisation Core	7
3	SE	Specialisation Elective	**12 (18)**
4	ME	Program Electives	**6 (0)**
5	OE	Open Electives	6
6	MP	Project	16
7	NH	Non-Graded Compulsory	4
		Total (Graded)	**57**
		Total (Graded + Non-graded)	**61**

M.Tech. Program Courses

List of Program Core courses

Course Number	***Course Title***	***L-T-P-D***	***Credits***
MTL7XX0	Computational Thermodynamics and Kinetics of Materials	3-0-2-0	4
MTL7XX0	Structure and Characterization of Materials	3-0-2-0	4
MTL7XX0	Industry 4.0: Applications in Metallurgical and Materials Engineering	2-0-0-0	2

List of Specialization Core courses

(a) Computational Materials Engineering

Course Number	***Course Title***	***L-T-P-D***	***Credits***
CSL7XX0	Fundamentals of Machine Learning	3-0-2-0	4
MTL7XX0	Modelling in Materials Engineering	2-0-0-0	2
MTL7XX0	Computational Materials Engineering Laboratory	0-0-2-0	1

List of Specialization Elective courses

List of specialization elective courses to be offered for M.Tech. students under different specializations:

(a) Computational Materials Engineering

Course Number	***Course Title***	***L-T-P-D***	***Credits***
MTL7XX0	First-Principles Calculations	2-0-2-0	3
MTL7XX0	Alloy Design: Computational Thermodynamic approach	3-0-2-0	4
MTL7XX0	Principles of Continuum Mechanics	3-0-0-0	3
MTL7XX0	Continuum Plasticity	3-0-0-0	3
MTL7XX0	Crystal Plasticity and Its Applications	3-0-0-0	3
MTL7XX0	Modelling of Metallurgical Processes	3-1-0-0	4
7XX0	Microstructure Image Processing	2-0-0-0	2
MTL7XX0	Machine Learning for Materials Design	2-0-2-0	3
MTL7XX0	Phase-Field Modelling	3-0-0-0	3
MTL7XX0	Symmetry, Structure, and Tensor Properties	3-0-0-0	3
MTL7XX0	Advanced Molecular Dynamics	3-0-0-0	3
MTL7XX0	Single and Multi-objective Evolutionary and Nature Inspired Algorithms	1-0-0-0	1
MTL7XX0	Data Visualisation in Materials Modelling	1-0-0-0	1
Courses from other Departments			
PHL7XX0	Computational Materials Science	3-0-0-0	3
MEL7XX0	Finite Element Methods in Engineering	3-0-0-0	3
MEL7XX0	Computational Fluid Dynamics and Heat Transfer	3-1-0-0	4
CHL7XX0	Advanced Process Control and AI Applications	3-0-0-0	3
CHL7XX0	Data Analytics in Process Modelling and Simulation	2-0-2-0	3
CHL7XX0	Molecular Simulations (2-0-0)	2-0-0-0	2

Program Elective courses

A student from a given specialization should opt for Program Elective courses from the other specialization courses (core and elective).

Open Elective courses

The open elective courses can be taken from courses offered by any Department.

DETAILED SYLLABUS FOR PROGRAM CORE COURSES

Title	**Computational Thermodynamics and Kinetics of Materials**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3–0–2 [4]
Offered for	M.Tech.	Type	Program Core
Pre-requisite			

Objectives

1. Provide a basis for describing and understanding the stability of various forms of matter.
2. Provide a basis for predicting the properties of an equilibrated system as a function of its content and characteristics.

Learning Outcomes

1. Understanding of the conditions for stability of a material and derive its properties.
2. Knowledge of parameters to control the evolution of microstructures.

Course Content

Laws of thermodynamics and Chemical reactions (14 lectures)
First, second and third laws (3 lectures), statistical interpretation of entropy (3 lectures) Free energy functions and criteria for equilibrium (3 lectures), reaction equilibrium, the equilibrium constant; applications to materials and metallurgical systems (5 lectures).

Thermodynamics of solutions and phase diagrams (14 lectures)
Ideal and non-ideal solutions, partial and molar quantities, quasi-chemical model and regular solutions (3 lectures), Phase rule and binary phase diagrams (2 lectures), free energy composition diagrams (5 lectures), phase equilibrium calculations. (4 lectures)

Thermodynamics of interfaces and kinetics (14 lectures)
Interfaces, surface tension and surface energy (3 lectures), equilibrium at interfaces, nucleation (3 lectures), coherency (1 lecture), thermal activation, diffusion, concentration gradients, thermal gradients (3 lectures), Fick's laws, mechanisms of interface migration (3 lectures)

Computational Tutorials (Thermocalc and DICTRA):
1. Single-Point Equilibrium calculations
2. Calculation of thermodynamic properties of elements
3. Calculation Thermodynamic Properties of Compounds
4. Calculation Thermodynamic Properties of Solution Phases
5. Computation of Phase equilibria
6. Stepping in Temperature in the Fe-C System,
7. Fe-C Phase Diagrams calculations,
8. Fe-Cr-C Ternary Phase Diagram at 1000 K,
9. Stable and the Metastable Fe-C Phase Diagrams
10. Thermodynamics of reactions
11. Calculation of activation energy
12. Calculation of partition coefficient

Text Books

1. Gaskell, D.R., *Introduction to Metallurgical Thermodynamics*, McGraw-Hill 1995.
2. Swalin, R. A., *Thermodynamics of Solids*, reprint Edition, Wiley, 1962.
3. Balluffi, R. W., Samuel, M. A., Carter, W. C., *Kinetics of Materials*, Wiley, 2005.
4. Porter, D. A., Easterling, K. E., and Sherif, M. Y., *Phase Transformation in Metals and Alloys*, 3rd edition, CRC Press, 2009.

Self-Learning Material

1. Bird, R.B., Stewart, W.E. and Lightfoot, E.N., *Transport Phenomena*, Wiley, 1960.

2. Hillert, M., *Phase Equilibria, Phase Diagrams and Phase Transformations Their Thermodynamic Basis,* Second edition, Cambridge University Press 2008.

Title	**Structure and Characterization of Materials**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3–0–2 [4]
Offered for	M.Tech.	Type	Program core
Pre-requisite			

Objective

1. Understanding the principles of instruments and methods for characterising different materials and their properties.

Learning Outcomes

1. Basic working knowledge of various instruments.
2. Ability to identify and choose different characterization techniques for specific property analysis.

