

## Department of Metallurgical and Materials Engineering

### Specialization 3: Computational Materials Engineering

**Table 2:** List of Specialization Core and Electives as per Senate approved document

|   | <b>List of core courses [8 Credits]</b>                         |    | <b>List of Elective courses [12 Credits]</b>  |
|---|---|----|---|
| 1 | MTL4XXX: Introduction to Dislocation Dynamics [2-0-2]           | 1  | MTL7XXX: Modelling of Metallurgical Processes [3-1-0]                                   |
| 2 | MTL7XXX: Modelling in Materials Engineering [2-0-0]             | 2  | 7XXX: Machine Learning for Materials Design [2-0-2]                                     |
| 3 | Microstructure Image Processing [2-0-0]                         | 3  | MTL7XXX: Single and Multi-objective Evolutionary and Nature Inspired Algorithms [1-0-0] |
| 4 | MTP7XXX: Computational Materials Engineering Laboratory [0-0-2] | 4  | MTL7XXX: Principles of Continuum Mechanics [3-0-0]                                      |
|   |   | 5  | MTL7XXX: Continuum Plasticity [3-0-0]   |
|   |   | 6  | MTL7XXX: Crystal Plasticity and Its Applications [3-0-0]                                |
|   |   | 7  | CHLP4XX0: Process Control and AI Applications [3-0-2]                                   |
|   |   | 8  | CHL4XXX0: Molecular Transport Phenomena [2-0-0]   |
|   |   | 9  | PHL7XXX: Computational Materials Science [3-0-0]  |
|   |   | 10 | MEL7XXX: Finite Element Methods in Engineering [3-0-0]                                  |
|   |   | 11 | MEL7XXX: Computational Fluid Dynamics and Heat Transfer [3-0-0]                         |
|   |   | 12 | CHL7XX0: Data Analytics in Process Modelling and Simulation [2-0-2]                     |
|   |   | 13 | CHL7XX0: Molecular Simulations [2-0-0]  |
|   |   | 14 | MTL7XXX: Data visualization in Materials Modelling [1-0-0]                              |
|   |   | 15 | MTD 7XXX: Project [0-0-6] /[0-0-8]/[0-0-12]   |

**Table 3:** Proposed Semester-wise Structure of **20 Graded Credits** and positioning of core courses for Computational Materials Engineering Specialization

|    | <b>Courses</b>   | <b>GC</b> |   | <b>Courses</b>                                 | <b>GC</b> |
|----|--|-----------|---|--|-----------|
|    | <b>V Semester</b>  |           |   | <b>VI Semester</b>                             |           |
|    | One 400 level 3 credit course may be placed in this semester for overloading |           | SC  | Introduction to Dislocation Dynamics           | 3         |
|    |  |           |   |  |           |
|    |  |           | <b>Overload this semester 3-4 credits</b> |  |           |
|    |  |           |   | Total  | <b>3</b>  |
|    | <b>VII Semester</b>  |           |   | <b>VIII Semester</b>                           |           |
| SC | Modelling in Materials Engineering   | 2         | SC  | Computational Materials Engineering Laboratory | 1         |
| SC | Microstructure Image Processing  | 2         | SE  | Specialization Electives                       | 3         |
| SE | Specialization Elective  | 3         | SE  | Specialization Electives                       | 3         |
| SE | Specialization Electives   | 3         |   |  |           |
|    |  |           |   |  |           |
|    | <b>Overload this semester 4-3 credits</b>                                    |           | <b>Overload this semester 3 credits</b>   |  |           |
|    |  | Total     |   | Total  | <b>7</b>  |
|    |  | <b>10</b> |   |  |           |

**Note:** Students will also be required to complete any non-graded credits associated with a minor programme.

### Dual Degree in Computational Materials Engineering

**Table 4:** Credit requirements for dual degree

|   | <b>Specialization Core</b>        | <b>Programme Core Credits</b> | <b>Specialization Elective</b> | <b>Programme Elective Credits</b> | <b>Open Electives Credits</b> | <b>M.Tech Project</b> | <b>Non-Graded Credits</b> |
|---|-----------------------------------|-------------------------------|--------------------------------|-----------------------------------|-------------------------------|-----------------------|---------------------------|
| Semester VI and VII during Specialization     | 7                                 | 0                             | 6                              | 0                                 | 0                             | 0                     | 0                         |
| Semester VIII - X                             | 1                                 | 2                             | 15                             | 0                                 | 3                             | 20                    | 2                         |
| <b>Total (As per Dual Degree requirement)</b> | 8                                 | 2                             | 21                             | 0                                 | 3                             | 20                    | 2                         |
|   | <b>31 (Compulsory + Elective)</b> |                               |                                |                                   | <b>3</b>                      | <b>20</b>             | <b>2</b>                  |

