Course Outline

MATS6102

Kinetics and Phase Transformations

Materials Science and Engineering

Faculty of Science

T3, 2022

1. Staff

Position	Name	Email	Consultation times and locations	Contact Details
Course Convenor	Prof. Charles C Sorrell	c.sorrell@unsw.edu.au	Room 248, School of Materials Science and Engineering (Building E10), by appointment	Phone: 9385-4421
Lecturer	Dr. Rakesh Joshi	r.joshi@unsw.edu.au	Room 448, School of Materials Science and Engineering (Building E10), by appointment	Phone: 9385-4324
Lecturer	Dr. Christopher Hansen	christopher.hansen@unsw.edu.au	Room 602, Science and Engineering Building (E8), School of Chemistry, by appointment	Phone: 9065-3085

2. Course information

Units of credit: 6

Pre-requisite(s): None

Timetabling website: http://timetable.unsw.edu.au/2021/MATS6102.html#S3-8385

Teaching times and locations:

Part 1	Lecture	Lecture	Lecture	Lab
Day	Monday	Wednesday	Friday	See Moodle for details
Time	09:00-11:00	11:00-13:00	09:00-11:00	
Weeks	1-3, 5	1-5	1-5	

Part 2	Lecture	Lecture
Day	Monday	Thursday
Location	On-line	On-line
Time	12:00-14:00	13:00-15:00
Weeks	7-10	7-10

2.1 Course summary

Part 1 of this course covers the background for the relationships between kinetics, diffusion, phase transformations, and the prediction of materials microstructure. Students will understand how to predict materials structures based on the principles of phase transformations and apply this knowledge to commercial alloys.

Kinetics - Reaction rate definition, the rate law, rate constant and order. Experimental determination of the rate law: the method of initial rates, methods using integrated rate equations for 1st order and 2nd order reactions; rate constants, half-life. Effect of temperature on reaction rates: the Arrhenius equation, activation energy and frequency factor. Elementary reactions, mechanism, rate-determining step; relation to the rate law. Complex reactions: opposing, consecutive, and parallel reactions; catalysis and catalysts; enzyme catalysis; Michaelis-Menten mechanisms; molecular reaction kinetics; and collision theory.

Diffusion Fundamentals - Introduction to diffusion in gases and liquids, membrane transport, facilitated diffusion, osmosis, diffusion in solids and thin films, Fick's first and second laws and other factors affecting diffusion.

Part 2 of this course covers the roles of point defects in diffusion. The background for Kröger-Vink notation for metal oxides will be provided and this information will be applied to defect reactions and defect equilibria.

2.2 Course aims

In this course, you will be introduced to the fundamentals of kinetics and diffusion mechanisms pertinent to engineering materials. When successfully completed, you should be able to apply these fundamentals to quantify transport phenomena that occur in various materials processing applications.

2.3 Course learning outcomes (CLO)

Upon the successful completion of this course, you should be able to:

1. Understand the fundamentals of kinetics and diffusion
2. Apply kinetics and diffusion to prediction of phase transformations
3. Quantify chemical kinetics and diffusion in materials processing operations
4. Identify, formulate, and solve reaction engineering problems from first principles
5. Apply defect equilibria to interpret the roles of defects in diffusion

2.4 Program learning outcomes (PLO)

Upon the successful completion of this course, you should be able to:

1. Knowledge: Understanding of kinetics, diffusion, and defect equilibria
2. Skills: Ability to apply computational skills to kinetics, diffusion, and defect equilibria data
3. Application of Knowledge and Skills: Ability to apply the knowledge and skills to:
    a) Predict phase transformations
    b) Quantify kinetics and diffusion data applied to materials processing
    c) Address reaction engineering problems
    d) Interpret the roles of defects in diffusion

2.5 Relationship between course and program learning outcomes and assessments

Course Learning Outcome (CLO)	LO Statement	Program Learning Outcome (PLO)	Related Tasks & Assessment
CLO 1	Understand…	1	1 & 2
CLO 2	Apply…	2 & 3	1 & 2
CLO 3	Quantify…	2 & 3	1 & 2
CLO 4	Identify…	2 & 3	1 & 2
CLO 5	Apply…	2 & 3	3

3. Strategies and approaches to learning

3.1 Learning and teaching activities

(Based on UNSW Learning Guidelines)

- *Students are engaged actively in the learning process.*

It is expected that, in addition to attending classes, students will read, write, discuss, and engage in analysing the course content.

