# ACADEMIC AFFAIRS OFFICE INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

No. Acd./ 3/60 /IAPC-78

Dated: February 65, 2020

## <u>Head, Department of Metallurgical & Materials Engineering</u> (through e-mail)

The IAPC in its 78<sup>th</sup> meeting held on 31.12.2019 vide **Item No. 78.2.2 (1)** considered the proposal to revise curriculum of PCC MTN-502: Modelling, Simulation and Computer Applications.

The IAPC accepted the proposal with minor modifications. The modified syllabus is attached as **Appendix-A**.

**Assistant Registrar (Curriculum)** 

Encl: as above

#### Copy to (through e mail):-

- 1. All faculty
- 2. All Heads of Departments/ Centres
- 3. Dean, Academic Affairs
- 4. Associate Dean of Academic Affairs (Curriculum)
- 5. Channel I/ Academic webpage of iitr.ac.in

#### INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT: Department of Metallurgical and Materials Engineering

1. **Subject Code**: MTN-502 **Course Title**: Modelling, Simulation and Computer Applications

2. Contact Hours: L: 3 T: 0 P: 2

3. Examination Duration (Hrs): Theory: 3 Practical: 0

4. Relative Weightage: CWS: 10-25 PRS: 25 MTE: 15-25 ETE: 30-40 PRE: 0

5. Credits: 4 6. Semester: Spring 7. Subject Area: PCC

**8. Pre-requisite:** Nil

9. Objective: To introduce various approaches used for modeling and simulation of materials

#### 10. Details of the Course:

S.No.	Particulars	Contact Hours
1.	<b>Introduction:</b> Need for modelling and simulation. Concepts of length and time scales in different materials phenomena, and choosing the appropriate modelling schemes to tackle them.	2
2.	Brief review of classical and statistical mechanics: Concepts of Lagrangian, Hamiltonian, and equations of motion from classical mechanics. Statistical mechanical concepts of Microstates, Phase space, Ensembles and the Ergodic hypothesis.	5
3.	Interatomic potentials and Boundary Conditions: Concept of cohesive energy and its formulation using semi-empirical potentials, Pair potentials like Lennard-Jones, Morse and Born-Mayer, Limitations of Pair Potentials, Embedded atom model potentials (EAM) for metals and alloys. Stillinger-Weber (SW) potential for covalent solids, Modeling coulombic interactions in ionic materials and challenges, Transferability of semi-empirical potentials, Boundary conditons: periodic and free, Cut-off distances for potentials.	7
4.	Molecular statics (MS) and dynamics (MD): Fundamentals of MS, Energy minimization algorithms like Steepest Descent and Conjugate Gradient, Applications of MS in calculating defect energies, Fundamental concepts of MD, Numerical algorithms for time integration of equations of motion, Properties of MD simulations, Analyzing MD simulations using spatial and time correlation functions, MD in different ensembles, Applications of MD, Limitations of MD.	10
5.	Monte-Carlo simulations (MC): Metropolis algorithm and its application to study the Ising model, Monte-Carlo in the mesoscopic scale: Q-state Potts Model, MC across different ensembles, Concept of time in MC, Analyzing MC simulations, Applications and Limitations of MC.	8
6.	Phase-field modeling: The diffuse interface and its advantages, Concepts of conserved and non-conserved order parameters to describe microstructure, Allen-Cahn and Cahn-Hilliard equations for microstructure evolution, Concepts of interfacial energy and width, Numerical algorithms and analysis of simulation results, Ways to construct free energy functions.  Total	10
	42	

#### **List of Practicals:**

- 1. Defect energy calculation using Molecular Statics
- 2. Molecular Dynamics simulation of melting
- 3. Simulations of deformation using Molecular Dynamics
- 4. Metropolis Monte-Carlo study of the Ising model
- 5. Employing Q-state Potts model to simulate grain growth
- 6. Phase-field simulation of spinodal decomposition

### 11. Suggested Books:

S.No.	Name of Author (s) / Book/ Publisher	Year of
		Publication
1.	Lesar R., An introduction to computational material science –	2013
	Fundamentals to Applications, Cambridge University Press	
2.	Landau D. P., and Binder K., A Guide to Monte-Carlo Simulation in	2014
	Statistical Physics, Cambridge University Press	
3.	Frenkel D., and Smit B., Understanding Molecular Simulation, Academic	2001
	Press	
4.	Provatas N., and Elder K., Phase-field methods in Material Science and	2011
	Engineering, Wiley-VCH	