**Table 5:** List of Dual Degree Programme Core

| List of core courses [Credits] |  |
|--------------------------------|--|
| 1                              | Industry 4.0: Applications in Metallurgical and Materials Engineering [2-0-0] (MC) |

**Note:** List of Specialization Core up to VIII Semester will be as per B.Tech. (Specialization) curriculum  
List of Specialization Electives up to VIII Semester will be as per B.Tech. (Specialization) curriculum  
List of Specialization Electives in IX th Semester will be as per M.Tech. Computational Materials Engineering Course Bouquet

**Table 6a:** Proposed Semester-wise Structure of **54-56 Graded and 4 Non-Graded Credits** and positioning of core courses for the specialization leading to dual degree [B.Tech.+M.Tech.]

|    | Courses  | NC       | GC        |    | Courses  | NC       | GC        |
|----|--|----------|-----------|----|--|----------|-----------|
|    | V Semester   |          |           |    | VI Semester                                    |          |           |
|    | One 400 level 3 credit course may be placed in this semester for overloading |          | -         | SC | Introduction to Dislocation Dynamics           |          | 3         |
|    |  |          |           |    |  |          |           |
|    |  |          |           |    | <b>Overload this semester 4 credits</b>        |          |           |
|    |  |          |           |    | Total  |          | <b>3</b>  |
|    | VII Semester   |          |           |    | VIII Semester                                  |          |           |
| SC | Modelling in Materials Engineering   |          | 2         | SC | Computational Materials Engineering Laboratory |          | 1         |
| SC | Microstructure Image Processing  |          | 2         | SE | Specialization Elective                        |          | 3         |
| SE | Specialization Elective  |          | 3         | SE | Specialization Elective                        |          | 3         |
| SE | Specialization Elective  |          | 3         |    |  |          |           |
|    | <b>Overload this semester 3 credits</b>                                      |          |           |    | <b>Overload this semester 3 credits</b>        |          |           |
|    | Total  |          | <b>10</b> |    | Total  |          | <b>7</b>  |
|    | IX Semester  |          |           |    | X Semester                                     |          |           |
| MC | Industry 4.0: Applications in Metallurgical and Materials Engineering        |          | 2         | MO | Open Elective                                  |          | 3         |
| SE | M.Tech. Specialization Elective  |          | 3         | MP | M.Tech. Project                                |          | 15        |
| SE | M.Tech. Specialization Elective  |          | 3         |    |  |          |           |
| SE | M.Tech. Specialization Elective  |          | 3         |    |  |          |           |
| MP | M.Tech. Project  |          | 5         |    |  |          |           |
|    | Non-graded PG courses  | 1        | -         |    | Non-graded PG courses                          | 1        | -         |
|    | Total  | <b>1</b> | <b>16</b> |    | Total  | <b>1</b> | <b>18</b> |

|              |   |           |   |
|--------------|---|-----------|---|
| Title        | <b>Introduction to Dislocation Dynamics</b> | Number    | MTL4XX0   |
| Department   | Metallurgical and Materials Engineering     | L-T-P [C] | 2-0-2 [3]   |
| Offered for  | B.Tech.                                     | Type      | Specialisation core for Computational Materials Engineering |
| Prerequisite | Nil   |           |   |

### Objective

1. Introduce basic concepts of discrete dislocation dynamics simulations

### Learning Outcomes

The student will be able to

1. Create a simulated system with various dislocation configurations.
2. Determine the properties associated with the dislocations by running simulations.

### Course Content

1. Crystal dislocations, The burgers vector, Motion of a crystal dislocation, Atomistic mechanism of dislocation motion, introduction to atomistic simulations (6 lectures)
2. Static simulations: setting up initial configuration, boundary conditions, data analysis and visualisation: Energy filtering and centro-symmetry deviation (6 lectures)
3. Dynamic simulations: Creation of dislocation through misfit at interfaces, stress control and temperature control, extraction of dislocation velocity (6 lectures)
4. Periodic boundary conditions: Displacement field induced by a dislocation, dislocation core energy, Peierls stress (6 lectures)
5. Free energy calculations: harmonic approximation, a Vacancy in the Dislocation Core, beyond harmonic approximation (4 lectures)

