MATS2008

Thermodynamics and Phase Equilibria

Course Outline
Session 1, 2014
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Course staff

<table>
<thead>
<tr>
<th>Name</th>
<th>Position</th>
<th>Dates</th>
<th>Room</th>
<th>Contact Information</th>
<th>Consultation hours:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dr Ron S Haines</td>
<td>Lecturer and Lab Demonstrator</td>
<td>1-4, 7-11 (labs)</td>
<td>Room 128, School of Chemistry (Dalton Building F12)</td>
<td><a href="mailto:r.haines@unsw.edu.au">r.haines@unsw.edu.au</a></td>
<td>by appointment</td>
</tr>
<tr>
<td>Dr Danyang Wang</td>
<td>Lecturer and Coordinator</td>
<td>4-9</td>
<td>Room 211 School of Materials Science and Engineering (Building e8)</td>
<td><a href="mailto:dy.wang@unsw.edu.au">dy.wang@unsw.edu.au</a></td>
<td>by appointment</td>
</tr>
<tr>
<td>Professor Charles C. Sorrell</td>
<td>Lecturer</td>
<td>9-12</td>
<td>Room 211 School of Materials Science and Engineering (Building e8)</td>
<td><a href="mailto:c.sorrell@unsw.edu.au">c.sorrell@unsw.edu.au</a></td>
<td>by appointment</td>
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</tbody>
</table>

Course Objectives:

To understand basic thermodynamic principles and to gain the capability of applying these principles to phase transitions and the chemical and electrochemical processes of pure substances, solutions, and multiphase systems. To understand the principles of binary phase diagrams and to apply this understanding to the interpretation and application of these diagrams to conditions of processing and performance.
Your Course at a Glance

<table>
<thead>
<tr>
<th>What you will learn</th>
<th>Weeks</th>
<th>Assessment task</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1</strong></td>
<td>Language of thermodynamics: System, surroundings, and processes. Heat, work, and internal energy. The first law and its applications. Heat capacity at constant volume and constant pressure. Enthalpy. Enthalpy of formation and Enthalpy of reaction. Temperature dependence of enthalpy changes.</td>
<td>1 – 4</td>
</tr>
<tr>
<td><strong>2</strong></td>
<td>Entropy changes and irreversible processes. The second and third laws and their applications. Statistical interpretation of entropy. Helmholtz and Gibbs energies.</td>
<td>7 – 11 (labs)</td>
</tr>
<tr>
<td><strong>4</strong></td>
<td>Equilibrium between two phases of a pure substance. First order transitions. Clapeyron equation. Second order transitions.</td>
<td>4 – 6</td>
</tr>
<tr>
<td><strong>6</strong></td>
<td>Ellingham diagrams. Variation of equilibrium constant with temperature.</td>
<td></td>
</tr>
<tr>
<td><strong>9</strong></td>
<td>Regular solutions.</td>
<td></td>
</tr>
<tr>
<td><strong>10</strong></td>
<td>Calculation of thermodynamic properties of a solution from phase diagrams.</td>
<td></td>
</tr>
<tr>
<td><strong>11</strong></td>
<td>Gibbs phase rule. Unary systems.</td>
<td>9 – 12</td>
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<tr>
<td><strong>12</strong></td>
<td>Binary systems: Principles, features, interpretation, microstructures, applications.</td>
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</table>
Timetable