MTL7XX1 Introduction to Diffraction [1-0-0]

Structure of Materials (7 Lectures): Crystal structure, Symmetry elements and point group notations, Miller indices and Weiss zone law, Stereographic projections, Reciprocal space, Brillouin Zone

Diffraction based characterization *(7 Lectures)*: Structure of crystalline and non-crystalline materials by X-ray diffraction, structure factor, indexing of lattice planes and lattice parameter determination, electron and neutron diffraction, small angle scattering

MTL7XX2 Characterization Using Electron Microscopy [1-0-0]

Scanning electron microscope (7 Lectures): Basis of image contrast and various operating modes, sample-electron interaction, cathodoluminescence, voltage contrast mode, Magnetic contrast mode, FEGSEM, Environmental SEM, Low voltage SEM. Electron back scattered diffraction/OIM, micro-textural analysis.

Transmission electron microscope (7 Lectures): Lens defects, aberration corrected TEM, Mass-thickness contrast, diffraction contrast and crystal defect, BF, DF, Weak beam DF images. Electron Diffraction: SADP. Phase contrast and HRTEM.

MTL7XX3 Spectroscopic Surface Analysis [1-0-0]

Chemical Analysis (5 Lectures): Optical emission spectroscopy, energy dispersive spectroscopy, Wavelength dispersive spectroscopy, X-ray fluorescence spectroscopy, Electron Probe Microanalysis, Electron energy loss spectroscopy.

Surface analysis (5 Lectures): X-ray photoelectron spectroscopy, UPS, Dynamic SIMS and static SIMS.

Spectroscopic characterization (4 Lectures): FTIR, and Raman spectroscopy, Mössbauer spectroscopy.

Lab Experiments

Calculation of thermodynamic parameters using DSC analysis;
Functional group analysis using FTIR;
XRD Pattern Indexing;
Lattice parameter and crystallite size calculation;
XRD Profile fitting;
SEM/EDS analysis;
UV-visible analysis and band gap calculation;
Electron Diffraction Pattern Indexing;

Image Analysis.

Text Books

1. Zhang, S., Li, L. and Kumar, A., *Materials Characterization Techniques*, CRC Press, 2008.
2. Brandon D., Kaplan W.D., Microstructural Characterization of Materials, 2nd Edition, Wiley, 2008
3. Barrett C. S., Massalski T. B., Structure of Metals. 3rd revised edition. Pergamon Press, 2006

Self-Learning Material

1. Evans, C., Brundle. R. and Wilson, *Encyclopaedia of Materials Characterization: Surfaces, Interfaces, Thin Films (Materials Characterization Series),* Butterworth-Heinemann, 1992.
2. Kaufmann, E.N., *Characterization of Materials, 3 Volume Set, 2nd Edition,* Wiley, 2012.

Online Course Material

1. Shankaran, S., Materials Characterization, Department of Metallurgical & Materials Engineering, Indian Institute of Technology, Madras, NPTEL http://nptel.ac.in/courses/113106034/
2. Biswas, K. and Gurao, N.P., Advanced Characterization Techniques, Department of Materials Science and Engineering, Indian Institute of Technology, Kanpur, NPTEL http://nptel.ac.in/courses/113104004

Title	**Industry 4.0: Applications in Metallurgical and Materials Engineering**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	2-0-0 [2]
Offered for	M.Tech. Materials Engineering	Type	Program core
Prerequisite	Nil		

Objectives

The Instructor will:

1. Introduce the importance of Industry 4.0 in context with Metallurgical and Materials Engineering
2. Provide a thought process to move from conventional to emerging technology in production and quality control

Learning Outcomes

The students are expected to gain:

1. Appreciation towards the evolutionary technology as a disruptive industrial growth
2. Knowledge to divide and integrate the production line steps and develop an inclination to for optimising the production lines.

Contents

Introduction: Concept of Industry 4.0, Types of metallurgical and materials industries, Product range, Present production practice (4 Lectures)

Process and Product Line Analysis: Typical flow charts from raw materials to processing of intermediate and final products, Their quality control at different stages of production, Product qualification methods, Property and performance evaluation, Product life prediction, Recyclable and repair options, Methods for data collection and processing (6 Lectures)

Automation:

Introduction to IoT: Sensing, Actuation, Basics of IoT Networking, IoT Architecture, Integration of Sensors and Actuators for Implementation of IoT (6 Lectures);

Basics of Industrial IoT: Industrial Processes, Industrial Sensing & Actuation, Industrial Internet Systems, Basics of Predictive maintenance (6 Lectures)

Application of Industry 4.0 in Metallurgical & Materials Engineering:

Optimized energy costs, Adaptive manufacturing, Preventive maintenance,

Defect detection and minimisation, Yield optimisation (6 lectures)

Laboratory Experiments

NA

Textbook

1. Rana, R. and Singh, S.B., *Automotive Steels: Design, Metallurgy, Processing and Applications*, Woodhead Publishing, 2016.
2. Vignes, A., *Extractive Metallurgy 3: Processing, Operations and Routes*, John Wiley & Sons, 2013.
3. Kamal, R., Internet of Things - Architecture and Design Principles, 1st Edition, Mcgraw Hill, 2017.

Online Course Material

1. Misra, S., 2018, *Introduction to Industry 4.0 and Industrial Internet of Things*, IIT Kharagpur. https://nptel.ac.in/courses/106/105/106105195/

DETAILED SYLLABUS FOR THE SPECIALIZATION CORE COURSES

(a) Computational Materials Engineering

Title	**Fundamentals of Machine Learning**	Number	CSLXXX0
Department	Computer Science and Engineering	L–T–P: C	3–0–2: 4
Offered for	Masters and Ph.D. in Non-CSE Programs	Type	Specialization core
Prerequisite	Bridge Course of Programming (Python)		
Antirequisite	ML, IML, PRML		

Objectives

1. To introduce the fundamental theories of machine learning.
2. To equip the students with the implementation data analysis and evaluation of machine learning algorithms.