- *Effective learning is supported by a climate of inquiry, where students feel appropriately challenged.*

Students are expected to be challenged by the course content and to challenge their own preconceptions, knowledge, and understanding by questioning information, concepts, and approaches during class and study.

- *Learning is more effective when students' prior experience and knowledge are recognised and built on.*

Coursework, tutorials, assignments, laboratories, examinations, and other forms of learning and assessment are intended to provide students with the opportunity to cross reference these activities in a meaningful way with their own experience and knowledge.

- *Students become more engaged in the learning process if they can see the relevance of their studies to professional and disciplinary contexts*

The course content is designed to incorporate both theoretical and practical concepts, where the latter is intended to be applicable to real-world situations and contexts.

3.2 Expectations of students

- Students must attend on-line at least 80% of all classes with the expectation that students miss classes only as a result of illness or unforeseen circumstances.
- Students must read through lecture notes and lab sheets prior to class.
- During class, students are expected to engage actively in class discussions.
- Students should work through lecture, tutorial, and textbook questions.
- Students should read through the relevant chapters of the prescribed textbooks.
- Students should complete all assessment tasks and submit them on time.
- Students are expected to participate in online discussions verbally and/or through the Moodle page.

4. Course schedule and structure

This course consists of 48 hours of class contact hours. You are expected to engage in an additional 102 hours of non-class contact hours in order to complete assessments, reading, and exam preparation.

Week	Course Section	Topics	Activity
1	Kinetics	Introduction and Reaction Rates Catalysis, Enzymes, and Molecular Reactions	
2		Catalysis, Enzymes and Molecular Reactions Tutorial Session and Practice Exam Questions	1) Exam
3	Diffusion	Introduction to Diffusion, Diffusion in Liquids	
4		Diffusion in Gases, Solids, and Thin Films	
5		Tutorial	2) Exam
6	Defects	Structural and Microstructural Background	
7		Point Defects	
8		Defect Reactions	
9		Defect Equilibria	
10		Summary and Review	3) Exam*

* Exam during exams period

5. Assessment

Assessment Task	Description	Weighting	Due Date
Kinetics Exam	The exam covers all kinetics content. Students will be asked to understand simple and complex kinetic systems, determine and apply rate equations, and interpret real data in terms of the theory provided.	20%	In Class, Week 2
Diffusion Exam	The exam covers all diffusion fundamentals. Students will be asked to understand the basic principles of diffusion, fundamental theory, examples of diffusion processes, and possible applications.	30%	In Class, Week 5
Defects Exam	The exam covers all aspects of the application of defect equilibria in the intrinsic defect equilibria of metal oxides and the extrinsic defect equilibria of doped metal oxides.	50%	In Exams Week

Further information

UNSW grading system: https://student.unsw.edu.au/grades

UNSW assessment policy: https://student.unsw.edu.au/assessment

5.2 Assessment criteria and standards

Assessment criteria and standards for each assessment tasks are available on the course Moodle page.

5.3 Submission of assessment tasks

UNSW operates under a Fit to Sit/Submit rule for all assessments. If a student wishes to submit an application for special consideration for an exam or assessment, the application must be submitted prior to the start of the exam or before an assessment is submitted. If a student sits the exam/submits an assignment, this is an implicit statement of being well enough to do so. Information on this process can be found at: https://student.unsw.edu.au/special-consideration. Medical certificates or other appropriate documents must be included. Students also should advise the lecturer of the situation.

Unless otherwise specified in the task criteria, all assignments must be uploaded via Moodle prior to the due date for submission.

Assignments/lab reports submitted after the due date for submission will receive a penalty of 10% deduction from the maximal grade for every day late or part thereof.

