



AME 599: Computational Mechanics and Thermodynamics of Energy Materials

Units: 4

Fall 2021—Tue, Thu—Time: 9:00-10:50am

Location: TBA (with DEN option)

Instructor: Ananya Renuka Balakrishna ([link](#))

Office: OHE 430J

Office Hours: T, Thu, 11:00am - 12:00 noon

Contact Info: renukaba@usc.edu

Teaching Assistant: TBD

Office:

Office Hours:

Contact Info:

Course Description

This course aims to provide graduate-level aerospace and mechanical engineering (and materials science) students with an in-depth introduction to *computational* mechanics and thermodynamics of energy materials. Topics covered will include: thermodynamics and kinetics of energy conversion and storage; material models; phase transformations; continuum mechanics of crystalline solids; phase field modeling of microstructural evolution; as well as several applications to battery electrodes, ferroelectrics, and soft magnets;

Learning Objectives

This course will:

- Introduce the concept of phase transformations for energy conversion and storage
- Provide exposure to hands-on analytical and computational methods to model energy-related problems:
 - o Mathematical interpretation of thermodynamic potentials
 - o Phase field modeling of spinodal decomposition
 - o Origins and analysis of material microstructures
- Teach problem-solving strategies in engineering applications of energy conversion and storage
- Enable students to identify the most appropriate methodology for solving engineering problems
- Integrate phase transformations, basic numerical methods, computational design and testing, data collection and post-processing.

Recommended Preparation: The recommended preparation for this course are familiarity with linear algebra and matrix mathematics. Any working knowledge of Mathematica would accelerate the learning process.

Textbook and Other Resources

There is no required textbook for this class. Course notes will be provided in electronic format via Blackboard. Readings will be suggested from the following books to supplement course notes:

- *Balluffi, Robert W., Samuel M. Allen, and W. Craig Carter. Kinetics of materials. John Wiley & Sons, 2005.*
- *Tadmor, Ellad B., Miller, Ronald E., and Elliot, Ryan S., Continuum Mechanics and Thermodynamics*
- *Bhattacharya, Kaushik, Microstructure of martensite*

Grading Breakdown

Assignment	% of Grade
Homeworks (2 total)	20
Quiz 1	25
Quiz 2	25
Final	30
TOTAL	100

Discussion board

Piazza will be used for all electronic discussions. Please post your questions (regarding homework assignments, class logistics, exams, etc.) on these forums instead of using email. You can access these through the Blackboard page for this course.

Assignment Submission Policy

There will be a total of 2 homework assignments.

- No late homework will be accepted without prior arrangement.
- Discussion of homework assignments with your classmates is allowed (and encouraged!) but each student should develop and write their own original solution.
- Assignments should be submitted electronically, with legible and logically organized solutions that explicitly include all necessary steps and assumptions (if any) made.
- Course grading policy and letter grade equivalence:

<http://arr.usc.edu/services/grades/gradinghandbook/gradingpolicies.html>

Course Schedule: A Weekly Breakdown

	Topics/Daily Activities	Notes
Week 1 8/23	T: Introduction to modern energy technologies & energy materials Th: Review of thermodynamics, First law and work differentials	
Week 2 8/30	T: Second law, Definition and use of enthalpy, entropy Th: Entropy of materials, combined first and second law	HW #1 Due
Week 3 9/6	T: Equilibrium conditions Th: Computational interpretation of thermodynamic potentials	Computational session
Week 4 9/13	T: Properties of mixtures, solution equilibria Th: Energy and entropy: microscopic origins and models	
Week 5 9/20	T: Quiz 1 Th: Mathematical background (order parameter, fields, variations)	
Week 6 9/27	T: Diffuse interface theory, phase transformation Th: Evolution equation, energy minimization	
Week 7 10/4	T: Regular solution model, Phase transformation Th: Spinodal transformation, nucleation and growth	
Week 8 10/11	T: Driving forces and fluxes for diffusion Th: Diffusion in crystalline solids and application for energy storage	HW #2 Due
Week 9 10/18	T: Computational understanding of spinodal decomposition Th: Quiz 2	Computational session
Week 10 10/25	T: Crystallography of phase transformations Th: Tensor Properties of energy materials (elastic, piezoelectric, magnetic)	
Week 11 11/1	T: Phase transformations in crystalline solids Th: Continuum theory of Crystalline Solids	
Week 12 11/8	T: Interpretation of variants, twins, transformations Th: Origin and analysis of microstructures	

Week 13 11/15	T: Linearized kinematics Th: Computational session on microstructural evolution	
Week 14 11/22	T: Computing phase transformations in battery electrodes Th: <i>Thanksgiving Holiday (no classes)</i>	Computational session
Week 15 11/29	T: Modeling phase transformations in energy conversion materials Th: Computing microstructures in ferroelectrics, soft magnets	Computational session
FINAL	Final exam TBD	

