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

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tr>
<td>MATSCEN</td>
<td>Materials Science and Engineering</td>
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Course Goals

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<th>Course Goals</th>
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<tr>
<td>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.</td>
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<tr>
<td>Introduce students to materials databases, graphical representation of material properties, and elementary case studies in materials selection.</td>
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<tr>
<td>Introduce students to modeling and simulation of crystal structures and diffraction spectra.</td>
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<tr>
<td>Introduce students to modeling and simulation of simple (e.g., isomorphous binary) phase diagrams and more advanced (e.g., binary eutectic) phase diagrams.</td>
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<tr>
<td>Introduce students to atomistic modeling and simulation methods to estimate energies of perfect crystals and energies of defects.</td>
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Define limitations of models and simulations and methods by which to assess accuracy.

**Course Topics**

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<tr>
<th>Topic</th>
<th>Lec</th>
<th>Rec</th>
<th>Lab</th>
<th>Cli</th>
<th>IS</th>
<th>Sem</th>
<th>FE</th>
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<tr>
<td>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.</td>
<td>4.0</td>
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<td>2.0</td>
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<td>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.</td>
<td>6.0</td>
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<td>3.0</td>
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<tr>
<td>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.</td>
<td>6.0</td>
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<td>3.0</td>
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<td>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.</td>
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<td>3.0</td>
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<tr>
<td>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.</td>
<td>6.0</td>
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<td>3.0</td>
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**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**

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<tr>
<th>Aspect</th>
<th>Percent</th>
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<tr>
<td>In-class assessment</td>
<td>40%</td>
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<tr>
<td>Homework assignments and Projects</td>
<td>60%</td>
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**Representative Textbooks and Other Course Materials**

<table>
<thead>
<tr>
<th>Title</th>
<th>Author</th>
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<tbody>
<tr>
<td>Manual: Cambridge Engineering Selector Software</td>
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<tr>
<td>Manual: CrystalMaker and CrystalDiffract Software</td>
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### ABET-EAC Criterion 3 Outcomes

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