# MS&E 330 Fall 2016: Thermodynamics of Materials

**Instructor:**

**Paul Evans**
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Office Hours: Monday, 1-2 PM, or by appointment. Also, please feel free to drop in or email.

**Teaching Assistant:**

**Kyle McElhinny** email: mcelhinny@wisc.edu

Office Hours: Mondays 2-3 PM, location to be announced.

## Course Meetings

*Lecture*: MWF 11-11:50 AM, Engineering Centers Building Room 1003.

*Required Discussion and Activity Section*: Th 1:20-2:10 PM Engineering Centers Building Room 1003

Attendance at all of these course meetings is required and will be accounted for in the Homework/Participation component of the grade. Attendance at office hours is not required.

## Course Homepage

Handouts, readings, assignments, and solutions are available on the course web page at the University of Wisconsin Canvas site: https://canvas.wisc.edu/courses/437

Course emails will come from mse330-1-f16@lists.wisc.edu.

## Course Description

MS&E 330 will cover the basic concepts of thermodynamics that underpin all areas of materials science and engineering. We will discuss the ideas that allow the thermodynamic state of a system to be described quantitatively and develop methods for describing materials of increasing complexity, including systems with multiple phases and multiple components.

## Course Requirements

*Exams*

**Two midterm exams:** Tentatively scheduled for October 10 and November 14, in class.

**Final exam:** December 21, 12:25 PM- 2:25 PM. The final exam will focus material from the later part of the class.

Please let me know right away if you will not be able to be present for the midterm exams.

*Homework*

We will have 11 homework assignments. Follow the requirements in the "*MS&E 330 Homework Guidelines and Requirements*" handout.

*Project*

There will be a final project involving the modeling and interpretation of phase diagrams.

*Grading*

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|---|---|
| Homework/Participation | 25% |
| Project | 10 |
| Midterm Exam 1 | 20 |
| Midterm Exam 2 | 20 |
| Final Exam | 25 |

**Resources**

*Course Text*

D. R. Gaskell, *Thermodynamics of Materials 5th edition*, Taylor and Francis, 2008. ISBN 9781591690436, library catalog number TN673 G33 2008.

*Books on Reserve (Wendt Library)*

Library course homepage: https://www.library.wisc.edu/course-pages/viewer/show/13862

1. P. Atkins and J. de Paula, *Physical Chemistry: Thermodynamics, Structure, and Change 10th edition,* Freeman, 2014. ISBN 9781429290197.

2. D. V. Ragone, *Thermodynamics of materials vols. 1 and 2*, Wiley 1995. ISBN 9780471308850 and 9780471308867. Catalog number TA418.52 R34 1995.

*Other resources*

1. *ASM Handbook Vol. 3 Alloy Phase Diagrams*, available at: http://products.asminternational.org.ezproxy.library.wisc.edu/hbk/index.jsp
2. University of Wisconsin Writing Center (writing.wisc.edu) and Writer's Handbook, available at: http://writing.wisc.edu/Handbook/index.html

