MSE 0051: THERMODYNAMICS OF MATERIALS Spring 2019
Course Syllabus

Catalog Description

This course covers basic concepts and laws of thermodynamics, work and heat, free energy, entropy, the basic problems of conditions for equilibrium and treatment of heterogeneous equilibrium. The relation between thermodynamics and the various types of phase diagrams is discussed and applied to unary and multi-component systems. Thermodynamics is introduced as a tool applicable to understand the phase stabilities and phase reactions in metal alloys and other solid solutions. The way to put thermodynamics to practical use for scientific and technical problems is emphasized.

It requires only a basic knowledge of physics and chemistry, but the second part of the course does rely on a strong basis in differential equations, especially partial differentials. All necessary math will be developed in the course alongside the concepts that employ the math. We will begin with an introduction to key concepts like temperature and heat, go through ideal gas behaviors, and equilibrium phase diagrams, and electrochemistry.

3 credit hours.

Schedule

Lecture Room 204

Section 01-03 Wednesdays 9:10 – 11:55am

SCUPI
Sichuan University - Pittsburgh Institute

Instructor

Prof. Charles Hua charleshua@scu.edu.cn
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Teaching Assistants

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When emailing the instructor or TAs, include "MSE 0051" in the subject field of your message. Use your university email account (student_ID_number@stu.scu.edu.cn), since mails from other accounts might be stopped by the SCU spam filter.

Textbook

Introduction to the Thermodynamics of Materials, 5th Edition, by David R. Gaskell, 2008, CRC Press, ISBN 9781591690436 - CAT# GS1076.

Or 6th Edition, by David R. Gaskell and David E. Laughlin, 2016, CRC Press, ISBN-13: 978-1498757003, ISBN-10: 1498757006

Reference Books

- David V. Ragone, *Thermodynamics of Materials*, vol. I, MIT Series in Materials Science and Engineering, John Wiley & Sons, Inc., 1995.
- Mats Hillert, *Phase Equilibria, Phase Diagrams and Phase Transformations: Their Thermodynamic Basis*, Cambridge University Press, 1998.
- N. Saunders and A. P. Miodownik, *CALPHAD: Calculation of Phase Diagrams A Comprehensive Guide*, Pergamon, 1998.

We will cover approximately one chapter per week. Read the assigned chapter BEFORE class.

Course Outline

1. Introduction and Definition of Terms
2. The Laws of Thermodynamics
3. The Statistical Interpretation of Entropy
4. Fundamental Equations and Their Relationships
5. Heat Capacity, Enthalpy, Entropy, and the Third Law of Thermodynamics
6. Phase Equilibrium in a One-Component System (Unary Systems)
7. The Behavior of Gases

8. The Behavior of Solutions
9. Gibbs Free Energy Composition and Phase Diagrams of Binary Systems
10. Reactions Involving Gases
11. Reactions Involving Pure Condensed Phases and a Gaseous Phase
12. Reaction Equilibria in Condensed Solution
13. Electrochemistry
14. Thermodynamics of Phase Transformation
15. Computational Thermodynamics and Materials Science

Course Web Site

This course uses the Blackboard system; the web site is

https://learn.scupi.cn/

or

https://learn.scupi.cn/webapps/blackboard/content/listContentEditable.jsp?content_id=_8633_1&course_id=_379_1&mode=reset

There you will find the course syllabus, studio and homework assignments, and other materials. Current announcements and assignments will be posted on the home page. All assignments will be uploaded through the Blackboard system. Please check the class page frequently.

Class Format

INTRODUCTION TO THE THERMODYNAMICS OF MATERIALS is taught using a combined lecture/quiz format. The class in the afternoon begins with a session lecture to review material from the text and introduce new concepts. In the second session, the lecturer may ask questions to as many students as possible and then continue with textbook. Session 3 may finish the chapter with highlighted concepts and even a few in-class quiz.

