



THE UNIVERSITY OF
NEW SOUTH WALES

SCHOOL OF MATERIALS SCIENCE AND ENGINEERING

MATS1282

THERMODYNAMICS OF MATERIALS

Course Outline

Session 2, 2009

Course staff

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Timetable

Lecture/Tutorial	Day	Time	Location
Lecture	Wednesday	9:00-11:00 pm	Webster 251
	Thursday	9:00-11:00 am	Webster 250

Course outline

- Thermodynamic functions and systems. Chemical system, stretched wire, galvanic cell and paramagnetic solid. Mechanical, electrical and magnetic work.
- The first thermodynamic law and its applications. Formulation of the first thermodynamic law for chemical system, stretched wire, reversible cell. Enthalpy. Heat capacity at constant volume and pressure. Heat capacity of gas and solid. Heat of formation and heat of reaction.
- The second and third thermodynamic laws and their applications. Entropy and its change in the irreversible process. Statistical interpretation of entropy. Helmholtz and Gibbs free energies.
- Equilibrium between two phases of a pure substance. First order transitions. Clapeyron equation. Second order transitions.
- Chemical equilibrium. Direction and extent of chemical reaction. Standard thermodynamic values. Fugacity and thermodynamic activity. Gaseous equilibria. Solid-vapour equilibria.
- Ellingham diagram. Variation of equilibrium constant with temperature.
- Galvanic cell. Chemical and electrical driving forces. Electrode potential. Nernst equation. Pourbaix diagram.
- Thermodynamics of solutions. Partial and integral thermodynamic properties. Perfect solution. Excess thermodynamic properties. Thermodynamic activity. Gibbs-Duhem equation.
- Raoult's and Henry's laws. The Raoultian and Henrian standard states. Activity in different standard states. Activity measurements.
- Calculation of thermodynamic properties of binary metallic solutions. Ideal substitutional solutions and regular solutions.
- Thermodynamic stability. Spinodal decomposition. Miscibility gap.
- Calculation of thermodynamic properties of a solution from phase diagrams. Calculation of phase diagrams.

The learning and teaching philosophy underpinning the course (based on UNSW Learning Guidelines)

- Students are actively engaged in the learning process.**
It is expected that in addition to attending classes, students read, write, discuss, and are engaged in solving thermodynamic problems, in analysis, synthesis, and evaluation of materials properties in context of thermodynamics.
- Effective learning is supported by a climate of inquiry where students feel appropriately challenged.**
Thermodynamic problems are challenging; student will be given assignments which require research and will motivate deep analysis of different phenomena in materials science.
- Learning is more effective when students' prior experience and knowledge are recognised and built on.**
This course will be built on chemical thermodynamics which is a part of Physical Chemistry.
- Students become more engaged in the learning process if they can see the relevance of their studies to professional and disciplinary contexts**
Students will be asked to analyse role and place of thermodynamics in materials science, and the use of thermodynamics to understand different phenomena in materials science and properties of materials.

Course information

Units of credit	6
Parallel teaching involved in this course	None
How the course relates to other course offerings and overall program(s) in the discipline	<ul style="list-style-type: none"> • Elements of chemical thermodynamics including thermodynamic laws are taught as a part of Physical Chemistry, while Thermodynamics of Materials discusses application of thermodynamics to materials science and engineering. • This course will give intellectual framework for a number of materials science courses such as phase equilibria, phase transformation, materials processing, kinetics and diffusion, and others.
Course aims	To extend and apply the knowledge of thermodynamics to materials science and engineering
Graduate attributes which will be gained through the course	<ul style="list-style-type: none"> • Research, inquiry and analytical thinking abilities • Capability and motivation for intellectual development • Communication • Information literacy.
Expected learning outcomes	<p>Students should gain:</p> <ul style="list-style-type: none"> • Enhanced critical thinking, analytical and problem solving skills in materials science and engineering • Understanding of thermodynamic principles and laws in application to broad range of materials including stretched wire, paramagnetic solid,

	<p>electrochemical cell, and others.</p> <ul style="list-style-type: none"> • Understanding of properties relationships and thermodynamics of magnetostriction, superconductivity, thermoelasticity and other phenomena in materials science. • Understanding of phase and chemical equilibria, calculation of conditions for transitions of the first and second order. • Calculations of equilibrium conditions in the gas phase and solid-gas equilibrium. • Calculation of electrochemical equilibrium and construction of the Pourbaix diagram. • Knowledge of thermodynamic properties of solutions, calculation of thermodynamic properties of ideal and regular solutions. • Calculation of chemical equilibrium for reactions involving solutions. • Calculation of thermodynamic properties of solutions from phase diagrams and construction of phase diagrams using thermodynamics of solutions.
Teaching strategies	<ul style="list-style-type: none"> • Core concepts, theories and approaches to numerous thermodynamic problems will be covered in lectures. Several examples will be offered to demonstrate the use of thermodynamics in materials science and engineering. A number of tutorial classes will be conducted to enhance problem solving skills. A number of problems will be offered for home work. • It is expected that students come to classes prepared for discussion. • Teaching material, including course outline, notes, problems, assignments, examples of solutions of problems, and course announcements are available on the Course Vista website.

Assessment

Assignments	20%
Test	30%
Final exam	50%

Assignments will include 4-6 problems, some of them quite challenging, to achieve learning outcomes and develop graduate attributes.

