THE OHIO STATE UNIVERSITY
COLLEGE OF ENGINEERING

Modeling and Simulation Lab I

MATSCEN 2321

Credit Hours:
3.00

Course Levels:
Undergraduate (1000-5000 level)

Course Components:
Lecture
Lab

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

Prerequisites and Co-requisites:
Prereq: 2010, Physics 1250 or 1260, Math 1151 or 1161, and Chem 1210 or 1250; and enrollment as MatScEn-BS student; or permission of instructor.

Course Goals / Objectives:
- 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:

- 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.
- 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.
- 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.
- 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.
- 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.

Designation:
Required