Learning Outcomes

The students are expected to have the ability to:

1. Explain the basic concepts of ML driven data analysis
2. Utilize the tools and techniques for collecting, storing, securing, retrieving, and analyzing data of different modalities

Contents

Introduction to Probability, Bayes Theorem, Random Variable, Distribution Function and Probability Density (Mass) Function, Linear algebra. (8 lectures)

Evaluating ML Models: Precision, recall, specificity, sensitivity, predictive value, ROC curve, Cross-validation, Overfitting Underfitting, Bias, and interpretability of ML models (4 lectures)

Unsupervised Learning, Feature Selection, Clustering, Missing data (6 Lectures)

Supervised Machine Learning Models: Regression Analysis, Bayes Classification, Parameter Estimation, Maximum Likelihood Estimator, k-nearest neighbor, Decision trees, Gradient Descent, Neural Networks, Ensemble Learning (16 lectures)

Introduction to Deep learning: CNN, Autoencoder, RNN (8 Lectures)

Textbook

1. Mitchell Tom (1997). Machine Learning, Tata McGraw-Hill
2. Richard Duda, Peter Hart, David Stork (2007). Pattern Classification, Wiley

Reference Materials

1. Wu, G., (2016), Machine Learning and Medical Imaging, Elsevier
2. Bertrand Braunschweig, Malik Ghallab (2021), Reflections on Artificial Intelligence for Humanity, Springer.

Online Course Material

1. Sarkar, S., 2021, *Introduction to Machine Learning*, IIT Kharagpur. https://nptel.ac.in/courses/106105152

Title	**Modeling in Materials Engineering**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L–T–P [C]	2–0–0 [2]
Offered for	M.Tech.	Type	Specialization Core
Pre-requisite	-		

Objectives
1. Introduce first-principles calculations and molecular dynamics.
2. Introduce crystal plasticity and phase-field modelling techniques.

Learning Outcomes
1. Able to use quantum and atomistic simulation tools
2. Awareness of modelling techniques at meso and macro-length scales.

Course Content
First-principles calculations (7 lectures)
Introduction, Periodic Structures, Supercells, Electronic kinetic energy cut-off, Total Energy, Geometry Optimization, Electronic Structure and Magnetic Properties, Calculations for Surfaces, Defects in solids

Molecular dynamics simulations (7 lectures)
Introduction, Application of various distribution functions in amorphous and crystalline materials, Study of Diffusion and activation energy barrier, Application of MD in studying the kinetics of battery electrodes and electrolytes, Steered molecular dynamics: Theory and application.

Phase-Field Modelling (7 lectures)
Microstructure evolution, Continuum vs sharp interface description, The Ginzburg-Landau free energy functional, Equilibrium interfaces and surface tension, Conserved and non-conserved order parameters, Driving forces, fluxes, Spinodal decomposition in a binary alloy

Introduction to Crystal Plasticity (7 lectures)
Deformation gradient and finite strain, rotation and stretch, elastoplastic decomposition, Flow rules, hardening rules, slip systems and resolved shear stress, Pole figures and stereographic projection, Euler angles and orientation distribution, Phenomenological models, dislocation based constitutive laws, geometrically necessary dislocations

Text Books
1. Lee, J., Computational Materials Science: An Introduction, 2nd Edition, CRC Press 2016.
2. Sholl, D. S., and Steckel, J. A., Density Functional Theory: A Practical Introduction, 1st Edition, Wiley, 2009.
3. Provatas, N., Elder, K., Phase-Field Methods in Materials Science and Engineering, John Wiley & Sons, 2011.
4. Roters, F., Eisenlohr,P., Bieler, T., Raabe, D., *Crystal Plasticity Finite Element Methods* in Materials Science and Engineering, WILEY-VCH Verlag GmbH & Co. KGaA, 2010.
5. LeSar, Richard, *Introduction to Computational Materials Science: Fundamentals to Applications*, Cambridge University Press, 2013.

References
1. Raabe, D., *Computational Materials Science: The Simulation of Materials, Microstructures and Properties*, Wiley VCH, 1998.
2. Hull, D., and Bacon, D. J., Introduction to Dislocations, Butterworth-Heinemann (Elsevier), 5th Ed., 2011.

Online Course Materials

1. Gururajan, M.P., *Phase field modeling: the materials science, mathematics and computational aspects*, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, https://www.youtube.com/watch?time_continue=11&v=wXCra9_bGSU

2. MIT open courseware: Gerbrand Ceder, and Nicola Marzari. 3.320 Atomistic Computer Modeling of Materials (SMA 5107). Spring 2005. Massachusetts Institute of Technology: MIT OpenCourseWare, https://ocw.mit.edu. License: Creative Commons BY-NC-SA

Title	**Computational Materials Engineering Laboratory**	Number	MTL7XX0
Department	Department of Metallurgical and Materials Engineering	L-T-P [C]	0-0-2 [1]
Offered for	M.Tech.	Type	Specialization Compulsory
Prerequisite	NA		

Objectives

1. To provide hands-on experience of using computer simulations for studying materials.
2. To provide experience in analysing the simulation results for understanding materials.

Learning Outcomes

1. Familiarity with the advantages and limitations of computational tools available for studying materials.
2. Able to run the simulations and study materials' behaviour/properties from the simulation results.

Course Content (Computer Simulations)

1. Calculation of the electronic band structure and density of states in a semiconductor
2. Calculation of the electronic band structure and density of states in a metal
3. Calculate glass transition temp of polymer
4. Yield mechanism of an Au nanowire
5. Determination of the elastic stiffness tensor
6. Spinodal decomposition in a binary alloy
7. Modeling of grain growth
8. Generation of synthetic 3D polycrystalline grain structure from Electron Backscatter Diffraction (EBSD) data
9. Simulation of uniaxial compressive stress-strain response of a polycrystalline FCC single-phase metal based on strain rate-independent and strain rate-dependent 3D Crystal Plasticity constitutive laws
10. Materials data visualization

Textbook

1. Sholl, D. S., and Steckel, J. A., Density Functional Theory: A Practical Introduction, 1st Edition, Wiley, 2009
2. Provatas, N., Elder, K., *Phase-Field Methods in Materials Science and Engineering*, John Wiley & Sons, 2011

Online Course Material

1. Voorhees, P.W., *Phase Field methods: From fundamentals to applications*, Department of Material Science and Engineering, Northwestern University, https://www.youtube.com/watch?v=FTiBq1o-8e4

DETAILED SYLLABUS FOR THE SPECIALIZATION ELECTIVE COURSES
(a) Computational Materials Engineering

Title	**First-Principles Calculations**	**Number**	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	2–0–2 [3]
Offered for	M.Tech.	Type	Specialization Elective
Pre-requisite			

Objective

1. Introduce different features of electronic and phonon band structure.

Learning Outcomes

1. Understand the working principles of the first-principles calculations.
2. Simulate the electronic and phonon band structure in materials using first-principles calculations.

