MAHATMA GANDHI INSTITUTE OF TECHNOLOGY (AUTONOMOUS)

B.Tech. Minor in Al & ML in MATERIALS ENGINEERING (4 Semesters)

COURSE STRUCTURE & SYLLABUS
(MR 25 Regulations)
Applicable for the batches admitted from AY 2025-26

S. No.	Semester	Course Code	Course Title	L	T	P	Credits
1	IV Semester	M154AI	Fundamentals of Materials Engineering	3	0	0	3
2	IV Semester	M15408	Materials Characterisation Lab	0	0	2	1
3	V Semester	M155AI	Artificial Intelligence and its Applications in Materials Engineering	3	0	0	3
4	VI Semester	M156AJ	Machine Learning and its Applications in Materials Engineering	3	0	0	3
5	VI Semester	M15609	Artificial Intelligence and Machine Learning for Materials Design Lab	0	0	2	1
6	VII Semester	M157AY	Data Science for Materials Design and Selection	3	0	0	3
7	VII Semester	M15709	Project	0	0	4	4
			Total	**12**	**0**	**8**	**18**

L	T	P	C
3	0	0	3

B.Tech., Minor in AI & ML in Materials Engineering
IV Semester Syllabus
M154AI: Fundamentals of Materials Engineering

Course Objectives:

To introduce the concepts of engineering materials, mechanical and microstructural characterization, design, selection and applications of materials.

Course Outcomes:

1. Outline the significance of materials in current day Industry
2. Design an alloy system for a specific engineering application
3. Understand the importance of non-metallic materials
4. Recommend the techniques of characterization for a specific material
5. Use modern tools for design and selection of materials for engineering applications

UNIT I: Introduction to Materials Engineering

Conceptualization of Materials Science and Engineering, classification, properties and applications of materials, scope and importance and applications of materials engineering to the current day industry, ASTM standard testing procedures for materials, a brief insight into advances in materials engineering.

UNIT-II: Metals and Alloys

Bonds in solids, metallic bonding, concept of solid solution alloys: purpose and significance, classification and general guidelines of constitution of alloys, novel methods of processing of alloys. Advanced alloy systems: Superalloys, Shape Memory Alloys.

UNIT-III: Nonmetallic Materials

Concepts and classification of nonmetallic materials, brief insight into ceramics, polymers, classification, properties and applications of ceramics and polymers, concept of composite technology, an overview on composite materials: classification, characteristics, and applications.

UNIT-IV: Characterization of Materials

Need for materials characterization, techniques of characterization of materials, principles, equipment used for characterization, advances in materials characterization techniques.

UNIT-V: Design and Selection of Materials

Fundamentals of materials design for specific engineering applications, criteria for selection of materials for technology driven applications, a brief insight into computer aided tools, softwares and methods for design of engineering materials.

Text Books and References:

1. George Murray, Charles V. White, Wolfgang Weise, “Introduction to Engineering Materials”, CRC Press, 2007.
2. William. D. Callister, David G. Rethwisch, “Materials Science and Engineering: An Introduction”, John Wiley & Sons, 2018.
3. Machine Learning for Materials Discovery: Numerical Recipes and Practical Applications" (Krishnan et al., 2024): A practical guide covering algorithms from regression to generative modeling.

L	T	P	C
0	0	2	1

B.Tech., Minor in AI & ML in Materials Engineering
IV Semester Syllabus
M15408: Materials Characterisation Lab

Course Objectives:

To understand the mechanical behaviour of materials by conductiong mechanical and microstructural characterization.

Course Outcomes:

1. Understanding the utilization of Optical Microscope for Microsturctural characterization.
2. Understanding the Microsturcture and fracture surface by Scanning Electron Microscope.
3. Understand the mechanical behavior materials by conducting hardness and tensile tests
4. Understand the phases present in the microstructure by chemical analysis by using SEM.

List of Experiments:

1. Understanding the Principles of Optical Microscope and Metallographic Examination by Optical Microscope.
2. Understanding the Principles of Scanning Electron Microscope and Metallographic Examination by Scanning Electron Microscope.
3. Analysis of Microstructue by using Image-J – Phase Analysis, Grain Size, Volume Fraction calculation, and other Microstructural Features.
4. Hardness Measurement of different metals using Rockwell and Vicker's Hardness Testers.
5. Fractography analysis using Scanning Electron Microscope (SEM)
6. Analysis of XRD data and determination of Crystal Structure from diffraction pattern and Miller indices (hkl) using digital tools.
7. Analysis of TEM data and to determine Crystal Structure, Grain Size, and Microstructural features using digital tools.
8. Study of Crystal Structures and Calculation of crystal structure parameters through python programming.

