

MSE 3070 Kinetics and Phase Transformation in Materials

Spring 2024

Department of Materials Science and Engineering
University of Virginia

- Instructor:** Dr. Bi-Cheng Zhou
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Office: Wilsdorf Hall (WDF) 303D
Personal Zoom link: <https://virginia.zoom.us/j/6983482198>
- Lectures:** TuTh 3:30 pm - 4:45 pm
Jesser Hall 171
All the lectures will be recorded on Canvas via Zoom Recordings.
- Office Hours:** Instructor: Fri 1:30 – 2:30 pm at WDF 303D, or by appointment
TA: Mon 2:00 – 3:00 pm at WDF 303A, or by appointment
- Prerequisite:** MSE 2090 and MSE 3050 or instructor permission
- Textbooks:** **Required:**
Ryan O'Hayre, “*Materials Kinetics Fundamentals*”, 1st ed. ([UVA online library](#) and UVA bookstore inclusive access, see the last page of syllabus for details)
Optional:
Porter, Easterling, Sherif, “*Phase Transformations in Metals and Alloys*”, 3rd ed.
- TA:** Peter Connors (pc5mx@virginia.edu), personal Zoom link:
<https://virginia.zoom.us/j/5957305728>
- Homework:** HWs will be assigned all together at the beginning of the first half and second half of the semester (6 HWs in total) so that students will be able to pace their own progress more easily. Only one late HW will be allowed. No credit will be given for HW submitted after solutions are posted to Canvas (2 days after the due date). Homework should be uploaded to the *Assignments* section on Canvas. You are encouraged to discuss the problems with your classmates, but you should hand in your unique version.
- Exam:** There will be two exams: one midterm exam and one comprehensive final exam. Both are in take-home format. Details will be announced in class.
- Grading:** Homework: 40%
Midterm exam: 20%
Comprehensive final exam: 40%
- Course Website:** UVA Canvas site: 24Sp Kinetics of Materials
- Course Email:** 24sp_kinetics_of_materials-9491501@mail.canvas.its.virginia.edu

Course Description:

This course will cover three main topics (see individual classes in course schedule on page 3 with corresponding colors): **1) chemical reaction kinetics**, **2) diffusion (mass transport)**, **3) phase transformation and microstructure evolution**.

In this course we will build on the understanding of thermodynamic driving forces and of phase diagrams you developed in MSE 3050 and apply these concepts to the analysis of the key kinetic processes, phase transformations, and the development of microstructure in materials. We will start with discussing chemical reaction kinetics in the gas phase. Most kinetic phenomena in condensed matter involve diffusion, and we will consider the phenomenological descriptions as well as atomic-scale mechanisms of diffusion in materials. We will then discuss the kinetics of phase transformations and microstructure evolution, including the classical nucleation theory, mechanisms of growth and coarsening, theory of capillary, grain growth and so on. By the end of the course we will see how the interplay of thermodynamic driving forces and kinetics of mass transfer is defining the formation of complex microstructures of real materials.

Course Objectives:

1. Comfortably and concisely use the materials science language pertaining to kinetic processes.
2. Estimate rates based on order of magnitude understanding of length scales, rate constants, and activation energies.
3. Precisely describe the evolution of a given materials system using both atomistic and phenomenological approaches with the help of computational tools.
4. Relate your knowledge of kinetics to key concepts in thermodynamics, crystal structure, defects, and microstructure.

Course schedule (subject to change):

Date	Topic	Reading (O'Hayre chapters)	Remark
Jan. 18	No class due to Northwestern trip		
23	Introduction, brief review of thermodynamics	Ch 1,2	HW 1-3 out
25	1 st and 2 nd order reactions	Ch 3 - 3.2	
30	Reaction constant, T dependence	Ch 3.3	
Feb. 1	TST, heterogeneous reaction kinetics	Ch 3.4	HW1 due Feb. 4
6	Diffusion, Fick's 1 st law	Ch 4 - 4.4.1	
8	Fick's 2 nd law, semi-infinite	Ch 4.4.2	
13	Thin film solution	Ch 4.4.2	
15	Finite systems	Ch 4.4.2	HW2 due Feb. 18
20	Random walk, diffusion mechanism	Ch 4.5.3	
22	Atomistics of solid-state diffusion Midterm review Midterm exam covers until here	Ch 4.5.3	HW3 due Feb. 25
27	Midterm exam (take home)		
29			
Mar. 5	Spring recess, no class		
7	Spring recess, no class		
12	Defect chemistry in ionic solids	Ch 4.5.3	HW 4-6 out
14	Diffusion in ionic solids, generalized transport	Ch 4.4.5	
19	Different diffusion coefficients, short-circuit diffusion	Ch 4.4.3, 4.5.4	
21	Gas phase diffusion	Ch 4.5 - 4.5.2	HW4 due Mar. 24
26	Gas-solid kinetic processes	Ch 5.1 - 5.2	
28	CVD, ALD, oxidation	Ch 5.3 - 5.5	
Apr. 2	Driving force for transformation	Ch 6.1 - 6.2, 6.4	
4	Nucleation theory	Ch 6.5	HW5 due Apr. 7
9	Nucleation and growth rate	Ch 6.5 - 6.6	
11	Combined nucleation and growth	Ch 6.7	
16	Solidification, spinodal decomposition	Ch 6.3, 6.8	
18	Precipitation	Ch 7.1 - 7.3	
23	Capillarity and coarsening	Ch 7.1 - 7.3	
25	Grain growth and sintering	Ch 7.4 - 7.5	HW6 due Apr. 28
30	Final review		
May 2-8	Comprehensive final exam (take home)		

Resources

Honor

<https://honor.virginia.edu/>

I trust every student in this course to fully comply with all the provisions of the University's honor Code. By enrolling in this course, you have agreed to abide by and uphold the Honor System of the University of Virginia, as well as the following policies specific to this course.