Assignments

	Issue	Submission
Assignment 1	week 3	week 5
Assignment 2	week 5	week 7
Assignment 3	week 9	week 11

Mid-session exam. The aim of this test is to assess students' skills in solving of problems on the use of thermodynamic laws in application to materials science and engineering, phase and chemical and electrochemical equilibria. It will be conducted in Week 7/8.

Final exam will cover thermodynamics of solutions, the use of phase diagrams for calculation of thermodynamic properties of solutions and construction of phase diagrams.

Academic honesty and plagiarism

What is Plagiarism?

Plagiarism is the presentation of the thoughts or work of another as one's own.*

Examples include:

- direct duplication of the thoughts or work of another, including by copying material, ideas or concepts from a book, article, report or other written document (whether published or unpublished), composition, artwork, design, drawing, circuitry, computer program or software, web site, Internet, other electronic resource, or another person's assignment without appropriate acknowledgement;
- paraphrasing another person's work with very minor changes keeping the meaning, form and/or progression of ideas of the original;
- piecing together sections of the work of others into a new whole;
- presenting an assessment item as independent work when it has been produced in whole or part in collusion with other people, for example, another student or a tutor; and
- claiming credit for a proportion a work contributed to a group assessment item that is greater than that actually contributed.†

For the purposes of this policy, submitting an assessment item that has already been submitted for academic credit elsewhere may be considered plagiarism.

Knowingly permitting your work to be copied by another student may also be considered to be plagiarism.

Note that an assessment item produced in oral, not written, form, or involving live presentation, may similarly contain plagiarised material.

The inclusion of the thoughts or work of another with attribution appropriate to the academic discipline does *not* amount to plagiarism.

The Learning Centre website is main repository for resources for staff and students on plagiarism and academic honesty. These resources can be located via:

www.lc.unsw.edu.au/plagiarism

The Learning Centre also provides substantial educational written materials, workshops, and tutorials to aid students, for example, in:

- correct referencing practices;
- paraphrasing, summarising, essay writing, and time management;
- appropriate use of, and attribution for, a range of materials including text, images, formulae and concepts.

Individual assistance is available on request from The Learning Centre.

Students are also reminded that careful time management is an important part of study and one of the identified causes of plagiarism is poor time management. Students should allow sufficient time for research, drafting, and the proper referencing of sources in preparing all assessment items.

* Based on that proposed to the University of Newcastle by the St James Ethics Centre. Used with kind permission from the University of Newcastle

† Adapted with kind permission from the University of Melbourne.

Recommended Reference Materials

- Lupis, C.H.P. Chemical Thermodynamics of Materials, North-Holland, 1983
- Ragone, D.V. Thermodynamics of Materials, Volumes 1& 2, John Wiley & Sons, Inc., 1995
- Kubashevski, O., Alcock, C.B., and Spencer, P.J. Materials Thermochemistry, Pergamon Press, 1993
- Gaskell, D.R. Introduction to the Thermodynamics of Materials, 4th Edition, Taylor & Francis, 2003
- Gokcen, N.A. and Reddy, R.G., Thermodynamics, 2nd Edition, Plenum Press, 1996
- Moore, J.J. Chemical Metallurgy, 2nd Ed. Butterworth & Co., 1990
- Zemansky, M.W. Heat and Thermodynamics, McGraw-Hill Book Company
- Espinola, T. Introduction to Thermophysics, Wm. C. Brown Publishers, 1994
- Sears, F.W., and Salinger, G.L. Thermodynamics, Kinetic Theory, and Statistical Thermodynamics, 3rd Ed., Addison Wesley Publishing Co., 1986.
- Swalin, R.A. Thermodynamics of Solids, John Wiley & Sons, Inc., 1972.
- Hillert, M. Phase Equilibria, Phase Diagrams and Phase Transformations, Their Thermodynamic Basis, Cambridge University Press, 1998.
- S. Stolen, T. Grande and N. L. Allan: Chemical Thermodynamics of Materials. Wiley, Chichester, 2004.

Continual course improvement

- We welcome feedback at all times on presentation of course materials and any other course-related matters, and will be happy to discuss any issues raised in the lectures.
- You will be asked to provide evaluative feedback through the UNSW's Course and Teaching Evaluation and Improvement (CATEI) Process at the end of the course. Feedback from prior assessments will be discussed in lecture 1.
- Students are encouraged to address any problems regarding teaching of this course at the annual staff-student meeting.

Administrative Matters

- Students should attend at least 80% of all classes.
- Assignments submitted after the deadline will receive a 10% of max. grade penalty for every day late, or part thereof.
- Students unable to submit assignments on time or attend the final exams on health grounds should make a request for special consideration by submitting the form available from the Student Desk in the Chancellery. Medical certificates or other appropriate documents must be included. Students should also advise the lecturer.
- 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 convener prior to, or at the commencement of, their course, or with the Equity Officer (Disability) in the Equity and Diversity Unit (9385 4734 or www.equity.unsw.edu.au/disabil.html). Early notification is essential to enable any necessary adjustments to be made. Information on designing courses and course outlines that take into account the needs of students with disabilities can be found at:

www.secretariat.unsw.edu.au/acboardcom/minutes/coe/disabilityguidelines.pdf