

# **Course Outline**

# MATS6102

## **Kinetics and Phase Transformations**

Materials Science and Engineering

Faculty of Science

T3, 2022

## 1. Staff

Position Name Email

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

#### **Further information**

UNSW grading system: <u>https://student.unsw.edu.au/grades</u> 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: <u>https://student.unsw.edu.au/special-consideration</u>. Medical certificates or other appropriate documents must be included. Students also should advise the lecturer

**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.<sup>1</sup> 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: <u>https://student.unsw.edu.au/conduct</u>.

## 7. Reading and resources

#### **Kinetics**

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

#### Diffusion

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

Paul Shewmon, *Diffusion in Solids, 2<sup>nd</sup> 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/

## 9. Additional support for students

The Current Students Gateway:

https://student.unsw.edu.au/