Technical Elective: Computational Materials Science
Spring 2025

Instructor

Dr. Liwei Geng
RM N402
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Meeting Time & Location

Lecture & Lab: Mondays 13:50-16:25 at RM S506

Office Hours

Wednesday & Thursday: 13:00-17:00

TA Information

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Course Catalog Description

Theories of materials science from first principles to constitutive laws. Materials modeling and computer simulation at multiple length and time scales. Laboratory practice of various computational methods. Hands-on experience in code development and programming.

Prerequisites

Basic programming skill in at least one of the following environments: Mathematica, Matlab, Fortran, C, C++, Python …

Course Objectives

Upon successful completion of this course, a student will be able to

1. apply some fundamental theories of materials science from first principles to continuum constitutive laws;
2. model and simulate basic material structure and property at multiple length and time scales;
3. select appropriate computational tools for specific problems based on the advantages and limitations of different computational methods;
4. perform computational materials research by using available software;
5. develop custom code of selected materials topics in one computing environment.

Learning Outcomes

1. An ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics.
2. An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors.

3. An ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions.
4. An ability to acquire and apply new knowledge as needed, using appropriate learning strategies.

Course Materials

Lecture notes and handouts; No textbook.

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Topics Covered

1. First-Principles Calculation based on DFT
2. Molecular Dynamics
3. Statistical Thermodynamics & Monte Carlo Method
4. Binary Solid Solution
5. Phase Field Modeling
6. Finite Element Method

Grading

10%: Participation
15%: Homework (Chapters 3-5)
45%: Lab reports
30%: Final project (report and presentation)

Late Assignment Policy

10% deduction/day

Grade Policy

A: 90 – 100	A−: 85 – 89	B+: 80 – 84	B: 76 – 79	B−: 73 – 75
C+: 70 – 72	C: 66 – 69	C−: 63 – 65	D: 60 – 62	F: < 60

Academic Integrity

All students are expected to adhere to the standards of academic honesty. Any student engaged in cheating, plagiarism, or other acts of academic dishonesty would be subject to disciplinary action. Any student suspected of violating this obligation for any reason during the semester will be required to participate in the procedural process, initiated at the instructor level, as outlined in the University Guidelines on Academic Integrity. This may include but is not limited to the confiscation of the examination of any individual suspected of violating the University Policy.

Tentative Lecture/Lab Schedule

Week	Date	Lecture & Lab Content
1	2/24	Introduction, Quantum Mechanics; Lab 1
2	3/03	First-Principles and DFT; Lab 2
3	3/10	Crystal Structure; Lab 3
4	3/17	First-Principles Calculation Examples; Lab 4
5	3/24	Molecular Dynamics Theoretical Basis, Lab 5
6	3/31	General Algorithm of MD, Lennard-Jones Potential; Lab 6
7	4/07	Statistical Thermodynamics; Lab 7
8	4/14	Monte Carlo Method; Lab 8
9	4/21	Binary Solid Solution; Lab 9
10	4/28	Mathematical Foundation of Phase Field Modeling; Lab 10
11	5/05	Finite Difference Method, Spinodal Decomposition; Lab 11
12	5/12	Calibration of Length/Time Scales, Grain Growth; Lab 12
13	5/19	Finite Element Method; Lab 13
14	5/26	Examples of Finite Element Method; Lab 14
15	6/02	Seminar of Final Project
16	6/09	Final Project Presentation
17	6/16	Final Project Presentation

Final Project

Requirement: Written Report + Oral Presentation

Idea:

1. Use what you learn in this course to find a topic/problem and solve it. (must be your own idea, never cheat or plagiarize)
2. Try to learn a new software we don't show in class and apply it to a specific problem. (DFT: VASP, ABINIT …; Molecular dynamics: feram, AMBER, OPLS …; Monte Carlo: BOSS, MacroModel …)
3. Try to reprogram the Spinodal Decomposition code by using a different language. (C, C++, Matlab …)
4. Build your own mathematical model and develop a program by yourself to solve the problem in materials science.

Written Report Format:

1. Introduction

Brief description of the background of your project research topic, with a few relevant references. You are expected to understand the general concepts of the topic and identify at least one problem to solve (not necessarily unsolved in literature), into which you propose to gain some insight by using computer modeling and simulation.

2. Methodology

Mathematical formulation of the model of your research problem (if relevant), numerical method used to solve the equations (if relevant), and input parameters used in your simulations (if relevant).

3. Results and Discussion

Simulation results to shed some light on the problem(s) of your interest. Discussion is What you want to say about your research project (limited to/based on your results).

4. Conclusion

Briefly summarize your main findings.

5. References

Key references.

<u>Oral Presentation:</u>

10 minutes' seminar-style computer-based presentation, followed by a question-and-answer part in class.