Course Content

Potentials: Construction method, advantages, types of pseudopotentials, Bloch theorem: Expression for Bloch wave, Finite plane-wave basis, energy convergence with the size of basis (5 lectures)

Electronic band structure: Fermi-Dirac distribution, Metals: charge sloshing, numerical issues, smearing methods (5 lectures)

Lattice dynamics: Dynamical properties, harmonic approximation, phonon dispersion curves, force constants, small-displacement methods, density functional perturbation theory, applications: normal mode analysis (10 lectures)

Electron transport: Boltzman transport equation for electrons, constant relaxation time approximation, transport coefficients (4 lectures)

Phonon transport: Boltzman transport equation for electrons, self-consistent phonon lifetimes, mean-free-path spectrum, lattice thermal conductivity (4 lectures)

Laboratory (Computer simulations):
1) Calculation of optical properties.
2) Calculation of magnetic moment in a system.
3) Calculation of the surface energy.
4) Calculation of stacking fault energy.
5) Calculation of stiffness tensor.
6) Performing an ab initio Molecular dynamics simulation.
7) Calculation of the phonon dispersion relation.
8) Calculation of the thermodynamic properties from the phonon dispersion relation.
9) Calculation of Raman spectra
10) Calculation of IR spectra

Text Books

1. Lee, J. G., Computational Materials Science: An Introduction, 2nd edition, CRC Press, 2016
2. Dove, M.T., Introduction to Lattice Dynamics, 1st Edition, Cambridge University Press, 1993
3. Sholl, D. S., and Steckel, J. A., Density Functional Theory: A Practical Introduction, 1st Edition, Wiley, 2009

References

1. Parr, R.G., and Yang, W., Density-Functional Theory of Atoms and Molecules, 1st Edition, Oxford Science Publications, 1994
2. Szabo, A., and Ostlund, N. S., *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Courier Corporation, 1996

Online Course Material

1. Ceder, G. and Marzari, N., 3.320 Atomistic Computer Modeling of Materials (SMA 5107). Spring 2005. Massachusetts Institute of Technology: MIT OpenCourseWare, https://ocw.mit.edu. License: Creative Commons BY-NC-SA

Title	**Alloy Design: Computational Thermodynamic Approach**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3–0–2 [4]
Offered for	M.Tech	Type	Specialization Elective
Prerequisite			

Objectives

1. Understanding the correlation between the phase diagram and chemical thermodynamics for alloy design.

Learning Outcomes

2. Ability to construct multicomponent phase diagrams using computational thermodynamic approach.
3. Ability to learn the assessment of binary phase diagram using PARROT module.

Contents

1. *Thermodynamics of Solution:* Ideal solution, configurational entropy, regular solution model, chemical potential, free energy composition diagram, evolution of phase diagrams quasichemical theory, Sub regular solution model. (8 Lectures)
2. *Alloy Design of multicomponent system:* Redlitch-kister polynomial, Muggianu and kohler extrapolation. Crystallography in thermodynamics, Order and disorder structure, antisite defect and vacancies. Compound energy formalism. Modeling of Interstitial and substitutional phases, stoichiometric and non-stoichiometric compounds. (14 Lectures)
3. CALPHAD modeling of non-metallic system. Cluster variance model. (6 Lectures)
4. *Calculation of thermodynamic parameters:* First principle calculation, Semi-empirical-Miedema approach. Calorimetric measurement, electrochemical measurement, Diffusion couple method. (8 Lectures)
5. *Assessment of thermodynamic system:* Optimization of binary isomorphous and eutectic phase diagram using PARROT module. (6 Lectures)

Lab Experiments

Construction of equilibrium and non-equilibrium phase diagram, Vertical section phase diagram and Property diagram for multi-component alloys, Scheil and equilibrium solidification simulation, Liquidus projections and monovariant reactions in ternary phase equilibria, Creation of user defined thermodynamic database for Solid solution, Stoichiometric compounds, non-stoichiometric compounds.

Textbooks

1. Saunders and Miodownik, *CALPHAD (Calculation of Phase Diagrams): A Comprehensive Guide,* 1st Edition, Pergamon Press, 1998.
2. Hans Lukas, Suzana G. Fries, Bo Sundman, *Computational Thermodynamics: The Calphad Method,* Cambridge University Press, 2007.
3. Oates, W. Alan., Chang, Y. Austin, *Materials Thermodynamics*, Wiley, 2010.

Self-Learning Material

1. Porter, D.A., Easterling, K. E., and Sherif, M.Y., *Phase Transformation in Metals and Alloys*, 3rd edition, CRC Press, 2009.
2. Hillert, M., *Phase Equilibria, Phase Diagrams and Phase Transformations Their Thermodynamic Basis,* Second edition, Cambridge University Press 2008.

Online Course Materials

1. Murty, B.S., Advanced Metallurgical Thermodynamics, NPTEL Course Material, Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, https://nptel.ac.in/courses/113106031/.

