Course Outline

MATS6101

Thermodynamics and Phase Equilibria

Materials Science and Engineering

Science

T2, 2022

1. Staff

Position	Name	Email	Consultation times and locations	Contact Details
Course Convenor	Dr Rakesh Joshi	r.joshi@unsw.edu.au	Room 448, School of Materials Science and Engineering (Building E10) by appointment	Phone: 9385 6726
Lecturer	Dr. Nima Haghdadi	nima.haghdadi@unsw.edu.au	**Room 302**, School of Materials Science and Engineering (Building E10), by appointment	Phone: 9385 5918
Lecturer	Dr Ron S Haines	r.haines@unsw.edu.au	Room 128, School of Chemistry (Dalton Building F12)	Phone: 9385 4653

2. Course information

Units of credit: 6

Pre-requisite(s): None

Timetabling website: http://timetable.unsw.edu.au/2021/MATS6101.html

Lectures will be online - check Moodle for announcements about how these will be delivered.

2.1 Course summary

Fundamentals of thermodynamics (thermodynamics basics; heat, work, and internal energy; heat capacity; enthalpy, entropy, and free energy; three laws of thermodynamics; redox processes).

Equilibrium and gas-solid phase transitions (chemical equilibrium, first- and second-order phase transitions, fugacity and activity, gas-solid equilibria, Ellingham diagrams).

Solution thermodynamics and phase diagram construction (Gibbs-Duhem equation. Raoult's and Henry's laws. Solutions and activity and phase diagram construction).

Interpretation and applications of binary and ternary phase diagrams (unary systems, binary systems, ternary effects on microstructures, phase calculations, drawing isothermal and vertical sections of real ternary systems).

2.2 Course aims

To understand basic thermodynamic principles and to gain the capability of applying these principles to phase transformations and the chemical and electrochemical processes of pure substances, solutions, and multiphase systems.

To understand the features and principles of unary systems, binary and ternary phase diagrams.

To understand the graphical representation of phase equilibria in real materials systems and to understand the thermodynamic stabilities of phases.

2.3 Course learning outcomes (CLO)

At the successful completion of this course you (the student) should be able to:

1. Understand and apply the laws of thermodynamics
2. Have an understanding of how to apply thermodynamics to the construction of phase diagrams
3. Be able to predict material microstructure from phase diagrams
4. Understand the effect of materials microstructure on materials properties

2.4 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…	3	1 & 2
CLO 2	Have…	5	3 & 4
CLO 3	Be able to…	5	2, 3 & 4
CLO 4	Understand…	3	2, 3 & 4

3. Strategies and approaches to learning

3.1 Learning and teaching activities

(based on UNSW Learning Guidelines)

- *Students are actively engaged 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.

Lectures: The core concepts will be taught in lectures, students will have access to the lectures notes before class for annotation during the lecture. Students will be engaged in the learning process through class discussions and problem-solving questions independently and working together with partners and groups.

3.2 Expectations of students

- Students must attend at least 80% of all classes with the expectation that students only miss classes due to 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 textbook.
- Students should complete all assessment tasks and submit them on time.
- Students are expected to participate in online discussions through the Moodle page

4. Course schedule and structure

This course consists of 34 hours of class contact hours. You are expected to take an additional 116 hours of non-class contact hours to complete assessments, readings and exam preparation.

Week	Topics	Activity
1	Language of thermodynamics	
2	Entropy changes and irreversible processes	
3	Entropy changes and irreversible processes	Quiz 1
4	Redox processes	
5	Solution thermodynamics. Gibbs-Duhem equation. Raoult's and Henry's laws. Solutions and activity	

6		Assignment 1 (Joshi's Part)
7	Gibbs phase rule. Principles and features of Unary systems and binary systems. Lever rule. Phase diagram calculations. Microstructure development and applications	
8	Thermodynamics of binary phase diagrams	
9	Principles and features of ternary phase diagram. Introduction of software for thermodynamic calculations.	
10	Summary **Haghdadi's** part	Assignment 2 (**Haghdadi**' s Part)

5. Assessment

5.1 Assessment tasks

Assessment task	Description	Weight	Due date
Assignment 1:	Students will be required to complete a problem-based assignment in the areas of equilibrium and gas-solid phase transitions. **Assignment 1 will be posted on Moodle in Week 4 (Joshi's part).** Submissions after deadline will not be assessed.	15%	Week 6
Quiz:	The quiz will be of 2 h in duration in the area of fundamentals of thermodynamics **(Haines's part)**	25%	Week 3
Assignment 2:	Students will be required to complete one problem-based assignment in the area of phase diagrams. Students will be given the problem set on Monday week 8.	20%	Monday Week 10
Final exam:	**The examination will be 2 h in duration and held in the final exam period. The area covered will be Haghdadi's part.**	40%	Final exam period

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.

Assignment 2 and the final exam: Questions will be graded on a rating scale of (1)-(5), where the highest rating (1) denotes: (i) a correct mathematical solution to the problem together with a logical 2-5 line written explanation of the meaning of the result, or (ii) a thorough written explanation of the question if it is an essay-type one (full marks), through to (5), which indicates that no attempt was made to answer the question (no marks). This rating is converted to the value of the mark for each question.

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, they are declaring themselves well enough to do so. Information on this process can be found here: https://student.unsw.edu.au/special-consideration. Medical certificates or other appropriate documents must be included. Students should also 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 10% of maximum grade penalty for every day late, or part thereof.

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

5.4. Feedback on assessment

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

Quizzes: 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. Feedback for the quiz will be provided before the Census date.

Final exam: Students will receive their final mark.

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. Not referencing other people's work can constitute plagiarism. If you compare a calculated result in an assignment with an experimental value taken from the literature, please reference the source: Authors, publication & date.

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, this means that your work must be your own, and others' ideas should be appropriately acknowledged. If you don't 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**,** and
- 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. Readings and resources

P.W. Atkins and J. de Paula, *Elements of Physical Chemistry, 6th Edition*. Oxford University Press, Oxford, 2013.

P.W. Atkins and J. de Paula, *Physical Chemistry, 9th Edition*. Oxford University Press, Oxford, 2010.

W.D. Callister, Jr., Materials Science and Engineering: An Introduction, 8th Edition. John Wiley & Sons, New York, 2007.

D.R. Gaskell, Introduction to the Thermodynamics of Materials, 4th Edition. Taylor & Francis, Oxford, 2003.

R.A. Higgins, Engineering Metallurgy. Part I: Applied Physical Metallurgy, 6th Edition. Edward Arnold, London, 1993.

M. Hillert, Phase Equilibria, Phase Diagrams and Phase Transformations: Their Thermodynamic Basis. Cambridge University Press, Cambridge, 1998.

C.H.P. Lupis, *Chemical Thermodynamics of Materials*. North-Holland, Amsterdam, 1983.

D.V. Ragone, *Thermodynamics of Materials, Volume 1* & *Volume 2*. John Wiley & Sons, New York, 1995.

S. Stolen, T. Grande, and N.L. Allan, *Chemical Thermodynamics of Materials*. John Wiley & Sons, New York, 2004.

8. Administrative matters

School Office: Room 137, Building E10 School of Materials Science and Engineering
School Website: http://www.materials.unsw.edu.au/
Faculty Office: Robert Webster Building, Room 128
Faculty Website: http://www.science.unsw.edu.au/

[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