# Lecture Schedule

| Week | Date | Day | Lecture | Topic/Activity | Reading (Chapter numbers refer to the textbook by Gaskell) | Assignment |
|---|---|---|---|---|---|---|
| 1 | 9/7 | W | 1 | **Introduction, Basic Concepts**: System, components, phases, phase diagrams | Chapter 1 and Math Review Handout | |
| | 9/8 | Th | *Discussion/Activity Section* | *Math review, homework 1 activities* | Chapter 1 and Math Review Handout | |
| | 9/9 | F | 2 | **Basic Concepts:** State, equation of state, properties, extensive, intensive parameters. Background Math: logarithms, differentials, exact differentials, partial derivatives, relationships among partials | Chapter 1 and Math Review Handout | |
| 2 | 9/12 | M | 3 | **First Law of Thermodynamics:** Work and heat: mechanical equilibrium, simple equilibrium, heat and energy | Chapter 2 | |
| | 9/14 | W | 4 | **Constant volume and Constant Pressure Processes, Enthalpy H:** Constant volume and constant pressure heat capacity | Chapter 2 | **Homework 1 Due** |
| | 9/15 | Th | *Discussion/Activity Section* | *Homework 2 activities* | Chapter 2 | |
| | 9/16 | F | 5 | **Reversible Processes:** Reversible adiabatic and isothermal processes, heat conduction | Handouts | |
| 3 | 9/19 | M | 6 | **Thermochemistry, Phase Transformations, and Reactions Calorimetry:** Cooling curves, differential scanning calorimetry, heats of reaction, specific heat | Handouts | |
| | 9/21 | W | 7 | **Chemical Reactions:** Chemical equilibria, rate of reactions, Arrhenius relation | Chapter 3 | **Homework 2 Due** |
| | 9/22 | Th | *Discussion/Activity Section* | *Homework 3 activities* | Chapter 3 | |
| | 9/23 | F | 8 | **Second Law of Thermodynamics Reversible and Irreversible Processes:** Heat engines and Entropy, thermodynamic temperature scale | Chapter 3 | |
| 4 | 9/26 | M | 9 | **Entropy and the Requirement for Equilibrium:** Energy maximized for fixed U, V | Chapter 4 | |
| | 9/28 | W | 10 | **Statistical Interpretation of Entropy:** Entropy and disorder: microstates, configurational entropy, thermal entropy | Chapter 4 | **Homework 3 Due** |
| | 9/29 | Th | *Discussion/Activity Section* | *Homework 4 activities* | Chapter 4 | |
| | 9/30 | F | 11 | Example: Statistical mechanics of polymers | Handouts | |
| 5 | 10/3 | M | 12 | **Statistical Interpretation of Temperature:** Equilibrium between system and heat reservoir | Chapter 5 | |
| | 10/5 | W | 13 | **Auxiliary Functions:** Enthalpy, H, Helmholtz Free Energy, A, and Gibbs Free Energy, G | Chapter 5 | **Homework 4 Due** |
| | 10/6 | Th | *Discussion/Activity Section* | *Review for Exam 1* | | |
| | 10/7 | F | 14 | Chemical potential | Chapter 5 | |
| 6 | 10/10 | M | 15 | | | **Exam 1 in Class** |
| | 10/12 | W | 16 | Maxwell's equations and relations among the auxiliary parameters | Chapter 5 | |
| | 10/13 | Th | *Discussion/Activity Section* | *Homework 5 activities* | Chapter 5 | |
| | 10/14 | F | 17 | **Heat Capacity and 3rd Law of Thermodynamics** | Chapter 6 | |
| 7 | 10/17 | M | 18 | Theoretical Calculation of Heat Capacity: Crystal Vibrations, Phonons, Einstein and Debye models | Chapter 6 | |
| | 10/19 | W | 19 | Enthalpy as function of temperature and composition: Thermochemical data, Richard's Rule | Chapter 6 | **Homework 5 Due** |
| | 10/20 | Th | *Discussion/Activity Section* | *Homework 6 activities* | Chapter 6 | |
| | 10/21 | F | 20 | **Phase Equilibria in a One-Component System:** Gibbs Free Energies of the phases; Clapeyron and Clausius Clapeyron Equations | Chapter 7 | |
| 8 | 10/24 | M | 21 | Equilibria among and vapor pressures of condensed phases | Chapter 7 | |
| | 10/26 | W | 22 | Solid-solid phase equilibria | Chapter 7 | **Homework 6 Due** |
| | 10/27 | Th | *Discussion/Activity Section* | *Homework 7 activities* | | |
| | 10/28 | F | 23 | **Behavior of Gases:** P-V-T relationships for ideal and non-ideal gases: Van der Waals, definition of fugacity | Chapter 8 | |
| 9 | 10/31 | M | 24 | Gibbs Free Energies of Ideal Gases and Mixtures of Gases | Chapter 8 | |
| | 11/2 | W | 25 | | | **Homework 7 Due** |
| | 11/3 | Th | *Discussion/Activity Section* | *Homework 8 activities* | | |
| | 11/4 | F | 26 | **Behavior of Solutions:** Activity, Chemical Potential, ideal solutions, Henry's and Raoult's Laws | Chapter 9 | |
| 10 | 11/7 | M | 27 | Regular Solutions and Regular Solution Theory | Chapter 9 | |
| | 11/9 | W | 28 | Partial Molar Quantities and the Gibbs-Duhem relations | Chapter 9 | **Homework 8 Due** |
| | 11/10 | Th | *Discussion/Activity Section* | *Review for Exam 2* | | |
| | 11/11 | F | 29 | **Phase Diagrams of Binary Systems:** Construction of Binary Phase Diagrams from Gibbs Free Energy Curves: Common tangent | Chapter 10 | |
| 11 | 11/14 | M | 30 | | | **Exam 2 in Class** |
| | 11/16 | W | 31 | Construction of Binary Phase Diagrams II: Effects of Regular Solution Parameters | Chapter 10 | |
| | 11/17 | Th | *Discussion/Activity Section* | *Homework 9 activities* | | |
| | 11/18 | F | 32 | Interpretation of phase diagrams, ternary diagrams | Chapter 10 and Handouts, Chapter 14 | |
| 12 | 11/21 | M | 33 | **Reactions Involving Gases:** Law of mass action and standard free energy for a chemical reaction | Chapter 11 | |
| | 11/23 | W | 34 | Examples: SO2-SO3-O2 , H2O-H2, and CO2-CO systems | Chapter 11 | **Homework 9 Due** |
| | 11/24 | Th | **No Meeting: Thanksgiving Recess** | | | |
| | 11/25 | F | **No Meeting: Thanksgiving Recess** | | | |
| 13 | 11/28 | M | 35 | **Equilibrium in Reactions Involving Pure Condensed Phases and a Gaseous Phase:** Ellingham Diagrams I | Chapter 12 | |
| | 11/30 | W | 36 | **Reaction Equilibria in Systems Containing Components in Condensed Solution:** Ellingham Diagrams II | Chapter 13 | **Homework 10 Due** |
| | 12/1 | Th | *Discussion/Activity Section* | *Homework 11 activities* | | |
| | 12/2 | F | 38 | Gibbs Phase Rule I | Chapter 13 | |
| 14 | 12/5 | M | 38 | Gibbs Phase Rule II, Phase Diagram Project Assignment | Chapter 13 | |
| | 12/7 | W | 39 | **Electrochemistry:** Electron transfer, Oxidation and Reduction reactions, Nernst Equation | Chapter 15 | **Homework 11 Due** |
| | 12/8 | Th | *Discussion/Activity Section* | *Homework 12 activities, project discussion* | | |
| | 12/9 | F | 41 | Electrochemical Cells and the Electrochemical Series | Chapter 15 | |
| 15 | 12/12 | M | 41 | Effect of Acidity, and Pourbaix Diagrams | Chapter 15 | |
| | 12/14 | W | 42 | Corrosion | Handouts | **Homework 12 Due** |
| | 12/15 | Th | *Discussion/Activity Section* | *Review for Final Exam* | | **Phase Diagram Project Due** |
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| | **Final Exam: December 21, 12:25 PM- 2:25 PM** | | | | | |
| | **Chapters and Refer to the Textbook by Gaskell** | | | | | |