Title	**Principles of Continuum Mechanics**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3-0-0 [3]
Offered for	M.Tech. (MT)	Type	Specialization Elective
Prerequisite			

Objectives

The Instructor will:

1. Provide background on the fundamentals of the mechanics of continuous media.

Learning Outcomes

The students are expected to understand:

1. Concepts and general principles of material mechanics
2. Mathematical formulations and tensor notations for understanding and developing constitutive equations

Contents

Mathematical Foundation: [6 lectures] Tensors and indicial notations, coordinate transformation, Transformation of cartesian tensors, Tensor multiplication, Vector and Tensor calculus

*Kinematics of Continuum: [8 lectures]*Lagrangian and Eulerian description of motion, Analysis of Deformation- Deformation gradient, stretch and rotation tensors, Deformation Tensors, Finite strain tensors, small deformation theory, Polar Decomposition, compatibility conditions

Analysis of Stress: [8 lectures] Body forces and surface forces, traction vector-stress tensor, stress equilibrium, stress transformation, principal axes, invariants, spherical and deviatoric stress tensors, maximum and minimum shear stress, other stress measures: 1st and 2ndPiola-Kirchhoff stress, Mohr's circle

Motion and Flow: [6 lectures] Material derivative, notations of velocity, acceleration and instantaneous velocity field, Rate of deformation and Spin, material derivative of volume, area and line elements

Fundamental Laws of Continuum Mechanics: [8 lectures] Tensor notation of conservation of mass, linear momentum and angular momentum principle, Equations of motion, Conservation of energy, First Law and Second Law of Thermodynamics, Clausius-Duhem inequality and Dissipation function

Constitutive Relation: [6 lectures] Generalized Hooke's law, Stiffness and compliance tensor, crystal symmetry and its effect on stiffness tensor, Frame indifference, Jaumann stress-rate

Laboratory Experiments

NA

Textbook

1. Reddy, J.N, (2013) *An Introduction to Continuum Mechanics*, 2nd Edition, Cambridge University Press
2. Malvern, L.E. (1969) *An Introduction to the Mechanics of Continuous Medium,* 1st Edition, Prentice Hall

Reference Books

1. Fung, Y.C., (1994) *A First Course in Continuum Mechanics: For Physical and Biological Engineers and Scientists*, Prentice Hall

Online Course Material

1. Reddy, A.N., Continuum Mechanics, NPTEL Course Material, Department of Mechanical Engineering, Indian Institute of Technology Guwahati, https://nptel.ac.in/courses/112/103/112103167/

Title	**Continuum Plasticity**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3-0-0 [3]
Offered for	M.Tech. (MT)	Type	Specialization Elective
Prerequisite	UG level Mechanics of Solids, Mechanical Behavior of Materials		

Objectives

The Instructor will:

1. Provide background on fundamentals of the mechanics of continuous media.

Learning Outcomes

The students are expected to:

1. Understand basic concepts of plasticity and damage mechanics and understand the capabilities and limitations of the different constitutive models
2. Identify the material parameters associated with material models and prepare material input data for finite element modeling

Contents

Introduction and Background: [6 lectures] Index notation, Stress, deformation, and strain tensor, Generalized Hooke's Law, stress and strain deviators, crystal slip, critical resolved shear stress

Rate Independent Plasticity for Isotropic Solids: [8 lectures] Yield criteria, Physical interpretation, Yield surface in 3D-space and normality, plastic flow rule- general formulation, associated flow, effective plastic strain increment, proportional and non-proportional loading

Evolution of Yield Surface: [8 lectures] Correlation between plastic strain evolution and yield surface, Strain hardening, consistency condition, pressure-dependent plasticity, loading and unloading criteria, Drucker's stability postulate, Isotropic hardening, Kinematic hardening, combined hardening

Solutions to Elastic-Plastic Problems [8 lectures]: Examples of elastic-plastic problems such as, Plane strain bending and compression, cylindrical bars under tension and torsion, thin walled tubes under combined loading, thermal stress in thick walled tube, etc.

Implicit and Explicit Integration of von Mises Plasticity [6 lectures]: implicit and explicit integration of constitutive equations, implicit integration-radial return method, material jacobian, isotropic, kinematic and combined hardening

Ductile Damage [6 lectures]: Yield criteria for spherical voids geometry, Application of Gurson's model to the analysis of damage distribution in notched specimen, Applications

Laboratory Experiments

NA

Textbook

1. Dunne, F, Petrinic, N., (2006) *Introduction to Computational Plasticity*, 1st Edition, Oxford University Press
2. Malvern, L.E. (1969) *An Introduction to the Mechanics of Continuous Medium,* 1st Edition, Prentice Hall

Reference Books

1. Cazacu, O., Revil-Baudard, B., (2019) *Plasticity-Damage Couplings: From Single Crystal to Polycrystalline Materials*, Springer International Publishing

Online Course Material

1. Bag, S., Introduction to Crystal Elasticity and Crystal Plasticity, NPTEL Course Material, Department of Mechanical Engineering, Indian Institute of Technology Guwahati, https://nptel.ac.in/courses/113/103/113103072/

Title	**Crystal Plasticity and Its Applications**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L–T–P: C	3–0–0 [3]
Offered for	M.Tech.	Type	Specialization Elective
Pre-requisite			

Objectives

1. The objective of this course is to learn different aspects of plasticity in relation to the crystallographic orientation of metallic materials.

Learning Outcomes

1. Fundamental understanding of the correlation between microstructural aspects and deformation aspects.
2. Apply the fundamental concepts to use crystal plasticity modeling for a better understanding of different microstructural evolution phenomena during deformation.

Course Content

Introduction: Metallurgical fundamentals of plastic deformation, Concepts of stress and strain, Introduction to continuum mechanics, Deformation gradient and deformation of line, Velocity gradient, Elastoplastic decomposition, Stress analysis and Yield surfaces (10 lectures)

Crystal orientation and its representation: Description of orientation and misorientation, Measurement techniques, Statistical representation of crystallographic texture (4 lectures)

Crystal plasticity modeling and numerical aspects:
Mean Field Models: Taylor Model, Grain Interaction Based Models, Viscoplastic Self consistent Models, Full Field Models : crystal plasticity finite element method, fast Fourier transformation method (10 lectures)

Work hardening models: Voce Model, extended Voce Model, Dislocation density based Kocks Mecking Model. Slip system interactions, latent hardening, Concepts of Taylor factor, Schmid factor and Single Crystal Yield Locus, Treatment of twinning in crystal plasticity. (10 lectures)

Examples of applications: Microscopic and Mesoscopic Examples: Plane strain deformation, Simple shear deformation, Single-and bicrystal deformation, Recrystallization, Multiphase steel (TRIP) deformation etc., Texture dependent properties and macroscopic examples such as deep drawing (8 lectures)

Books

1. Roters, F., Eisenlohr, P., Bieler, T., Raabe, D., *Crystal Plasticity Finite Element Methods in Materials Science and Engineering*, WILEY-VCH Verlag GmbH & Co. KGaA, 2010.
2. Hosford, W. F., *The mechanics of crystals and textured polycrystals*, Oxford University Press (USA), 1993.