### Laboratory (Computer simulations):

- 1) An atomistic simulation of an edge and a screw dislocation in BCC tantalum
- 2) Simulation of a system containing vacancy–interstitial pair and data analysis
- 3) Simulation of a perfect grain boundary and data analysis
- 4) Simulation of dislocation glide motion at different stress values
- 5) Simulation a system with a screw dislocation dipole and estimation of the excess energy associated with the dislocation dipole
- 6) Estimation of dislocation core energies
- 7) Estimation of a Peierls stress near dislocations
- 8) Compute the free energy of a silicon crystal containing a vacancy

### Text Books

1. Bulatov, Vasily, and Cai, Wei. Computer Simulations of Dislocations. United Kingdom, OUP Oxford, 2006.

### References

1. Cui, Yanan. The Investigation of Plastic Behavior by Discrete Dislocation Dynamics for Single Crystal Pillar at Submicron Scale. Singapore: Springer Nature Singapore, 2016.

|               |   |           |   |
|---------------|---|-----------|---|
| Title         | <b>Modelling in Materials Engineering</b>     | Number    | MTL7XX0   |
| Department    | Metallurgical and Materials Engineering       | L-T-P [C] | 2-0-0 [2], SC   |
| Offered for   | B.Tech., B.Tech.-M.Tech. Dual Degree, M.Tech. | Type      | Specialization Core for Computational Materials Engineering |
| 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), 5<sup>th</sup> 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](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        | <b>Microstructure Image Processing</b>                | Number    | 7XX0                                       |
| Department   | Department of Metallurgical and Materials Engineering | L-T-P [C] | 2-0-0 [2]                                  |
| Offered for  | B.Tech., B.Tech.-M.Tech. Dual Degree, 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**

Fractal 1:

Image Filtering and Feature Extraction

Colour spaces, Frequency domain representation, convolution, Image transforms, noise removal, restoration of degraded images, Texture Features: moments, correlation, frequency domain, wavelet transform, keypoints and line extraction, keypoint based features.

Fractal 2:

Image Segmentation and Image Registration

Region growing, Clustering, Mixture Models, graph partitioning, keypoint correspondence, image registration as an optimization problem, 2D and 3D registration, multimodal registration

**Textbook**

1. Gonzalez, R., Woods. R., Digital Image Processing, 4<sup>th</sup> Edition, Global Edition, 2017
2. Szeliski . R., Computer Vision: Algorithms and Applications, 2<sup>nd</sup> Edition, Springer, 2022.

**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., Niezgodna, 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        | <b>Computational Materials Engineering Laboratory</b> | Number    | MTL7XX0   |
| Department   | Department of Metallurgical and Materials Engineering | L-T-P [C] | 0-0-2 [1]   |
| Offered for  | B.Tech., B.Tech.-M.Tech. Dual Degree, M.Tech.         | Type      | Specialization Core for Computational Materials Engineering |
| 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>



|               |   |          |                         |
|---------------|---|----------|-------------------------|
| Title         | <b>Machine Learning for Materials Design</b>  | Number   | 7XX0                    |
| Department    | Metallurgical and Materials Engineering       | L-T-P: C | 2-0-2: 3                |
| Offered for   | B.Tech., B.Tech.-M.Tech. Dual Degree, M.Tech. | Type     | Specialization Elective |
| Pre-requisite | -   |          |                         |

## Objectives

- Objectives**
1. Introduce a selected set of Machine learning and Deep Learning techniques for Materials design
  2. Introduce hands-on experience with some practical methods and techniques in materials informatics for materials classification, regression, clustering, and adaptive design.
  3. Introduce hands-on experience in analyzing data and applying ML approaches through a set of case studies pertaining to Materials Engineering.

## Learning Outcomes

1. To be able to apply 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 Neural Networks (RNNs), Self-Supervised Learning, Few Shot Learning, adversarial Learning, and Transformers. (14 lectures)

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

Laboratory exercises:  
1. 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 alloys
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 Materials Design and Discovery: Basic Ideas and General Methods*, Morgan & Claypool Publishers, 2020.
2. *Machine Learning And Data Mining In Materials Science*, Edited by Huber, N., Kalidindi, S. R., Klusemann, B. and Cyron, C. J., Frontiers in Materials, 2020.
3. Mueller, T., Kusne, A.G. and Ramprasad, R., *Machine Learning in Materials Science*. In Reviews in Computational Chemistry, Edited by Parrill, A.L., and Lipkowitz, K.B., John Wiley & Sons, 2016.

