UNIVERSITY OF ILLINOIS
Grainger College of Engineering
Department of Materials Science and Engineering

Fall 2025: **MSE 498**
Computational Thermodynamics and Kinetics

Instructor:	Pascal Bellon, 312D MSEB, 265-0284, bellon@illinois.edu
Lecture:	TuTh 12:30 pm – 1:50 pm
Office Hours:	Pascal Bellon: by appointment
Websites:	https://canvas.illinois.edu/ ; www.campuswire.com

Prerequisites: MSE 401 and MSE 402 or equivalent courses or instructor approval.

Course description: Modeling of hard materials thermodynamics and kinetics, including diffusion in binary and multicomponent alloys, nucleation and precipitation, spinodal decomposition, solidification. Applications to practical situations and engineering materials using commercial software Thermo-Calc and open-source continuum-scale (phase-field) modeling.

Recommended books and sources:

CALPHAD: Calculation of Phase Diagrams, a comprehensive guide, N. Saunders, A.P. Miodownik, 530.474 Sa87c (online).

Computational Thermodynamics, H. Lukas, S. G. Fries, B. Sundman, 621.4021 L968c (online)

Computational Design of Engineering Materials, Y. Du, R. Schmid-Fetzer, J. Wang, S. Liu, J. Wang, Z. Jin (online)

Thermo-Calc: https://thermocalc.com (access via EWS)

Introduction to Computational Materials Science, R. LeSar, Cambridge Press, 620.110285 L56i

Phase Field Modeling Methods in Materials Science and Engineering, N. Provatas, K. Elder.

Phase transformations in metals and alloys, D. A. Porter and K. E. Easterling, 669.94P833p

Kinetics of materials, R. W. Balluffi, S. A. Allen, W. C. Carter, 620.11292B214k

Solidification, J. A Dantzig and M. Rappaz, 669.94 D236s

Course Objectives: For students to (i) learn fundamental concepts underpinning computational thermodynamics and kinetics in hard materials; (ii) become familiar with standard models for phase transformations and microstructure evolution; (iii) apply this knowledge to practical problems through the use of commercial software Thermo-Calc and phase-field modeling (PFM); (iv) practice critical reading of scientific literature.

Course Outline:

1. Introduction
   - 1.1 Introduction to the course
   - 1.2 Introduction to computational methods
   - 1.3 Introduction to the CALPHAD method Thermo-Calc
2. Phase diagrams
   - 2.1 Review of phase diagrams
   - 2.2 CALPHAD thermodynamics
   - 2.3 Ternary phase diagrams
   - 2.4 Compound and ordered phases
   - 2.5 Interfacial energies: Free surfaces
   - 2.6 Interfacial energies: Grain boundaries
3. Diffusion
   - 3.1 Review of diffusion
   - 3.2 Case studies: Homogenization and carburization
   - 3.3 Diffusion in ternary alloys
4. Solidification
   - 4.1 Review of solidification
   - 4.2 The Scheil model and beyond
   - 4.3 Case studies: Hot tearing in Al alloys
5. Solid-solid phase transformations
   - 5.1 Review of precipitation
   - 5.2 Precipitation in Al alloys
   - 5.3 Precipitation in steels
   - 5.4 Precipitation in superalloys
   - 5.5 Spinodal decomposition and phase field modeling
6. Phase evolution during additive manufacturing
   - 6.1 Review of additive manufacturing
   - 6.2 Applications to AM of ferritic and austenitic steels

GRADE BREAKDOWN:

- Homework assignments: 25%
- Paper review: 25%
- Term project: 50% (25% for report, 25% for presentation)

STUDENT ABSENCES

The Student Code outlines those circumstances in which a student may be eligible to obtain a letter from the Office of the Dean of Students for missed class. When eligible, students must submit an absence letter request within two weeks of returning to class following the absence.

HOMEWORK ASSIGNMENTS

There will be 5 homework assignments, which you will complete using the software Thermo-Calc. Your overall assignment grade will be the average of your 4 best scores.

