Syllabus for MTSE 4040 Computational Materials Science

Course Number: MTSE 5710/4040 Computational Materials Science
Time: Tuesday 2:30PM - 5:20pm
Classroom: Discovery Park D207B
Dates: Jan 20, 2016-May 15, 2016
Instructors: Dr. Jincheng Du, Dr. Srinivasan Srivilliputhur, Dr. Zhenhai Xia

Course Summary
Computational materials modeling has emerged as an increasingly important branch of materials science due to the evolution of modeling frameworks, invention of novel numerical algorithms, and increased computer capability. As a consequence, modeling and simulation are emerging as powerful complementary approaches to experiment and traditional theory. The aims of this course are to: (i) introduce students to materials modeling and simulation techniques that cover a wide time and length scales; (ii) show how these modeling methods can be used to understand fundamental material structure, material defects and the relationships between material structure and material behavior; and (iii) develop an understanding of the assumptions and approximations that are involved in the modeling frameworks at the various time and length scales. Students will be introduced to the basis for the simulation techniques, learn how to use computational modeling, and how to present and interpret the results of simulations. The students will work with simulation modules to reinforce concepts learned in the lectures. No computer programming will be required.

Course Requirements
Introduction to Materials Science or an equivalent course. Computer programming knowledge is NOT a prerequisite.

Grading

Class projects	(75%)
Course project	(25%)

Class projects: The class projects include three modules, in which class projects are signed. After the projects are completed, the students are required to write project reports summarizing his or her work on their class project modeling. This report must be typed, single spaced, 12 point Symbol and/or Times New Roman fonts, and with 1-inch margins around. The report will follow the style of a standard laboratory report and must include the following sections: Title, Author and affiliation, Abstract, Introduction (of the method used and properties calculated), Results, Discussions (comparing the results from simulations with corresponding experimental values, or theory), Conclusions, and References. You must include appropriate visual figures from the simulations (including charts and graphs, and material structures). All the legends and labels in the charts and graphs must be at least a 12-point font when scaled to fit to the report.

Course project includes a literature review (minimum seven pages, double space) on a selected area of computational material science. The topic is picked in consultation with one of the instructors and can be related to current research work you are carrying out.

Tentative timeline:
February 23th – turn in the first project report in Module one
March 29th – turn in the second project report in Module two

April 26th – turn in the third project report in Module three
March 1rd – Assign the Course report (review report) and discuss with instructor (optional)
April 29th (TBD) – turn in the review report

Codes to be provided:
Each student is required to bring his/her laptop to install the codes needed for class projects
o VASP code for DFT simulations
o LAMMP code for MD simulation
o ABAQUS code for FEA simulation

Brief list of topics to be covered

1. General introduction and overview; (Instructor: Dr. Xia)
Week 1: Introduction

2. Quantum Mechanics Module (4 weeks) (Instructor: Dr. Jincheng Du)
Week 2: Introduction to quantum mechanical methods
Week 3: Density function theory and application to solid materials
Week 4: First principles modeling of material surfaces
Week 5: Module projects on quantum mechanical calculations

3. Atomistic Modeling Module (4 weeks); (Instructor: Dr. Srinivasan Srivilliputhur)
Week 6: Introduction to Atomistic Modeling
Week 7: Interatomic Potentials, including computational exercises
Week 8: Molecular statics, including computational exercises
Week 9: Molecular dynamics, including computational exercises
4. Continuum Modeling Module (4 weeks) (Instructor: Dr. Zhenhai Xia)
Week 10: Introduction to continuum mechanics
Week 11: Computational methods
Week 12: finite element modeling of materials
Week 13: Finite element materials design project

5. Course project (1-2 weeks);
Week 14-15: Review of Computational Materials

Some details in Atomistic Modeling Module: Atomistic modeling will be covered from weeks six through nine (02/23, 03/01, 03/15, and 03/22). Students are expected to have a laptop to run their simulations. We will use open-source LAMMPS code for atomistic simulations and OVITO for visualization of results. Please download the executable for two codes from lammps.sandia.gov and ovito.org on your laptops.

The students will first learn the fundamentals of interatomic potentials, statics and dynamics simulations, and visualization and analyses of results using metals as a model system. This year we have chosen silver as the system of interest. They will also learn about the new directions in computational materials science, especially novel materials databases, under the Materials Genome Initiative (MGI). In addition to the above theoretical concepts, the students will conduct simulations at zero Kelvin (molecular statics) and at finite temperatures (molecular dynamics).

Molecular Statics Simulations: The students will calculate the following properties of silver– (a) energy versus volume relationship of fcc, bcc, and hcp crystals. From these curves, they will determine their equilibrium lattice constants and cohesive energy. (b) For only fcc crystals, they will calculate the equation of state, vacancy and interstitial formation energies, and excess energies of (100), (110), and (111) surfaces. Lastly, they will conduct molecular dynamics simulations

Molecular Dynamics Simulations: The students will calculate the thermal expansion coefficient and melting point of fcc Ag.

Student report for atomistic modeling is due on March 29, 2016. Each student must write an individual report summarizing his or her work on atomistic modeling. This report must be typed, single spaced, 12 point Symbol and/or Times New Roman fonts, and with 1-inch margins around. The report will follow the style of a standard laboratory report and must include the following sections: Abstract, Introduction (of the method used and properties calculated), Results, Discussions (comparing the results from simulations with corresponding experimental values), Conclusions, and References. You must include appropriate visual figures from the simulations (including charts and graphs, and crystal structures). **All the legends and labels in the charts and graphs must be at least a 12-point font when scaled to fit to the report**.

CAUTION: follow the timeline above; pace your effort and don't wait until the deadline.