References:

1. R. J. Asaro and Vlado A. Lubarda, *Mechanics of Solids and Materials*, Cambridge University Press, 2006.
2. A. F. Bower, *Applied Mechanics of Solids*, CRC Press, 2009.
3. A. S. Argone, *Strengthening Mechanisms in Crystal Plasticity*, Oxford University Press, 2008.
4. Raabe, D., Roters, F., Barlat, F., and Chen, L. Q. (Eds.)., *Continuum scale simulation of engineering materials: fundamentals-microstructures-process applications*. John Wiley & Sons, 2004.

Online Course Material:

1. Biswas, S. and Toth, L. S., *Crystallographic texture and crystal plasticity*, GIAN-MHRD, IIT Kharagpur course.
2. Biswas, S., *Texture in Materials,* https://nptel.ac.in/courses/113105103
3. Bag, S., *Introduction to crystal elasticity and crystal plasticity*, https://nptel.ac.in/courses/113/103/113103072/

Title	**Modeling of Metallurgical Processes**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3-1-0 [4]
Offered for	M.Tech. (MT)	Type	Specialization Elective
Prerequisite	None		

Objectives

The Instructor will:

1. Introduce methods for developing simple models of metallurgical processes considering important process variables
2. The models will be evaluated for their industrial adaptability

Learning Outcomes

The students are expected to have the ability to:

1. Apply the principles of thermodynamics and transport phenomena to understand and control metallurgical processes
2. Relate the basic phenomena and process output through modelling

Contents

Thermodynamic aspects: laws of thermochemistry, Ellingham diagram, solution thermochemistry (6 lectures)

Process metallurgy: transport phenomena, reaction kinetics, rate phenomena, chemical reaction kinetics, fluid flow, heat and mass transfer (12 lectures)

Metal-slag interactions: Thermo-physical properties of metals and slags, slag-metal equilibrium calculations, application of slag capacity during metal refining (12 lectures)

Process phenomena: bubble formation, foaming, gas-liquid reactions, reactions between liquid phases (10 lectures)

Process control in metallurgical processes: iron making, converter steel making, electric arc furnace, secondary steel making (12 lectures)

Textbooks

1. Sano N., Lu W., Riboud P., *Advanced Physical Chemistry for Process Metallurgy*, Academic Press, 1997.
2. Shamsuddin M., *Physical Chemistry of Metallurgical Processes*, John Wiley & Sons, 2016.
3. Roy, Sanat Kumar., Bose, Subir Kumar, *Principles of Metallurgical Thermodynamics*, Universities Press, 2014.
4. Mohanty, A. K., *Rate Processes in Metallurgy*, India: PHI Learning, 2009.
5. Ghosh, Sudipto., Ghosh, Ahindra, *A Textbook Of Metallurgical Kinetics*, India: PHI Learning, 2014.

Reference books

1. Seetharaman S.S., *Treatise on Process Metallurgy*, Volume 1: Process Fundamentals, Elsevier Ltd., 2014
2. Seetharaman S.S., *Treatise on Process Metallurgy*, Volume 2: Process Phenomena, Elsevier Ltd., 2014
3. Seetharaman S.S., *Treatise on Process Metallurgy*, Volume 3: Industrial Processes, Elsevier Ltd., 2014

Online Course Materials

1. Muzumdar, D., and Koria, S.C., *Steel Making*, NPTEL Course Material, Department of Material Science and Engineering, Indian Institute of Technology Kanpur, http://nptel.ac.in/courses/113104013/

Title	**Microstructure Image Processing**	Number	MTL7XX0
Department	Department of Metallurgical and Materials Engineering	L-T-P [C]	1-0-0 [1]
Offered for	B.Tech. (CME specialization), M.Tech.	Type	Specialization Core for UG and Dual Degree
Prerequisite	NA		

Objectives

1. Introduce the emergent field of image processing for better understanding the microstructure for material engineering.

Learning Outcomes

The students are expected to have the ability to acquire basic knowledge and understanding of image processing and their applications in metallurgy and materials engineering.

Course Content

Reconstruction: Mathematical models of image regularity, random fields, practical data sampling and acquisition schemes (3 lectures)
Restoration: Deconvolution, degradation models for corrupted and missing data, Bayesian graphical modelling and inference, regression methods for filtering of images (4 lectures)
Image segmentation, delineation & classification: Clustering, graph partitioning, classification, mixture models, expectation maximization, variational methods using geometric and statistical modelling, computer aided diagnosis (4 lectures)
Registration: Deformation models, optimization algorithms, 2D-3D registration, multimodal registration (2 lectures)
Specific to textures: n-point correlation functions, Frequency domain computations (e.g. DFT) (1 Lecture)

Textbook

1.

Reference

1. Cecen, A., Fast, T. & Kalidindi, S.R. Versatile algorithms for the computation of 2-point spatial correlations in quantifying material structure. Integr Mater Manuf Innov 5, 1–15 (2016). https://doi.org/10.1186/s40192-015-0044-x.

2. Kalidindi, S.R., Niezgoda, S.R. & Salem, A.A. Microstructure informatics using higher-order statistics and efficient data-mining protocols. JOM 63, 34–41 (2011). https://doi.org/10.1007/s11837-011-0057-7

Title	**Machine Learning for Materials Design**
Department	Metallurgical and Materials Engineering
Offered for	M.Tech.
Pre-requisite	-

Objectives

1. Introduce a selected set of Machine learning and Deep Learning techniques for Materials desi
2. Introduce hands-on experience with some practical methods and techniques in materials
3. Introduce hands-on experience in analyzing data and applying ML approaches through a set o

Learning Outcomes

1. Aware of different data-driven techniques for creating Materials Knowledge.
2. To use machine learning tools for solving problems in materials design

Course Content

Deep Learning Techniques:
Supervised Learning using deep networks: Convolutional Neural Networks (CNN), Recurrent N

Unsupervised Learning using deep networks: Auto encoders, Deep Belief Networks (5 lectures

Ensemble Classifiers: Random Forests, Gradient Boosted Decision Trees (4 lectures)

