

MSE 201: Phases and Phase Relations

Syllabus version January 15, 2021

Spring 2021, Fully on-line. Homepage <https://campuswire.com/c/GD73EE5D7>

3 credit hours

Credit is not given for both MSE 201 and MSE 280

Synchronous meeting times will be on MWF at 10:00-10:50 via Campuswire. Each class session will start with an approximately 30-minute lecture that will be recorded with no questions. Each lecture will be followed by 20 minutes of questions, answers, and discussion. The discussion will not be recorded. The recorded lectures and lecture notes will be made available for asynchronous viewing via Campuswire.

Instructor and TAs

Instructor: Prof. David Cahill (he/him)
Campuswire office hours: MWF 11-11:50
Phone: 217-333-6753
Email: d-cahill@illinois.edu

TA: Amlan Das (he/him)
Campuswire office hours: MWF 4:00-4:50
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Computational TA: Kisung Kang (he/him)
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Course Description

Introduction to bonding, crystal structures, phase equilibria and microstructure. Quantitative examination of phases (crystalline and non-crystalline structures) and the relationships between phases (phase diagrams and phase transitions).

Course Objectives

Upon completion of the course, students will be able to:

- Define a thermodynamic phase.
- Use density functional theory to calculate the cohesive energy and bulk modulus of a crystal.
- Use python to analyze and visualize one-dimensional data.
- Interpret a phase diagram and categorize transformations between phases.
- Use Thermocalc to calculate temperature versus composition phase diagrams.
- Describe and interpret the crystal structures of common metals, ceramics, and semiconductors.
- Use concepts of point defect diffusion, interface energy, and nucleation to predict the kinetics of phase transformations.
- Contrast the structure and properties of crystalline and non-crystalline materials.

Prerequisites

MSE 182; credit or concurrent enrollment in CHEM 104, MATH 231 and PHYS 211. (The prerequisite of MSE 182 is often waived for students that were not enrolled in the MatSE degree program in the fall semester of their freshmen year.)

Course Expectations and Teaching Philosophy

The focus of this course is on intermediate-level topics in materials science and engineering that bridge the introductory content of MSE 182 and the greater depth of the junior year curriculum. The primary textbook is "Materials Science, an Intermediate Text," by William Hosford. We will supplement this text with selected readings and exercises in python computation, crystallography and diffraction, and density functional theory. All the texts are free to download as ebooks for U. Illinois students.

The design of the course combines reading of texts, lectures, (virtual) classroom discussion, discussion forums, weekly homework, and assessment by two midterm exams and one final exam. We will strive to clearly articulate the assignments, due dates, and grading criteria.

MSE 201 is a 3 credit hour course and therefore requires a minimum commitment of 9 hours per week. I expect you to spend 2.5 hours per week attending the synchronous on-line lectures and discussions. You should spend a minimum of 6.5 hours per week reviewing lecture material, reading, doing homework, contributing to asynchronous discussions, and studying for exams. I recommend that you schedule a regular time to study.

Web Applications

URL	Purpose
Campuswire.com	Discussion forum; posting of text-based resources, e.g., syllabus, schedule, required readings; on-line synchronous lectures, office hours; posting of video recordings of lectures and lecture notes.
Gadescope.com	Assignments; rubrics; gradebook; exams
Teamup.com	Course schedule

Academic Integrity Policy

The University of Illinois at Urbana-Champaign Student Code should also be considered as a part of this syllabus. According to the Student Code, 'It is the responsibility of each student to refrain from infractions of academic integrity, from conduct that may lead to suspicion of such infractions, and from conduct that aids others in such infractions.'

Academic dishonesty may result in a failing grade. Every student is expected to review and abide by the Academic Integrity Policy: <http://studentcode.illinois.edu/>. Ignorance is not an excuse for academic dishonesty. It is your responsibility to read this policy to avoid any misunderstanding. Do not hesitate to ask the instructor if you are ever in doubt about what constitutes plagiarism, cheating, or any other breach of academic integrity.

See also this quick reference guide to academic integrity:

<https://provost.illinois.edu/policies/policies/academic-integrity/students-quick-reference-guide-to-academic-integrity/>

Academic Accommodations

To obtain disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact the course instructor and the Disability Resources and Educational Services (DRES) as soon as possible. To contact DRES, you may visit 1207 S. Oak St., Champaign, call 333-4603 (V/TDD), or e-mail a message to disability@uiuc.edu. <http://www.disability.illinois.edu>

Family Educational Rights and Privacy Act

Any student who has suppressed their directory information pursuant to Family Educational Rights and Privacy Act (FERPA) should self-identify to the instructor to ensure protection of the privacy of their attendance in this course. See <https://registrar.illinois.edu/academic-records/ferpa> for more information.

