MATSCEN 2321 (Approved): Modeling and Simulation Lab I

Course Description

A modeling and simulation laboratory appropriate to sophomore-level study in materials science and engineering.

Transcript Abbreviation: Mod Sim Lab I
Grading Plan: Letter Grade
Course Deliveries: Classroom
Course Levels: Undergrad
Student Ranks: Sophomore
Course Offerings: Spring
Flex Scheduled Course: Never
Course Frequency: Every Year
Course Length: 14 Week
Credits: 3.0
Repeatable: No
Time Distribution: 2.0 hr Lec, 1.0 hr Lab
Expected out-of-class hours per week: 6.0
Graded Component: Lecture
Credit by Examination: No
Admission Condition: No
Off Campus: Never
Campus Locations: Columbus
Prerequisites and Co-requisites: Prerequisite: MSE 2010; Calculus I
Co-requisites: MSE 2241, MSE 2251
or permission of instructor.
Exclusions:
Cross-Listings:

The course is required for this unit's degrees, majors, and/or minors: Yes
The course is a GEC: No
The course is an elective (for this or other units) or is a service course for other units: No

Subject/CIP Code: 14.1801
Subsidy Level: Baccalaureate Course

Programs

Abbreviation	Description
MATSCEN	Materials Science and Engineering

Course Goals

Introduce students to visualizing data and mathematical functions, numerical and symbolic differentiation/integration, matrix operations, coupled algebraic equations, and elementary programming constructs related to materials science and engineering.
Introduce students to materials databases, graphical representation of material properties, and elementary case studies in materials selection.
Introduce students to modeling and simulation of crystal structures and diffraction spectra.
Introduce students to modeling and simulation of simple (e.g., isomorphous binary) phase diagrams and more advanced (e.g., binary eutectic) phase diagrams.
Introduce students to atomistic modeling and simulation methods to estimate energies of perfect crystals and energies of defects.

Define limitations of models and simulations and methods by which to assess accuracy.

Course Topics

Topic	Lec	Rec	Lab	Cli	IS	Sem	FE	Wor
Lab A. Introduction to Visualization and Manipulation of Data and Functions: Visualization of data and functions in 2D and 3D; differentiation, integration, and extraction of data subsets; e.g., MatLab.	4.0		2.0					
Lab B. Introduction to Materials Selection: Databases/graphical representation of properties; materials selection (e.g., optimization of stiffness, strength, cost); case studies; software limitations; e.g., Cambridge Engineering Materials Selector.	6.0		3.0					
Lab C. Introduction to Crystal Visualization and Diffraction: Visualization of crystal structures and defects; computation of diffraction spectra; determining structure from diffraction spectra; software limitations; e.g., CrystalMaker, MatLab.	6.0		3.0					
Lab D. Introduction to Thermodynamic Modeling and Simulation: Theory/construction of isomorphous and binary phase diagrams; calculation of free energy vs. temperature, composition; software limitations; e.g., PANDAT, MatLab.	6.0		3.0					
Lab E. Introduction to Atomistic Modeling and Simulation: Construction of elementary crystal models, computation of internal energy of perfect crystals and defect energies; software limitations; e.g., MatLab.	6.0		3.0					

Representative Assignments

Lab A: Read in and manipulate data (e.g., spatial distribution of temperature or displacement as a function of time during casting or deformation); Produce movies of the function evolution (or derivatives thereof) with time; identify maxima and minima.
Lab B: Select optimal materials for a stiff, yet light component to be used in compression or in a 3-pt, 4-pt, or cantilevered application.
Lab C: Determine the crystal structure based on diffraction spectra; determine anisotropy in surface energy based on a bond cutting model; determine dimensions of interstitial sites in a crystal; determine atomic packing factors.
Lab D: Selection of a binary system and alloy composition based on desired physical properties.
Lab E: Estimate the free energy of a FCC vs. BCC crystal given an atomic bonding relation; estimate the free energy of a vacancy atom.

Grades

Aspect	Percent
In-class assessment	40%
Homework assignments and Projects	60%

Representative Textbooks and Other Course Materials

Title	Author
Manual: Cambridge Engineering Selector Software	
Manual: CrystalMaker and CrystalDiffract Software	

Title	Author
Manual: PANDAT Software	

ABET-EAC Criterion 3 Outcomes

Course Contribution		College Outcome
***	a	An ability to apply knowledge of mathematics, science, and engineering.
***	b	An ability to design and conduct experiments, as well as to analyze and interpret data.
**	c	An ability to design a system, component, or process to meet desired needs.
	d	An ability to function on multi-disciplinary teams.
***	e	An ability to identify, formulate, and solve engineering problems.
	f	An understanding of professional and ethical responsibility.
**	g	An ability to communicate effectively.
	h	The broad education necessary to understand the impact of engineering solutions in a global and societal context.
	i	A recognition of the need for, and an ability to engage in life-long learning.
	j	A knowledge of contemporary issues.
***	k	An ability to use the techniques, skills, and modern engineering tools necessary for engineering practice.

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