Academic Dishonesty: Sanction Guidelines

Violation	USC – Recommended sanction	AME – Recommended sanction
Copying answers from other students on any course work **	F for course	First offense: F on assignment Second offense: F for course
One person allowing another to cheat from his/her exam or assignment	F for course for both persons	If assignment: First offense: F on assignment Second offense: F for course If exam: F for course
Possessing or using material during exam (crib sheets, notes, books, etc.) which is not expressly permitted by the instructor.	F for course.	First offense: F on exam. Second offense: F for course.
Continuing to write after exam has ended.	F for course.	F on exam
Taking exam from room and later claiming that the instructor lost it.	F for course and recommendation for further disciplinary action (possible suspension).	F for course
Changing answers after exam has been returned.	F for course and recommendation for further disciplinary action (possible suspension).	F for course
Fraudulent possession of exam prior to administration.	F for course and recommendation for suspension.	F for course
Obtaining a copy of an exam or answer key prior to administration.	Suspension or expulsion from the university; F for course.	F for course
Having someone else complete course work for oneself.	Suspension or expulsion from the university for both students; F for course.	F for course
Plagiarism — Submitting other's work as one's own or giving an improper citation.	F for course.	First offense: F on assignment. Second offense: F for course.
Submission of purchased term papers or papers done by others.	F for course and recommendation for further disciplinary action (possible suspension).	F for course
Submission of the same assignment to more than one instructor, where no previous approval has been given.	F for both courses.	F for both courses
Unauthorized collaboration on an assignment.	F for the course for both students.	First offense: F on assignment. Second offense: F for course.
Falsification of information in admission applications (including supporting documentation).	Revocation of university admission without opportunity to reapply.	Revocation of university admission without opportunity to reapply.
Documentary falsification (e.g., petitions and supporting materials; medical documentation.)	Suspension or expulsion from the university; F for course when related to a specific course.	Suspension or expulsion from the university; F for course when related to a specific course.
Plagiarism in a graduate thesis or dissertation.	Expulsion from the university when discovered prior to graduation; revocation of degree when discovered subsequent to graduation.***	Expulsion from the university when discovered prior to graduation; revocation of degree when discovered subsequent to graduation.***

Statement on Academic Conduct and Support Systems

Academic Conduct:

Plagiarism – presenting someone else’s ideas as your own, either verbatim or recast in your own words – is a serious academic offense with serious consequences. Please familiarize yourself with the discussion of plagiarism in SCampus in Part B, Section 11, “Behavior Violating University Standards” policy.usc.edu/scampus-part-b. Other forms of academic dishonesty are equally unacceptable. See additional information in SCampus and university policies on scientific misconduct, policy.usc.edu/scientific-misconduct.

Support Systems:

Counseling and Mental Health - (213) 740-9355 – 24/7 on call (studenthealth.usc.edu/counseling)
Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

National Suicide Prevention Lifeline - 1 (800) 273-8255 – 24/7 on call (suicidepreventionlifeline.org)
Free and confidential emotional support to people in suicidal crisis or emotional distress 24 x 7.

Relationship and Sexual Violence Prevention Services (RSVP) - (213) 740-9355(WELL), press “0” after hours – 24/7 on call (studenthealth.usc.edu/sexual-assault)
Free and confidential therapy services, workshops, and training for situations related to gender-based harm.

Office of Equity and Diversity (OED) - (213) 740-5086 | *Title IX* – (213) 821-8298 (equity.usc.edu, titleix.usc.edu)
Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants.

Reporting Incidents of Bias or Harassment: (213) 740-5086 or (213) 821-8298
usc-advocate.symplicity.com/care_report: Avenue to report incidents of bias, hate crimes, and microaggressions to the Office of Equity and Diversity | Title IX for appropriate investigation, supportive measures, and response.

The Office of Disability Services and Programs - (213) 740-0776 (dsp.usc.edu)
Support and accommodations for students with disabilities. Services include assistance in providing readers/notetakers/interpreters, special accommodations for test taking needs, assistance with architectural barriers, assistive technology, and support for individual needs.

USC Campus Support and Intervention - (213) 821-4710 (campussupport.usc.edu)
Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

Diversity at USC - (213) 740-2101 (diversity.usc.edu)
Information on events, programs and training, the Provost’s Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

USC Emergency - UPC: (213) 740-4321, *HSC*: (323) 442-1000 – 24/7 on call (dps.usc.edu, emergency.usc.edu)
Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

USC Department of Public Safety - UPC: (213) 740-6000, *HSC*: (323) 442-120 – 24/7 on call (dps.usc.edu)
Non-emergency assistance or information.

Office of the Ombuds - (213) 821-9556 (UPC) / (323-442-0382 (HSC) (ombuds.usc.edu)
A safe and confidential place to share your USC-related issues with a University Ombuds who will work with you to explore options or paths to manage your concern.