Sexual Misconduct Policy and Reporting

The University of Illinois is committed to combating sexual misconduct. Faculty and staff members are required to report any instances of sexual misconduct to the University's Title IX and Disability Office. In turn, an individual with the Title IX and Disability Office will provide information about rights and options, including accommodations, support services, the campus disciplinary process, and law enforcement options. A list of the designated University employees who, as counselors, confidential advisors, and medical professionals, do not have this reporting responsibility and can maintain confidentiality, can be found at

<https://wecare.illinois.edu/resources/students/#confidential>

Other information about resources and reporting is available at <https://wecare.illinois.edu>

Community of Care

As members of the Illinois community, we each have a responsibility to express care and concern for one another. If you come across a classmate whose behavior concerns you, whether in regards to their well-being or yours, we encourage you to refer this behavior to the Student Assistance Center (217-333-0050 or <http://odos.illinois.edu/community-ofcare/referral/>). Based on your report, the staff in the Student Assistance Center reaches out to students to make sure they have the support they need to be healthy and safe. Further, we understand the impact that struggles with mental health can have on your experience at Illinois. Significant stress, strained relationships, anxiety, excessive worry, alcohol/drug problems, a loss of motivation, or problems with eating and/or sleeping can all interfere with optimal academic performance. We encourage all students to reach out to talk with someone, and we want to make sure you are aware that you can access mental health support at the Counseling Center (<https://counselingcenter.illinois.edu/>) or McKinley Health Center (<https://mckinley.illinois.edu/>). For mental health emergencies, you can call 911 or walk into the Counseling Center, no appointment needed.

Required Readings

Materials Science, an Intermediate Text, by William Hosford,

<https://www.cambridge.org/core/books/materials-science/6B4B4D3A43642B71F1B55CD585DEE3A5>

Paperback and hardback versions are also available. We will refer to this book as “Hosford”.

pycse - Python3 Computations in Science and Engineering. <https://kitchingroup.cheme.cmu.edu/pycse/>

We will refer to this book as “Kitchen”.

X-ray Diffraction Crystallography, <https://link.springer.com/book/10.1007%2F978-3-642-16635-8> We

will refer to this book as “Waseda”.

Density Functional Theory: A Practical Introduction,

<https://onlinelibrary.wiley.com/doi/book/10.1002/9780470447710> We will refer to this book as

“Sholl”.

Supplementary textbooks

Diffusion in Solids, by Paul Shewmon, <https://link.springer.com/book/10.1007%2F978-3-319-48206-4>

Introduction to Crystallography, by Frank Hoffmann, <https://link.springer.com/book/10.1007/978-3-030-35110-6>

Course Requirements

1. Use Campuswire for communicating with the instructor, TA, and peers.
2. Complete all assigned readings.
3. Attendance at the ethics lecture is mandatory.
4. Access the course materials and complete assignments within the guidelines established in the course calendar. Submit assignments via Gradescope.
5. Contribute questions, answers, or comments at least once per week to the real-time class discussions or the Campuswire discussion forum. So that we can more easily keep track of participation during the synchronous lecture, please state your question or comment briefly in writing in the chat, and if you want to elaborate, you can do that orally after we call on you.
6. Adhere to assignment deadlines. The deadlines are firm unless a student is given special permission by the instructor. Late submissions are subject to partial credit.
7. Contact the instructor immediately if special circumstances cause interruption of course activities.
8. Keep backup copies of all work.
9. Submit only original work. You are encouraged to communicate with your classmates about the homework assignments if needed but you must turn in your own work. Any form of plagiarism is strictly prohibited, as required by University policy. Violation of this rule will result in "no credit" for an assignment or "no credit" for the course.

Course Communication

Please contact the instructor or the TAs via the Campuswire discussion forum if you have questions at any time. Video or telephone consultations can be arranged outside of regularly scheduled office hours. The instructor and TAs will respond within one business day.

Announcements. The instructor and TAs will use Campuswire to make announcements. The default settings of Campuswire are that announcements are also sent by email. You can change that default setting within Campuswire if you prefer.