- All graded assignments must be pledged unless otherwise stated.
- Students must familiarize on the meaning of Citations, Plagiarism, and Paraphrasing, see: <https://honor.virginia.edu/plagiarism-supplement>
- All suspected violations will be forwarded to the Honor Committee, and you may, at my discretion, receive an immediate zero on that assignment regardless of any action taken by the Honor Committee.

Please let me know if you have any questions regarding the course Honor policy. If you believe you may have committed an Honor Offense, you may wish to file a Conscientious Retraction by calling the Honor Offices at (434) 924-7602. For your retraction to be considered valid, it must, among other things, be filed with the Honor Committee before you are aware that the act in question has come under suspicion by anyone. More information can be found at <http://honor.virginia.edu>. Your Honor representatives can be found at: <http://honor.virginia.edu/representatives>.

Accessibility

It is my goal to create a learning experience that is as accessible as possible. If you anticipate any issues related to the format, materials, or requirements of this course, please meet with me outside of class so we can explore potential options. Students with disabilities may also wish to work with the Student Disability Access Center to discuss a range of options to removing barriers in this course, including official accommodations. Please visit their website for information on this process and to apply for services online: <https://studenthealth.virginia.edu/sdac>. If you have already been approved for accommodations through SDAC, please send me your accommodation letter and meet with me so we can develop an implementation plan together.

Well-being

MSE serves as a safe space for its students and aims to promote their wellbeing. If you are feeling overwhelmed, stressed, or isolated, the Student Health Center offers Counseling and Psychological Services (CAPS) for students. Call 434-243-5150 (or 434-972-7004 for after hours and weekend crisis assistance) to get started and schedule an appointment.

<http://www.virginia.edu/studenthealth/caps.html>

Recording of classroom activities

I will be recording every lecture in order to accommodate students who will be learning remotely. Because lectures include fellow students, you and they may be personally identifiable on the recordings. These recordings may only be used for the purpose of individual or group study with other students enrolled in this class during this semester. You may not distribute them in whole or in part through any other platform or to any persons outside of this class, nor may you make your own recordings of this class unless written permission has been obtained from the Instructor and all participants in the class have been informed that recording will occur. If you want additional details on this, please see Provost Policy 008. If you notice that I have failed to activate the recording feature, please remind me!

Violence and discrimination prevention

The University of Virginia is dedicated to providing a safe and equitable learning environment for all students. To that end, it is vital that you know two values that I and the University hold as critically important:

- Power-based personal violence will not be tolerated.
- Everyone has a responsibility to do their part to maintain a safe community on Grounds.

If you or someone you know has been affected by power-based personal violence, more information can be found on the UVA Sexual Violence website that describes reporting options and resources available - www.virginia.edu/sexualviolence.

As your professor and as a person, know that I care about you and your well-being and stand ready to provide support and resources as I can. As a faculty member, I am a responsible employee, which means that I am required by University policy and federal law to report what you tell me to the University's Title IX Coordinator. The Title IX Coordinator's job is to ensure that the reporting student receives the resources and support that they need, while also reviewing the information presented to determine whether further action is necessary to ensure survivor safety and the safety of the University community. If you wish to report something that you have seen, you can do so at the **Just Report It** portal (<http://justreportit.virginia.edu/>). The worst possible situation would be for you or your friend to remain silent when there are so many here willing and able to help.

Religious accommodations

It is the University's long-standing policy and practice to reasonably accommodate students so that they do not experience an adverse academic consequence when sincerely held religious beliefs or observances conflict with academic requirements. Students who wish to request academic accommodation for a religious observance should submit their request in writing directly to me as far in advance as possible. Students who have questions or concerns about academic accommodations for religious observance or religious beliefs may contact the University's Office for Equal Opportunity and Civil Rights (EOCR) at UVAEOCR@virginia.edu or 434-924-3200.

Welcome to **MSE 3070!** This course will take part in the Inclusive Access program with The UVA Bookstore to provide your course material at a low price.

ALL students enrolled in the class will have immediate access to your digital course materials through UVA Canvas. Your student account will be charged **\$83.53 for *Materials Kinetics Fundamentals (perpetual access)***.

This program is optional for students, but you must actively opt-out before the deadline on **Wednesday January 31st** if you choose not to participate. Opting out will automatically generate a credit for the charged amount that will appear on your SIS student account after a few days. Additionally, you will lose access to your materials.

After January 31st, the charges will be finalized. Due to the special pricing, no refunds can be processed.

This program aims to offer all students accessibility and affordability. If you have any questions regarding the program, please email us at UVAInclusiveAccess@virginia.edu .

We wish you great success in your studies.

