

SEMESTER V

1. INTRODUCTION TO MODELING AND SIMULATION

Module I (11 hrs)

Mathematical Basics: length scales, flow chart of models, PDEs and boundary conditions (Neumann, Dirichlet, Robin, Cauchy), fourth order Runge Kutta Method, finite Difference method, Leap Frog Algorithm, Numerical errors;

Ab Initio Methods (DFT): Slater determinant, Hartee Fock method, Kohn Sham Equations;

Module II (9 hrs)

Statistical Mechanics: phase space, Micro Canonical, Canonical and Grand Canonical Ensembles, Ergodic Hypothesis;

Monte Carlo Simulation: basics, hit or miss technique, simple and importance sampling, Metropolis algorithm;

Molecular Dynamics: classical pair potentials, many body pair functional potentials, verlet algorithm,

Module III (9 hrs)

Grain continuum modelling: representations and models, grain continuum approach and examples;

Finite element modelling of materials: Computational micro-mechanics, Multiscale coupling;

Modelling dislocation behaviour: discretization, regularization, approximations, nonlocal and image fields, applications in bulk and film plasticity;

Module IV (9 hrs)

Phase field modelling: microstructure representation, thermodynamics, evolution equations, numerical simulation

Mesoscale Modelling of grain growth and microstructure in polycrystalline materials: molecular dynamics of grain growth, mesoscale simulation methodology and validation;

Modelling of structural materials: structural materials, metals, polymers, ceramics, time scales

Text and Reference Books:

1. Computational Material Science, Dierk Raabe, Wiley-VCH Verlag GmbH, 1998
2. Multiscale Materials Modelling: Fundamentals and Applications, Ed Z Xiao Guo, Woodhead Publishing Limited, Cambridge, 2007.
3. Introduction to Materials Modelling, Ed Zoe H. Barber, Maney Publishing, 2005
4. Computational Material Science From Ab Initio to Monte Carlo Methods, K. Ohno, K.Esfarjani, Y. Kawazoe, Springer, 1999
5. Multiscale Modelling & Simulation, Astringes & Coumoutsakos, Springer
6. Computational Materials Design, Tetsuya, Springer
7. Continuum Scale Simulation of Engineering Materials-Fundamentals, Microstructures, Process Applications, Dierk Rabbe, Barlat, Wiley, 2004
8. Combinatorial material Science, Balaji narasimhan, Surya K Mallaprajada, wiley, 2007