L	T	P	C
3	0	0	3

B.Tech., Minor in AI & ML in Materials Engineering
V Semester Syllabus
M155AI: Artificial Intelligence and its Applications in Materials Engineering

Course Objectives:

To interoduce the concepts of Artificial Intelligence and their applications in Materials Engineering.

Course Outcomes:

1. Know the concepts of Artificial Intelligence.
2. Know the fundamentals of artificial neural networks.
3. Solve the materials data problems using artificial neural networks.
4. Know genetic algorithms and their applications in materials engineering

Unit I: Fundamentals of Artificial Intelligence and Machine Learning

Introduction to Artificial Intelligence (AI) and Machine Learning (ML), Importance of AI in engineering and industry, Relationship between material structure, properties, processing, and performance.

Unit 2: Basics of Artificial Neural Networks and Deep Learning

Introduction to Artificial Neural Networks (ANN), Biological neuron and artificial neuron model, Architecture of neural networks: Input layer, Hidden layer, Output layer, Learning process in ANN, Activation functions and loss functions, Backpropagation algorithm, Introduction to Deep Learning and recent developments.

Unit 3: Data Handling and Model Validation

Importance of data in AI and ML, Data collection and preprocessing, Training, validation, and testing datasets, Data normalization and feature selection, Performance evaluation methods: Accuracy, Error analysis, Model validation. Introduction to Python tools for ANN applications, Simple demonstrations related to materials data analysis**.**

Unit 4: AI Applications in Materials Engineering

Application of ANN in materials property prediction, Process–structure–property relationship studies, AI applications in Metallurgical processes like Heat treatment, Rolling and forming, Welding, casting and Corrosion prediction, Prediction of mechanical properties of metals and alloys, AI-based process optimization in metallurgical industries.Case studies using Python.

Unit 5: Advanced AI Techniques and Industrial Case Studies

Introduction to Genetic Algorithms (GA), Single and multi-objective optimization, Constraints optimization problems, Industrial case studies.

Textbooks

1. S. Haykin, Neural Networks: A Comprehensive Foundation, 2nd Edition, Prentice Hall India, 2003.
2. Stuart Russell and Peter Norvig, Artificial Intelligence: A Modern Approach, Pearson Education, 2019.
3. Dan W. Patterson, Introduction to AI and Expert Systems, PHI Learning, 2015.
4. Krishna Rajan and Olga Kononova, Materials Informatics, Elsevier, 2021

Reference Book

1. Rajalingappa Shanmugamani, Deep Learning for Computer Vision, Packt Publishing, 2018.

L	T	P	C
3	0	0	3

B.Tech., Minor in AI & ML in Materials Engineering
VI Semester Syllabus
M156AJ: Machine Learning and its Applications in Materials Engineering

Course Objectives:

To learn the concepts of AI /ML Models & apply for prediction of mechanical properties of materils and alloys

Course Outcomes:

1. Understand Machine Learning & various algorithms used.
2. Understand Cyclic oxidation of Metals & application of ML to predict cyclic oxidation
3. Understand High Entropy Alloys (HEA) & use of Machine Learning to predict mechanical properties.
4. Understand Creep phenomena and use AI/ML to predict the creep behavior of superalloys.
5. Understand constitutive behavior of Materials and use Artificial Nural Networks (ANN) to predict constitutive behavior of metals and alloys.

UNIT I: Fundamentals of Machine Learning:

Definition, significance and salient features of Machine Learning, Types of Machine Learning: Supervised Learning, Unsupervised Learning, Reinforcement Learning, Basic concepts of data, features, and datasets. Critical applications of Machine Learning in science and engineering; Algorithmic approach to Machine Learning, A brief insight into various algorithms used in Machine Learning process**.**

UNIT II: **Oxidation of Metals and Alloys:**
Classification of oxidation, reasons and consequences of oxidation, critical methods of avoiding oxidation in metallic materials, phenomenological approach to predict oxidation of metals. Machine Learning approach to predict oxidation of metals with a case study of cyclic oxidation.