## Reference Books:

1. *Materials Informatics: Methods, Tools, and Applications*, Edited by Olexandr Isayev, Alexander Tropsha, Stefano Curtarolo, John Wiley & Sons, 2019

2. *Informatics for Materials Science and Engineering-Data-driven Discovery for Accelerated Experimentation and Application*, Edited by: Krishna Rajan, Butterworth-Heinemann, 2013

|              |  |           |   |
|--------------|--|-----------|---|
| Title        | <b>Data Visualisation in Materials Modelling</b>                   | Number    | MTL7XX0   |
| Department   | Department of Metallurgical and Materials Engineering              | L-T-P [C] | 1-0-0 [1]   |
| Offered for  | B.Tech. (CME specialization), B.Tech.-M.Tech. Dual Degree, M.Tech. | Type      | CME Specialization Elective (UG), CME Elective for M.Tech |
| 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.

|              |   |           |                         |
|--------------|---|-----------|-------------------------|
| Title        | <b>Modelling of Metallurgical Processes</b>   | Number    | MTL7XX0                 |
| Department   | Metallurgical and Materials Engineering       | L-T-P [C] | 3-1-0 [4]               |
| Offered for  | B.Tech., B.Tech.-M.Tech. Dual Degree, M.Tech. | 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 Korla, 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   | <b>Single and Multi-objective Evolutionary and Nature Inspired Algorithms</b> | Number    | MTL7XXX0                |
| Department  | Metallurgical and Materials Engineering                                       | L-T-P [C] | 1-0-0 [1]               |
| Offered for   | B.Tech., B.Tech.-M.Tech. Dual Degree, M.Tech.                                 | Type      | Specialization Elective |
| Prerequisite  |   |           |                         |
| <p><b>Objectives</b><br/> The Instructor will:<br/> 1. Introduce evolutionary algorithms for single and multi-objective optimization</p> <p><b>Learning Outcomes</b><br/> The students are expected to have the ability to:<br/> 1. Carry out Multi-objective optimization using evolutionary algorithms</p> <p><b>Contents</b><br/> 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)<br/> The 'Simple Genetic Algorithm'. The basic genetic operators: selection, crossover, mutation and their variants. (1 lecture)<br/> How Genetic Algorithm works: The Schemma Theorem. The problems of binary encoding: Hamming Cliff. Remedial measures: Gray encoding, real encoding, (1 lecture)<br/> Recent algorithms: Differential Evolution, Particle Swarm Optimization, Ant Colony optimization, Artificial Immune System Algorithms (2 lectures)<br/> Fundamentals of Multi-objective Optimization. The concept of Pareto Optimality (2 lectures)<br/> Major Evolutionary Multi-objective optimization Algorithms: SPEA, NSGAI, MOGA etc. (2 lectures)</p> <p>Genetic Programming (1 lecture)<br/> Data-driven modeling, Surrogate or metamodeling. Modeling data with random noise: EvoNN, BioGP and EvoDN2 algorithms. Commercial software like Kimmeme and ModeFrontier. (4 lectures)<br/> Term Project on a problem of student's choice.</p> <p><b>Textbook</b><br/> 1. Chakraborti Nirupam, <i>Data-driven evolutionary modelling in materials technology</i>, CRC Press, 2022.<br/> 2. Datta, Shubhabrata, <i>Materials design using computational intelligence techniques</i>. CRC Press, 2016.<br/> 3. Deb K. <i>Multi-objective optimization using evolutionary algorithms</i>. John Wiley &amp; Sons; 2001.</p> <p><b>Reference books</b><br/> 1. DE Goldberg, <i>Optimization &amp; Machine Learning</i>, Addison Wesley, 1989.<br/> 2. Melanie Mitchell, <i>An introduction to genetic algorithms</i>. MIT press, 1998.<br/> 3. Coello, Carlos A. Coello, and Gary B. Lamont. <i>Applications of multi-objective evolutionary algorithms</i>. Vol. 1. World Scientific, 2004.<br/> 4. Ant Colony Optimization by Marco Dorigo and Thomas Stützle, MIT Press, 305 pp.</p> |   |           |                         |

|               |  |          |                         |
|---------------|--|----------|-------------------------|
| Title         | <b>Crystal Plasticity and Its Applications</b> | Number   | MTL7XX0                 |
| Department    | Metallurgical and Materials Engineering        | L-T-P: C | 3-0-0 [3]               |
| Offered for   | B.Tech., B.Tech.-M.Tech. Dual Degree, 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.
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