Students who have a disability that requires some adjustment in the teaching or learning environment are encouraged to discuss their study needs with the course coordinator prior to, or at the commencement of, their course; alternatively, the Equity Officer (Disability) in the Equity and Diversity Unit may be contacted: https://student.unsw.edu.au/disability. Early notification is essential in order to enable any necessary adjustments to be made.

Rules governing conduct during exams are given at: https://student.unsw.edu.au/exam-rules.

5.4. Feedback on assessment

Assignments: Feedback will be given 2 weeks after submission of assignments and take the form of the mark for the assignment, overall comments on how the class performed, and discussion of any collective areas that were not answered correctly. Individual feedback and how each student performed may be given.

Exams: For Part 1 of the course, students will receive their marked exams, indicating what questions were answered correctly and incorrectly. Overall comments and worked solutions may be provided to the class.

6. Academic integrity, referencing and plagiarism

Referencing is a way of acknowledging the sources of information that you use to research your assignments. You need to provide a reference whenever you draw on someone else's words, ideas, or research. The general rule is: If the material is not your own original thought or common knowledge, then it must be referenced. Not referencing other people's work can constitute plagiarism.

Further information about referencing styles can be located at: https://student.unsw.edu.au/referencing.

Academic integrity is fundamental to success at university. Academic integrity can be defined as a commitment to six fundamental values in academic pursuits**:** honesty, trust, fairness, respect, responsibility, and courage.[1] At UNSW Sydney, this means that your work must be your own and others' ideas should be acknowledged. If you do not follow these rules, plagiarism may be detected in your work.

Further information about academic integrity and **plagiarism** can be located at:

- The *Current Students* site: https://student.unsw.edu.au/plagiarism
- The *ELISE* training site: http://subjectguides.library.unsw.edu.au/elise/presenting

The *Conduct and Integrity Unit* provides further resources to assist you to understand your conduct obligations as a student: https://student.unsw.edu.au/conduct.

7. Reading and resources

Kinetics

P.W. Atkins and J. De Paula, *Elements of Physical Chemistry, 5th Edition*. Oxford University Press, Oxford, UK, 2009.

Diffusion

M. Mulder, *Basic Principles of Membrane Technology, 2nd Editon*. Kluwer Academic Publishers, Amsterdam, Netherlands, 1996

Paul Shewmon, *Diffusion in Solids, 2nd Edition*. Springer International Publishers, Cham, Switzerland, 1989.

H.S. Ray, *Kinetics of Metallurgical Reactions*, International Science Publishers, New York, USA, 1993.

N.J. Themelis, *Transport and Chemical Rate Phenomena*, Gordon and Breach Publishers, London, UK, 1995.

Defects

P. Kofstad, *Nonstoichiometry, Diffusion, and Electrical Conductivity in Binary Metal Oxides*. John Wiley & Sons, Inc., New York, 1972.

P. Kofstad, *High-Temperature Oxidation of Metals*. John Wiley & Sons, Inc., New York, 1966.

B.I. Boltaks (Translated by J.I. Carasso), *Diffusion in Semiconductors*. Infosearch Limited, London, 1963.

8. Administrative matters

School Office: Room 137, School of Materials Science and Engineering, Grid E10

School Website: http://www.materials.unsw.edu.au/

Faculty Office: Room 128, Robert Webster Building, Grid K-G14

Faculty Website: http://www.science.unsw.edu.au/

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[1] International Center for Academic Integrity, 'The Fundamental Values of Academic Integrity', T. Fishman (ed), Clemson University, 2013.

9. Additional support for students

- The Current Students Gateway:

  https://student.unsw.edu.au/
- Academic Skills and Support:

  https://student.unsw.edu.au/academic-skills
- Student Wellbeing, Health, and Safety:

  https://student.unsw.edu.au/wellbeing
- Disability Support Services:

  https://student.unsw.edu.au/disability-services
- UNSW IT Service Centre:

  https://www.it.unsw.edu.au/students/index.html
- Assessment Implementation Procedure

  https://www.gs.unsw.edu.au/policy/documents/assessmentimplementationprocedure.pdf
- Special Consideration:

  https://student.unsw.edu.au/special-consideration