Lectures

<table>
<thead>
<tr>
<th>Day</th>
<th>Dates</th>
<th>Mondays</th>
<th>Tuesdays</th>
<th>Wednesdays</th>
<th>Thursdays</th>
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</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>9:00 – 11:00</td>
<td>12:00-14:00</td>
<td>13:00-15:00</td>
<td>14:00-17:00</td>
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<tr>
<td>Time</td>
<td></td>
<td>Location</td>
<td>Location</td>
<td>Location</td>
<td>Location</td>
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<tr>
<td>Location</td>
<td>Dates</td>
<td></td>
<td></td>
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<tr>
<td>Week 1</td>
<td>2 – 8 March</td>
<td>Haines</td>
<td>--</td>
<td>Haines</td>
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<tr>
<td>Week 2</td>
<td>9 – 15 March</td>
<td>Haines</td>
<td>--</td>
<td>Haines</td>
<td>--</td>
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<tr>
<td>Week 3</td>
<td>16 – 22 March</td>
<td>Haines</td>
<td>--</td>
<td>Haines</td>
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<tr>
<td>Week 4</td>
<td>23 – 29 March</td>
<td>Haines</td>
<td>Wang</td>
<td>Wang</td>
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</tr>
<tr>
<td>Week 5</td>
<td>30 Mar – 5 April</td>
<td>--</td>
<td>Wang</td>
<td>Wang</td>
<td>--</td>
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<tr>
<td>Week 6</td>
<td>6 – 12 April</td>
<td>--</td>
<td>Wang</td>
<td>Wang</td>
<td>--</td>
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<tr>
<td>Week 7</td>
<td>13 – 19 April</td>
<td>--</td>
<td>Wang</td>
<td>Wang</td>
<td>Haines</td>
</tr>
<tr>
<td>Break</td>
<td>20 - 26 April</td>
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<tr>
<td>Week 8</td>
<td>27 April - 3 May</td>
<td>--</td>
<td>Wang</td>
<td>Wang</td>
<td>Haines</td>
</tr>
<tr>
<td>Week 9</td>
<td>4 - 10 May</td>
<td>Sorrell</td>
<td>Wang</td>
<td>Sorrell</td>
<td>Haines</td>
</tr>
<tr>
<td>Week 10</td>
<td>11 - 17 May</td>
<td>Sorrell</td>
<td>--</td>
<td>Sorrell</td>
<td>Haines</td>
</tr>
<tr>
<td>Week 11</td>
<td>18 - 24 May</td>
<td>Sorrell</td>
<td>--</td>
<td>Sorrell</td>
<td>Haines</td>
</tr>
<tr>
<td>Week 12</td>
<td>25 – 31 May</td>
<td>Sorrell</td>
<td>--</td>
<td>Sorrell</td>
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</tbody>
</table>

Thursday Lecture and Laboratory Locations

Lectures

Mondays | Weeks 1 – 12 | Old Main Building 229
Tuesdays | Weeks 1 – 12 | Chemical Sciences Room M11
Wednesdays | Weeks 1 – 12 | The Michael Hintze Theatre

Laboratories

Thursdays | Weeks 7 – 11 | Chemical Sciences Room 162

Course Outline

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 (ideal and regular solution thermodynamics, Raoult's and Henry's laws, calculation of thermodynamic values, construction of binary phase diagrams); interpretation and applications of binary phase diagrams (unary systems, binary systems, effect on microstructures, applications for processing and performance)
Assessment

<table>
<thead>
<tr>
<th>Assessment Task</th>
<th>Fraction</th>
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<tbody>
<tr>
<td><strong>Laboratories:</strong> Students will undertake two laboratory experiments. These will illustrate the principles of (1) enthalpy of solution by calorimetry and (2) enthalpy of solution by variation of solubility with temperature.</td>
<td>15%</td>
</tr>
<tr>
<td><strong>Details:</strong> Students will be divided into two groups. There will be an induction in Week 7. Students in Group 1 will undertake the experiments in Weeks 8 and 10; students in Group 2 will undertake them in Weeks 9 and 11.</td>
<td>15%</td>
</tr>
<tr>
<td><strong>Assignment:</strong> Students will be required to complete a problem-based assignment in the areas of equilibrium and gas-solid phase transitions.</td>
<td>15%</td>
</tr>
<tr>
<td><strong>Details:</strong> Students will be given the problems in Week 4 and they will be due in Week 6.</td>
<td>15%</td>
</tr>
<tr>
<td><strong>Quizzes:</strong> The quizzes will be 2 h in duration in the areas of (1) fundamentals of thermodynamics and (2) solution thermodynamics and phase diagram construction.</td>
<td>(1) 15%  (2) 25%</td>
</tr>
<tr>
<td><strong>Details:</strong> Students will take quiz (1) in Week 4 and quiz (2) in Week 9.</td>
<td>15%</td>
</tr>
<tr>
<td><strong>Final Exam:</strong> The examination will be 2 h in duration and held in the final exam period. The only area covered will be the interpretation and applications of binary phase diagrams.</td>
<td>30%</td>
</tr>
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</table>