Association Analysis: Mining association rules, Graph Neural Networks (5 lectures)

Laboratory exercises:

1. A deep-learning technique for phase identification using synthetic XRD powder patterns
2. Physics-driven ML for catalysts design
3. Data-Driven Prediction of Interatomic Potentials
4. Automated Micrograph Analysis: Optical, SEM, TEM and EBSD analysis.
5. Data-Driven Approach for design and rapid screening of High Entropy and Amorphous allo
6. Materials Property Predictions Based on Data from Chemistry, Structure and Processing
7. Data Driven Modelling for Defect prediction during Additive Manufacturing Process
8. Fatigue life prediction using ML

Books

1. Pilania, G., Balachandran, P. V., Gubernatis, J. E., and Lookman, T., *Data-Based Methods for Mate*

2. *Machine Learning And Data Mining In Materials Science*, Edited by Huber, N., Kalidindi, S. R., Kluse

3. Mueller, T., Kusne, A.G. and Ramprasad, R., *Machine Learning in Materials Science.* In Reviews in C

Reference Books:

1. Materials Informatics: Methods, Tools, and Applications, Edited by Olexandr Isayev, Alexander Trop

2. Informatics for Materials Science and Engineering-Data-driven Discovery for Accelerated Experime

Title	**Phase Field Modelling**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L–T–P [C]	3–0–0 [3]
Offered for	M.Tech.	Type	Specialization Elective
Pre-requisite	-		

Objectives
1. Introduce different phase-field models for studying microstructural evolution.
2. Introducing relevant analytical equations for microstructural evolution.

Learning Outcomes
1. Understand the different parameters influencing the microstructure.
2. Know the usage of different simulation techniques in microstructural evolution study.

Course Content
Introduction: Solidification, precipitation, strain-induced transformations (5 lectures)

Simple lattice models: Phase separation in a binary mixture, Ising model of magnetism (5 lectures)

Landau theory: Order parameters and phase transformations, the Landau free energy functional, phase transitions with a symmetric phase diagram, phase transitions with a non-symmetric phase diagram, first-order transition with a critical point (5 lectures)

Spatial variations and interfaces, Non-equilibrium dynamics: Conserved and non-conserved order parameters, Ginzburg-Landau free energy functional, Driving forces, fluxes (6 lectures)

The diffusion equation, Dynamics of conserved order parameter, Dynamics of non-conserved order parameter, Equilibrium fluctuations of order parameters (6 lectures)

Stability and the formation of second phases*,* Interface dynamics of phase field models (5 lectures)

Solidification of pure metals, Solidification dynamics, anisotropy, non-isothermal solidification (6 lectures)

Properties of dendritic solidification in pure materials: Microscopic solvability theory, phase field predictions of dendrite operating states (4 lectures)

Text Books
1. Provatas, N., Elder, K., *Phase-Field Methods in Materials Science and Engineering*, John Wiley & Sons, 2011.
2. Emmerich, Heike, *The Diffuse Interface Approach in Materials Science: Thermodynamic Concepts and Applications of Phase-Field Models*, Springer, 2003.
3. Biner, S. Bulent, *Programming Phase-Field Modeling*, Springer International Publishing, 2017.

Online Course Material
1. Voorhees, P.W., *Phase Field methods: From fundamentals to applications*, Department of Material Science and Engineering, Northwestern University, https://www.youtube.com/watch?v=FTiBq1o-8e4
2. Gururajan, M.P., *Phase field modeling: the materials science, mathematics and computational aspects*, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, https://www.youtube.com/watch?time_continue=11&v=wXCra9_bGSU

Title	**Symmetry, Structure and Tensor Properties**	**Number**	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3–0–0 [3]
Offered for	M.Tech.	Type	Specialization elective
Pre-requisite	Linear Algebra and Matrix Mathematics, MATLAB/Mathematica		

Objectives
1. Introduce the concept of symmetry in crystal lattices; point groups, space groups, and use of symmetry in tensor representation of crystal properties, including anisotropy and representation surfaces; and applications to piezoelectricity and elasticity.

Learning Outcomes
1. Students would learn how to calculate different thermodynamic properties of different materials.
2. The student would understand how crystalline anisotropy affects/governs the property anisotropy.

Contents
Introduction: Spherical trigonometry and Applications in Crystallography: (5 lectures)
Crystal lattices: Direct lattice, Crystal systems, Bravais Lattice (2 lectures)
Point Groups: Stereographic projection, Proper Cubic point groups, Improper point groups (Dihedral angle, inversion symmetry), Types of point groups: 2D and 3D lattices (7 lectures)
Space Groups: Enumeration of the operations, Different space groups with specific materials examples (7 lectures)
Group Theory: Basic Concepts, Character Tables, Examples (5 lectures)
Symmetry and Lattice Vibrations: Symmetry and Local Mode Vibrations, Jahn-Teller Effect, IR and Raman Effect (6 lectures)
Tensor Properties of Materials: Basic Tensorial Operations: Transformation of Axis, Eulerian Angles, Orthogonality Neumann Principle, Pseudo Tensors, Symmetry and Mathematical Properties of Tensors, Different ordered tensors: 2^{nd} order(Stress-Strain, Permittivity, Permeability, Thermal Expansion), 3^{rd} order(Piezoelectricity), 4^{th} order (Elasticity Tensor) (10 lectures)

Text Books
1.Newnham, R. E., *Structure-property relations* (Vol. 2). Springer Science & Business Media, 2012.
2. Nye, J. F., *Physical properties of crystals: their representation by tensors and matrices*. Oxford university press, 1985.

Reference Books
1. International Tables for Crystallography Volume A: Space-group symmetry
2. Buerger, M. J., *Elementary crystallography*, John Wiley & Sons, 1956.

Online Course Material
1. Prof. Bernhardt Wuensch, Symmetry, Structure, and Tensor Properties of Materials, DMSE MIT, MIT OCW, https://ocw.mit.edu/courses/materials-science-and-engineering/3-60-symmetry-structure-and-tensor-properties-of-materials-fall-2005/syllabus/

Title	**Advanced Molecular Dynamics**	Number	MTL7XXX0
Department	Metallurgical and Materials Engineering	L–T–P [C]	3–0–0 [3]
Offered for	M.Tech.	Type	Specialization Elective
Pre-requisite	--		

Objectives
1. The aim of this course is to provide the student with an understanding of the various molecular dynamics methods, their capabilities, and their limitations.

