

MSE-341 Computational Materials Science

Credit Hours: 2-1

Pre-requisites: CS-117

Course Objectives

This course introduces the basic concepts, techniques, and applications of computational methods in materials engineering. The students will learn about different modelling and simulation tools to predict the behavior of materials at different length scales.

Course Contents

- Introduction to computational material science and engineering.
- Introduction to modelling and simulation software (Abaqus / Solidworks); 3D part and assembly modelling, finite element analysis; stress analysis using finite element modeling.
- 1D Structural Analysis (Truss Elements – Overhead Hoist); 3D Mechanical (Elastic/Plastic) Analysis; deformation of basic structure (Cantilever Beam); 3D Mechanical (Elastic) Analysis; deformation of mechanical parts (Connecting Lug); 2D Heat Transfer + Mechanical Analysis (Plane Stress/Strain) (2D Trapezoidal Plate); Tensile Test – Axisymmetric, 2D or 3D – Elastic, Elastoplastic with/without damage (Tensile Test of a Ductile Material); Contact analysis including rigid and deformable bodies (3 Points Bend Test); Modelling of elastic properties; plastic deformation and mechanical behavior of engineering materials. Data analysis and plotting.

Weekly Plan

Week	Topics
1	Introduction to computational material science and engineering
2	Introduction to modelling and simulation software (Abaqus / Solidworks)
3	
4	
5	3D part and assembly modelling, finite element analysis; stress analysis using finite element modeling.
6	
7	1D Structural Analysis (Truss Elements – Overhead Hoist)
8	
9	Mid-Semester Exams

10	3D Mechanical (Elastic/Plastic) Analysis; deformation of basic structure (Cantilever Beam)
11	
12	3D Mechanical (Elastic) Analysis; deformation of mechanical parts (Connecting Lug); 2D Heat Transfer + Mechanical Analysis (Plane Stress/Strain) (2D Trapezoidal Plate); Tensile Test – Axisymmetric, 2D or 3D – Elastic
13	
14	
15	Elastoplastic with/without damage (Tensile Test of a Ductile Material); Contact analysis including rigid and deformable bodies (3 Points Bend Test); Modelling of elastic properties; plastic deformation and mechanical behavior of engineering materials. Data analysis and plotting.
16	
17-18	End Semester Exams

Course Outcomes

At the end of the course, students will be able to:

- Explain the process of finite element analysis and interpret the role of modelling and simulation softwares in materials engineering.
- Apply modelling and simulating techniques to predict mechanical behavior of materials under various loading scenarios.
- Generate plots and graphs to effectively communicate the experimental findings.

Suggested Books

- Introduction to Computational Materials Science: Fundamentals to Applications by R. LeSar. 1st ed. Cambridge University Press (2013)
- Introduction to Materials Modelling by Z. H. Barber. Maney Publishing, (2005)
- Computational Materials Science by D. Raabe. Wiley VCH Verlag GmbH, (1998)
- An Introduction to Computer Simulation by M. M. Wolfson, G.J. Pert. Oxford, (1999)