References:

Learning and teaching philosophy underpinning the course
Based on UNSW Learning Guidelines

The course is designed for students to actively engage in the learning process and analyse and synthesise the content in a real world environment.

• **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.

### Course Information

<table>
<thead>
<tr>
<th>Units of credit</th>
<th>6</th>
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<tbody>
<tr>
<td>How the course relates to other course offerings and overall program(s) in the discipline</td>
<td>The course applies thermodynamic laws and principles and phase equilibria considerations to analyse and solve physical and chemical problems in materials processing and applications. Knowledge of chemical equilibria, chemical reactions, physical changes in systems, and mathematics will be used in the course.</td>
</tr>
</tbody>
</table>
| Graduate attributes that will be gained through the course¹ | • Ability to communicate effectively  
• Capacity for creativity and innovation  
• Ability to manage information and documentation  
• Understanding of professional and ethical responsibilities, and commitment to them  
• Ability to function effectively as an individual  
• Ability to work effectively in multidisciplinary and multicultural teams  
• Capacity for lifelong learning and professional development  
• Professional attitudes |

¹ Graduates will be expected to be able to:

- Communicate effectively in written and oral form
- Demonstrate creativity and innovation
- Manage information and documentation
- Understand professional and ethical responsibilities, and commit to them
- Function effectively as an individual
- Work effectively in multidisciplinary and multicultural teams
- Engage effectively in lifelong learning and professional development
- Demonstrate professional attitudes
### Expected learning outcomes

The goals of the course are:

- To introduce students to the basic concepts of thermodynamics applied to the gas, liquid, and solid states
- To provide the means for students to apply thermodynamic concepts to the behaviour of materials
- To allow students to understand the relation between thermodynamics and phase equilibria
- To enable students to interpret phase diagrams in terms of specifying materials processing parameters and predicting materials performance

Students also will learn:

- To think critically in decision making and problem-solving
- To communicate with correct terminology
- To conduct library and online research
- To work effectively to solve problems
- To communicate in writing

### Teaching strategies

- Core concepts, theories, and approaches will be covered in lectures.
- These principles will be illustrated through worked examples in class and a problem-based assignment.
- The practical applications of these principles will be demonstrated through clarification and demonstration of the use of thermodynamics and phase equilibria.
- Teaching material, including course outline, relevant notes, case studies, and course announcements will be available on the Course Moodle website.

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*Based on the professional attributes given in *Engineers Australia National Generic Competency Standards - Stage 1 Competency Standard for Professional Engineers* and UNSW Graduate Attributes.

### 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.

Continual course improvement

• Students 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
• Students are encouraged to address any problems regarding teaching of this course at the annual staff-student meeting
• Student comments on teaching during the session are welcome and will be appreciated
  At times students may be asked to answer a short questionnaire for feedback on the course

Administrative Matters

• Students should attend at least 80% of all classes.
• Students unable to submit assignments on time or attend the mid-session quizzes or final exams on health grounds should make a request for special consideration. Information on this process can be found here (https://my.unsw.edu.au/student/atoz/SpecialConsideration.html). Medical certificates or other appropriate documents must be included. Students should also advise the lecturer of the situation.
• Assignments/lab reports submitted after the deadline 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 (www.studentequity.unsw.edu.au). Early notification is essential to enable any necessary adjustments to be made.

Rules for Exams

Rules governing conduct during exams are given at: https://my.unsw.edu.au/student/academiclife/assessment/examinations/examinationrules.html - Rulesfortheconductofexaminations

Note that the use of mobile phones or music players in an exam room will constitute Academic Misconduct.