Each week you will turn in one assignment, which will be selected from the end of each chapter.

It is imperative that you come to class prepared. This will generally involve reading one or more chapters of the textbook, viewing tutorial videos, thinking, engaging with fellow students, practice and performing preliminary calculations. This is a three credit hour class, which means you should expect to devote at least 9 to 12 hours of effort outside the scheduled class time every week.

Homework Assignments

Homework problems will be assigned every week and posted on Blackboard. These are to be solved and turned in by **Tuesday 1:30 PM** the following week. You may work with other people on homework, but all writeups must be individual efforts. Homework will be graded on a 0-100 point scale.

All work will be submitted electronically through the Blackboard system. Late homework will not be accepted.

Unless specifically requested, emailed homework will not be accepted.

Please adhere to these homework guidelines:

- Your assignment must be typeset using Word and submitted electronically through Blackboard. Handwritten assignments will not be accepted.
- Put your name, ID number (last four digits), and class section at the top of the first page.
- List the names of other people you've worked with on the assignment.
- All work must be shown for each solution to receive full credit. Present your solution in a logical fashion, showing and explaining all steps in detail.

- A significant amount of the homework points is associated with obtaining the correct answer. This includes getting the correct quantity, **number of significant digits**, sign, and **unit**.

All of the homework scores will be used in your grade computation. Unless otherwise indicated, you can work with your fellow classmates in the class, but you must submit a distinct and independent write-up to receive credit.

If you're sick, or have a compelling emergency that prevents you from turning in the homework on time, email Prof. Charles Hua.

If you believe an error has been made in the grading of an assignment, bring it to the attention of your TA within ONE WEEK of its return.

Exams and Grading

The will be a midterm exam in March, and a comprehensive final examination at the end of the semester.

The test and exam are CLOSED BOOK, CLOSED NOTES, CLOSED COMPUTER. You will also find a calculator and a straightedge ruler helpful.

Your grade will be based on the homework (35%), class participation (5%), mid-term exam (30%), and final examination (30%).

Office Hours

If you don't understand something, and talking to your classmates doesn't help, then you should be seeking help from the instructor or teaching assistant.

Office hours are times we have specifically set aside to be available to students. During office hours, you can come to our office; you don't need an appointment. We are also available at other times; please email to schedule a time.

Current office hours will be Monday, Tuesday and Friday morning 9-11:30am. You are encouraged to make appointment.

Course Goals

- To explain the laws of thermodynamics in equations of state functions
- To understand the nature of entropy and chemical potential
- To be able to calculate certain phase diagrams, predict the microstructure and properties
- To explore how a chemical reaction can be designed to maximize productivity

Approximate Schedule

Week	Date	Topic
1		00 Course Introduction 01 Basic Concepts
2		02 0^{th} and 1^{st} Law of Thermodynamics
3		03 The 2^{nd} Law of Thermodynamics
4		04 The Statistical Interpretation of Thermodynamics
5		Happy Holiday
6		05 Auxiliary Functions, Entropy and Free Energy 06 Heat Capacity, Enthalpy, Entropy and 3rd Law
7		07 Phase Equilibrium in a One-Component System
8		08 Behavior of Gases
9		Mid-term Exam 09 Behavior of Solutions
10		10 Gibbs Free Energy Composition and Phase Diagrams of Binary Systems
11		11 Reactions Involving Gases Experimental Determination of Phase Diagrams
12		12 Reactions Inv. Pure Condensed Phases and a Gaseous Phase Computation of Phase Diagrams
13		13 Reaction Equilibria in Systems Containing Components in Condensed Solution Solidification Modeling
14		14 Phase Diagrams for Binary Systems in Pressure-Temperature-Composition Space
15		15 Electrochemistry
16		Final Exam

Extra lectures if time permits:

Experimental Determination of Phase Diagrams
Computation of Phase Diagrams
Solidification Modeling

Thermodynamics of surfaces