Learning Outcomes
1. Make sound judgements regarding the quality of molecular simulation studies reported in the literature
2. Have exposure to various advanced molecular dynamics techniques to reach experimental level times scale
3. Get an idea to set up the molecular dynamics simulations to solve realistic problems

Course Content
Molecular dynamics of hard spheres, demonstrating elementary concepts of temperature, ensemble averaging, error estimation, periodic boundaries, classical potentials and Machine learning potential. Equations of motion, integration schemes, Various ensembles and their applications, dynamical properties-Macroscopic Transport Phenomena (10 Lectures)

Limitations of Equilibrium Methods, Non-Equilibrium Molecular Dynamics, One (Disfavored) Approach, Basic theory and example of static and dynamic linear response, Diffusion: An Inhomogeneous Approach, Self-Diffusion: Perturbation, Thermostatting, Shear Viscosity: Boundary-Driven Algorithm, Limitations of Boundary-Driven Shear (14 Lectures)

Accelerated molecular dynamics, Parallel-Replica Dynamics, Hyperdynamics, Temperature-Accelerated Dynamics, Recent Advances and Applications, Overview of sampling methods (6 Lectures)

Ab-initio molecular dynamics, Basics of Nonadiabatic molecular dynamics, Different flavors of nonadiabatic molecular dynamics (6 Lectures)

Overview of various software to perform molecular dynamics, A model example of molecular dynamics calculation and its result analysis. (6 Lectures)

Books
1. Allen, M.P. and Tildesley, D.J., *Computer Simulation of Liquids*, Clarendon Press, Oxford 1987.
2. Frenkel, D. and Smit, B., *Understanding Molecular Simulation*, second edition, Academic Press, San Diego, 2002.
3. Marx, D. and Hutter, J., *Ab Initio Molecular Dynamics*, Cambridge University Press, Cambridge, 2009.

References:
1. Hiroki Nakamura, *Introduction To Nonadiabatic Dynamics*, World Scientific Press, 2019, https://doi.org/10.1142/11359
2. *Ab Initio Nonadiabatic Quantum Molecular Dynamics*, Chem. Rev. 2018, 118, 7, 3305–3336.
3. *Annual Reports in Computational Chemistry*, Volume 5, 2009, Elsevier B.V.,ISSN: 1574-1400, DOI 10.1016/S1574-1400(09)00504-0

Title	**Single and Multi-objective Evolutionary and Nature Inspired Algorithms**	Number	MTL7XXX0
Department	Metallurgical and Materials Engineering	L–T–P [C]	1–0–0 [1]
Offered for	M.Tech.	Type	Specialization Elective
Prerequisite			

Objectives

The Instructor will:

1. Introduce evolutionary algorithms for single and multi-objective optimization

Learning Outcomes

The students are expected to have the ability to:

1. Carry out Multi-objective optimization using evolutionary algorithms

Contents

Historical perspective of Evolutionary Algorithms: the American and German schools of thought. The scope of evolutionary algorithms and the advantages of a 'non-calculus' approach. (1 lecture)
The 'Simple Genetic Algorithm'. The basic genetic operators: selection, crossover, mutation and their variants. (1 lecture)
How Genetic Algorithm works: The Schemma Theorem. The problems of binary encoding: Hamming Cliff. Remedial measures: Gray encoding, real encoding, (1 lecture)
Recent algorithms: Differential Evolution, Particle Swarm Optimization, Ant Colony optimization, Artificial Immune System Algorithms (2 lectures)
Fundamentals of Multi-objective Optimization. The concept of Pareto Optimality (2 lectures)
Major Evolutionary Multi-objective optimization Algorithms: SPEA, NSGAII, MOGA etc. (2 lectures)

Genetic Programming (1 lecture)
Data-driven modeling, Surrogate or metamodeling. Modeling data with random noise: EvoNN, BioGP and EvoDN2 algorithms. Commercial software like Kimmeme and ModeFrontier. (4 lectures)
Term Project on a problem of student's choice.

Textbook

1. Chakraborti Nirupam, *Data-driven evolutionary modelling in materials technology*, CRC Press, 2022.
2. Datta, Shubhabrata, *Materials design using computational intelligence techniques*. CRC Press, 2016.
3. Deb K. *Multi-objective optimization using evolutionary algorithms*. John Wiley & Sons; 2001.

Reference books

1. DE Golderg, *Optimization & Machine Learning*, Addison Wesley, 1989.
2. Melanie Mitchell, *An introduction to genetic algorithms*. MIT press, 1998.
3. Coello, Carlos A. Coello, and Gary B. Lamont. *Applications of multi-objective evolutionary algorithms*. Vol. 1. World Scientific, 2004.
4. Ant Colony Optimization by Marco Dorigo and Thomas Stützle, MIT Press, 305 pp.

Title	**Data Visualisation in Materials Modelling**	Number	MTL7XX0
Department	Department of Metallurgical and Materials Engineering	L-T-P [C]	1-0-0 [1]
Offered for	B.Tech. (CME specialization), M.Tech.	Type	Specialization core (UG), Specialization Elective for PG
Prerequisite	NA		

Objectives

1. Introduce the emergent field of data visualization for better understanding and processing of scientific data for material engineering.

Learning Outcomes

1. Understand key methods and libraries for scientific data visualization.
2. Understand the data handling and efficiently visualize the data in 2D and 3D.
3. Performing the fits to the data and quantify the quality of the fit.

Course Content

Basics of data handling and visualization: Overview of python language, Data input and output, Organisation of big multidimensional data in numpy and pandas, and efficient data format conversion, Python IDE. (7 lectures)

Data visualization in Python for materials modelling: Data visualization in various python libraries, 2D and 3D data visualization, linear, matrix and multidimensional data visualization, *Data* visualization of density of states, band structure, charge density, spectroscopic data, numerical data fitting and its visualization in materials modelling (7 lectures)

Textbook

1. Landup. D, *Data visualization in python with pandas and matplotlib*, 2020.

Reference book

1. Beazley, D., Jones, B.K, *Python Cookbook: Recipes for Mastering Python 3 (English Edition)*, O'Reilly media, 2013.