TERM PROJECT

Students will work in groups of two on the Term project. Possible topics will be proposed by the Instructor, but other topics may be submitted by the students for review and approval from the instructor. Students will submit a 5-page written report and give an in-class presentation.

ABSENCE POLICY

You are expected to attend all lectures, all class presentations, and all exams. If you are absent and if your absence warrants it, please obtain an absence letter from the Office of the Dean of Students for missed classes. The above link provides more information regarding the circumstances in which a student may request a letter. Make sure also that you keep me informed of any situation that would prevent you from attending class, completing an assignment on time, or attending an exam.

ACADEMIC INTEGRITY

Academic dishonesty may result in a failing grade. Every student is expected to review and abide by the Academic Integrity Policy detailed in The University of Illinois Urbana-Champaign *Student Code.* Students should pay particular attention to Article 1, Part 4: Academic Integrity. Read the Code at the following URL: https://studentcode.illinois.edu/article1/part4/1-401/ . Ignorance is not an excuse for any academic dishonesty. It is your responsibility to read this policy to avoid any misunderstanding. Do not hesitate to ask me if you are ever in doubt about what constitutes plagiarism, cheating, or any other breach of academic integrity.

FAMILY EDUCATIONAL RIGHTS AND PRIVACY ACT (FERPA)

Please visit http://registrar.illinois.edu/ferpa for information about the Family Educational Rights and Privacy Act (FERPA).

MENTAL HEALTH

Significant stress, mood changes, excessive worry, substance/alcohol misuse or interferences in eating or sleep can have an impact on academic performance, social development, and emotional wellbeing. The University of Illinois offers a variety of confidential services including individual and group counseling, crisis intervention, psychiatric services, and specialized screenings which are covered through the Student Health Fee. If you or someone you know experiences any of the above mental health concerns, it is strongly encouraged to contact or visit any of the University's resources provided below. Getting help is a smart and courageous thing to do for yourself and for those who care about you.

Counseling Center (217) 333-3704
McKinley Health Center (217) 333-2700
National Suicide Prevention Lifeline (800) 273-8255

Rosecrance Crisis Line (217) 359-4141 (available 24/7, 365 days a year)
If you are in immediate danger, call 911.

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 regard to their well-being or yours, we encourage you to refer this behavior to the Connie Frank CARE Center (formerly the Student Assistance Center) in the Office of the Dean of Students. You may do so by calling 217-333-0050 or by submitting an online referral. Based on your report, staff in the Student Assistance Center will reach out to offer support and assistance.

Further, as a Community of Care, we want to support you in your overall wellness. We know that students sometimes face challenges that can impact academic performance (examples include mental health concerns, food insecurity, homelessness, personal emergencies). Should you find that you are managing such a challenge and that it is interfering with your coursework, you are encouraged to contact the Connie Frank CARE Center (formerly the Student Assistance Center) in the Office of the Dean of Students for support and referrals to campus and/or community resources.

STUDENTS WITH DISABILITIES

The University of Illinois is committed to ensuring that all students, including those with disabilities, do not experience barriers to learning and participating fully in class. If you have a letter of accommodation from DRES and have not already given it to me, please do so as soon as possible to ensure your accommodation needs are met.

To obtain disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact Disability Resources and Educational Services (DRES) as soon as possible. To contact DRES, you may visit 1207 S. Oak St., Champaign, call 333-1970, email: disability@illinois.edu, or go to the DRES website.

DISRUPTIVE BEHAVIOR

Behavior that persistently or grossly interferes with classroom activities is considered disruptive behavior and may be subject to disciplinary action. Such behavior inhibits other students' ability to learn and an instructor's ability to teach. A student responsible for disruptive behavior may be required to leave class pending discussion and resolution of the problem and may be reported to the Office for Student Conflict Resolution (https://conflictresolution.illinois.edu; conflictresolution@illinois.edu; 333-3680) for disciplinary action.