Campuswire feed. The Campuswire forum is an important part of the course. Please minimize the use of individual posts and emphasize posting to the entire class. If you want clarification of an assignment or help in understanding the reading, then it is likely that many of your classmates will benefit from your question and will benefit from the responses of classmates, the TAs, or instructor. Feel free to carry on an extended discussion with your classmates independent of feedback from the instructor or TAs. The TAs will intervene if the discussion gets off track. Significant and meaningful public posts will be counted toward the participation grade (see below); individual posts will not.

Netiquette. In any social interaction, certain rules of etiquette are expected and contribute to more enjoyable and productive communication. The following [tips for interacting online](#) are adapted from guidelines originally compiled by Chuq Von Rospach and Gene Spafford at UIS.

- Remember that the person receiving your message is someone like you, someone who deserves and appreciates courtesy and respect.
- Be brief; succinct, thoughtful messages have the greatest impact.
- Your messages reflect on YOU; take time to make sure that you are proud of their form and content.
- Use descriptive subject headings.
- Think about your audience and the relevance of your messages.
- Be careful with humor and sarcasm; without the voice inflections and body language of face-to-face communication, Internet messages can be easily misinterpreted.
- When making follow-up comments, summarize the parts of the message to which you are responding.
- Avoid repeating what has already been said; needless repetition is ineffective communication.
- Cite appropriate references whenever using someone else's ideas, thoughts, or words.

Diversity, Equity, and Inclusion

The University of Illinois, the Grainger College of Engineering, the Materials Science and Engineering department, and MSE201 operate under the guiding principle that "Our entire community benefits when individuals from different personal, cultural, and disciplinary perspectives are working together." (<https://grainger.illinois.edu/about/diversity>). MSE201 will be a safe and inclusive place for learning.

Assessment

Participation (15% of final grade): Records will be kept for significant and meaningful questions and comments during the discussion sessions that will follow each lecture. You will also receive participation credit for significant and meaningful questions, answers, and comments you post in the Campuswire forum. A TA will serve as a moderator of the discussion sessions that follow each lecture. You can either raise your hand in the Campuswire session or use the chat function. Only productive comments or genuine questions will receive credit. You must contribute to either the classroom discussion or the Campuswire forum once per week to receive participation credit for that week.

Homework (25% of final grade): homework is due by 5 pm on the assigned day. Late work will be accepted within 5 days of the due date. A penalty of 10% per day (linear, not compounded) will be applied for late submissions. Work submitted more than 5 days late will not be graded unless

arrangements were made with the instructor prior to the original due date. If an emergency arises, contact Prof. Cahill.

Exam I (15% of final grade): This will cover material from weeks 1-5.

Exam II (15% of final grade): This exam will cover material from weeks 6-10.

Final Exam (30% of final grade): The final exam will cover the entire semester.

Grading Rubrics for Assignments

Grading rubrics will be posted in gradescope with each assignment.

Grading Scale

Percent Range	Letter Grade
100-93	A
92-90	A-
89-87	B+
86-83	B
82-80	B-
79-77	C+
76-73	C
72-70	C-
69-67	D+
66-63	D
62-60	D-
59 and below	F

Course Schedule

A more detailed list of lecture topics, reading assignments, assignment due dates, and times of exams are available through a teamup calendar. <https://teamup.com/ks86vtqj5gb62f1try>

The schedule is subject to change.

Week. Topic	Readings
1. Calculations; introduction to python	Hosford 21 (p 214-223); Kitchen 2, 3
2. Calculations; data analysis and visualization in python	Hosford 21 (pp. 224-231); Kitchen 7.1-7.7; 11.1-11.2
3. Crystal structures and symmetries	Waseda 2.1-2.3; Hosford 3, 4
4. Scattering and diffraction	Waseda 3.1-3.3
5. Bonding; DFT cohesive energy and modulus	Hosford 13; Sholl 1, 2
6. Reciprocal space	Waseda 5.1; Sholl 3.1
7. Crystal defects	Hosford 5
8. Surfaces and interfaces	Hosford 12
9. Phase diagrams; Thermocalc	Hosford 6, 7
10. Diffusion	Hosford 9
11. Phase transformations	Hosford 10
12. Phase transformations	Hosford 11
13. Amorphous materials	Hosford 15
14. Magnetic phases and behavior	Hosford 18
15. Ethics; review	