UNIT III: Metals and Alloys:
An overview on metals and alloys, need and development of High Entropy Alloys, conceptualization of thermodynamic entropy, High entropy effect in metals and alloys, definition, classification and application of high entropy alloys, Machine learning application to predict mechanical properties of refractory high entropy alloys.

UNIT IV: Creep Behavior of Materials:
Definition of creep, importance in critical engineering applications, types of creep, modeling of creep behavior, Concept of superalloys, Artificial Intelligence application to predict creep behavior of Materials with a case study of superalloys.

UNIT V: **Constitutive Behavior of Materials:**
Insights of constitutive behavior, current models for understanding constitutive behavior of materials, related case studies, applications of Artificial Neural Networks (ANN) in constitutive behavior of meterials.

Text Books/ References:

1. John D. Kelleher, Brian Mac Namee, Aoife D' Arcy : Fundamentals of Machine Learing for Predictive Data Analytics.
2. T. Lookman, Stephan Eidenbennz, et al., Materials Discovery and Design by Means of Data Science and Optimal Learning, Springer , 2018
3. Y. Cheng, T. Wang ad G. Zhang; Artificial Intelligence for Materials Science, Springer ,2018
4. Phil Del Luna, Accelerated Materials Discovery, De Grutyer, 2022

L	T	P	C
0	0	2	1

B.Tech., Minor in AI & ML in Materials Engineering
VI Semester Syllabus
M15609: Artificial Intelligence & Machine Learning for Materials Design Lab

Course Objectives:

To apply the concepts of AI /ML in evaluating materials physical and mechanical properties for materials design.

Course Outcomes:

1. Understand the materials data with the concepts of Artificial Intelligence.
2. Data interpretation for Mechanical Testing Materials.
3. Classification metals and materials by using artificial neural networks.
4. To optimize the materials data to understand materials engineering

List of Experiments:

1. To perform basic Python operations using materials engineering data.
2. Ploting stress-strain data using Python.
3. Predicting tensile properites using linear regression using Python.
4. Classificaiton of metals and materials based on hardness values using Python.
5. To implement a simple Artificial Neural Network (ANN) using Python.
6. To normalize materials engineering data using Python.
7. Demonstration(s) of simple optimization algorithms using Python.

L	T	P	C
3	0	0	3

B.Tech., Minor in AI & ML in Materials Engineering
VII Semester Syllabus
M157AY: Data Science for Materials Design and Selection

Course Objectives:

To know the concepts of data science and data models to predict the mechanical properties for selection of a suitable material for applications.

Course Outcomes:

1. To understand the concepts of data science and its applications with respect to materials engineering.
2. The available data models should be used for designing the materials for applications.
3. To understand the modelling of materials and their applications by using AI/ ML approaches.
4. To develop the data science models for selection of a suitable materials based on the applications.

UNIT I: **Fundamentals of Data Science**:
Introduction to Data Science, Three pillars of data science, Types of Data, Measuring the Central Tendency: Mean, Median, and Mode, Measuring the Dispersion of Data: Range, Quartiles, Variance, Standard Deviation, and Interquartile Range, Graphic Displays of Basic Statistical Descriptions of Data, significance and applications of data science, methods of data generation, classification, design and analysis.

UNIT II: **Design of Materials:**
Necessity of designing of materials for engineering applications, methods and models involved in designing of materials, traditional procedures for design of materials, a brief insight into AI/ML based approaches for designing of materials.

UNIT III: Modelling Methods of Materials:
Fundamental approaches to modelling of materials, data driven methodologies for materials modelling, designing novel materials using artificial intelligence.

UNIT IV: **Selection of Materials based on the applications:**
Need and necessity for selection of materials for different technologies, methods of selection, Machine Learning based applications in selection of materials. Large Language Models (LLM) approach in selection of materials.

UNIT V: **Methods of Data Handling and Data Validation:**

Different methods of data handling, a brief insight into structure-property correlation techniques using Artificial Intelligence approach, case studies involving optimum solutions for design model for materials.

Textbooks / References:

1. John D. Kelleher, Brian Mac Namee, Aoife D' Arcy: Fundamentals of Machine Learning for Predictive Data Analytics.
2. T. Lookman, Stephan Eidenbennz, et al., Materials Discovery and Design by Means of Data Science and Optimal Learning, Springer, 2018
3. Y. Cheng, T. Wang ad G. Zhang; Artificial Intelligence for Materials Science, Springer ,2018
4. Phil Del Luna, Accelerated Materials Discovery, De Gruyter, 2022