EMERGENCY RESPONSE RECOMMENDATIONS

Emergency response recommendations and campus building floor plans can be found at the following website: https://police.illinois.edu/em/run-hide-fight/. I encourage you to review this website within the first 10 days of class.

RELIGIOUS OBSERVANCES

It is the policy of the University of Illinois Urbana-Champaign to reasonably accommodate its students' religious beliefs, observances, and practices that conflict with a student's class attendance or participation in a scheduled examination or work requirement, consistent with state and federal law. Students should make requests for accommodation in advance of the conflict to allow time for both consideration of the request and alternate procedures to be prepared. Requests should be directed to the instructor. The Office

of the Dean of Students provides an optional resource on its website to assist students in making such requests.

SEXUAL MISCONDUCT REPORTING OBLIGATION

The University of Illinois is committed to combating sex-based misconduct. Faculty and staff members are required to report any instances of sex-based misconduct to the University's Title IX Office. In turn, an individual with the Title IX 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 here: wecare.illinois.edu/resources/students/#confidential.

Other information about resources and reporting is available here: wecare.illinois.edu.

Tentative lecture schedule

Textbooks: Du = Computational Design of Engineering Materials
Saunders = CALPHAD: Calculation of Phase Diagrams
Lukas = Computational Thermodynamics: the CALPHAD method
Porter = Phase Transformations in Metals and Alloys

Homework assignments: In-Class paper reviews / Thermo-Calc problems

Week	Day	Date	Topic	Resource	Hmwk	Project
1	Tu	26-Aug	1.1 Intro to course, ICME, Materials Genome Initiative	D:1		
	Th	28-Aug	1.2 Intro to computational methods	D:2; LQChen		
2	Tu	2-Sep	1.3 Intro to the CALPHAD method and Thermo-Calc in class activities	Q. Chen lecture		
	Th	4-Sep	2.1 Review of phase diagrams	P:1; L:3		
3	Tu	9-Sep	2.2 CALPHAD Thermodynamics	S:5, L:5, D:5		
	Th	11-Sep	2.3 Ternary phase diagrams	L:5, D:5		
4	Tu	16-Sep	2.4 Compound and ordered phases	L:5, D:5		
	Th	18-Sep	Case studies: Fe-Cr and Al-Cu	L:5, D:5		
5	Tu	23-Sep	2.5 Interfacial energies: Free surfaces	LQChen	#1	
	Th	25-Sep	2.6 Interfacial energies: Grain boundaries	LQChen		
6	Tu	30-Sep	Term project: Goals and expectations			***
	Th	2-Oct	3.1 Review of kinetics: Diffusion			
7	Tu	7-Oct	In class activities: DICTRA examples		#2	
	Th	9-Oct	3.2 Case studies: homogenization, carburization (TC)			
8	Tu	14-Oct	3.3: Diffusion in ternary alloys: Thermal bonding in superalloys			
	Th	16-Oct	4.1 Review of Solidification			
9	Tu	21-Oct	4.2 Scheil model and beyond (TC)		#3	
	Th	23-Oct	4.3 Hot tearing in Al alloys			Proposal due
10	Tu	28-Oct	5.1 Review of precipitation: N+G+C			
	Th	30-Oct	In class activities: PRISMA examples			
11	Tu	4-Nov	5.2 Precipitation in Al alloys		#4	
	Th	6-Nov	5.3 Precipitation in steels: From global to non-partitioning equilibrium			
12	Tu	11-Nov	5.4 Precipitation in Superalloys			
	Th	13-Nov	5.5 Spinodal decomposition			
13	Tu	18-Nov	Guest lecture: Phase field modeling	D:3	#5	
	Th	20-Nov	Preparation of project report			
14	Tu	2-Dec	6.1 Review of additive manufacturing			
	Th	4-Dec	6.2 Application: AM of ferritic and austenitic steels			Written report due
15	Tu	9-Dec	Preparation of project presentation			
16	Tu	16-Dec	Final exam: In-class presentations			Presentations