Thermodynamics of Materials EN1410

Instructor Janet Rankin

I like to give students the option of meeting outside of scheduled office hours.

Office Hours

M & W 3-5PM, or by appointment

Consider wording your overview so that it is directed at the students: e.g., "You will learn...", etc.

Course Overview

The Big Idea in thermodynamics – and in this course is that Energy is conserved and minimized at equilibrium. Materials scientists and engineers must be able to apply thermodynamics (and the idea the energy is minimized at equilibrium) in order to understand and control the structure-properties-processing relationships that exist in physical systems. In this course you will learn how to effectively, and accurately manipulate the thermodynamic formalism to mathematically describe material behavior at equilibrium. In addition, you will learn how to utilize thermodynamic data to predict and optimize the behavior of complex physical systems.

Learning Outcomes¹

After successful completion of EN0141 students will understand how to define thermodynamic properties of solids, by:

- recognizing the difference between state functions and path-dependent (e.g. energy functions) quantities (e.g. work and heat);
- describing the consequences of entropy as a state function;
- explaining the implications (and the equivalence) of the entropy-maximum, and energy-minimum principles;
- constructing alternate energy functions, and utilizing particular alternate energy functions in the description and analysis of physical systems (e.g., the Gibbs free energy);
- demonstrating that all energy functions are minimized at equilibrium;
- relating partial derivatives of energy functions to measurable materials properties. Be able to describe equilibrium in multicomponent systems, by:
- implementing a variety of solution models;
- interpreting the meaning of curvature and slope of "G versus X" curves generated from various solution models
- applying the tangent construction to molar free energy curves for solutions;
- identifying single and multiphase regions of phase diagrams.

Note that the learning outcomes are based on course topics...notice the active verbs like: constructing, interpreting, performing.

Know how to perform equilibrium calculations, by:

¹ Several of these learning outcomes were adapted from Prof. Craig Carter's syllabus for 3.00 (MIT)

- determining equilibrium compositions in single and multiphase systems;
- evaluating equilibrium in systems where chemical reactions are occurring;
- performing calculations with FactSage software.

In addition, you will have increased confidence in your ability to:

- explain scientific concepts and ideas orally, and
- prepare and orally present original results and analyses

Note that the L.O.s relate to knowledge, skills, and abilities.

Required Text

Thermodynamics in Material Science, 2nd Edition Robert DeHoff, Taylor & Francis Publishers

Recommended Text

Thermodynamics and an Introduction to Thermostatistics, 2nd Edition Herbert B. Callen, Wiley

We will use parts of this book in the early stages of the course. However, there is *really no need for you to purchase this text*, however - I will provide copies/access to the I will provide copies/access to the relevant material through hard-copies or the course website.

If a text will only be used occasionally, or for a small part of the course – consider putting it on reserve at the Library, or making copies available to borrow.

Course Components *Problem Sets*

I think it's important to explain your reasons for including various course components, especially assignments and assessments). This is even more important for non-standard components.

As in most engineering classes – the problems sets will give you the opportunity to apply what we have been discussing each week in class. You should make notes of areas/topics/problems that give you particular difficulty, and make sure to speak to me or your peers about them.

Pre-Class Assignments

These assignments are intended to help you identify topics and concepts that you find particularly interesting, confusing, surprising, etc.

They are also meant to be a way to "jumpstart" each class period – so that we can begin with more interesting material, and in general, at a "higher level" than if you had come to class having not engaged with the pre-class assignment, and the associated readings.

The assignments themselves are definitely *not meant as a way for me to evaluate you*. I will, of course know whether you have or have not completed the assignment - based on your comments and participation in class – but I will not be "grading" the assignments themselves, in the traditional sense. Just as the questions are meant to *help you measure your level of understanding* – they are also a means for *me to measure your level of understanding* so that I can help you build that understanding if necessary.

Set the exam and due dates before the first class meeting. Students will be juggling multiple classes with multiples due dates. It also helps prevent students from missing exams (and saves you the agony of writing make-ups.)

Exam 1 (oral)

14 October (Wednesday)

Being able to think, clearly and logically under pressure is an important skill for an engineer. This oral exam will give you the opportunity to demonstrate your understanding of course material by answering a few short questions orally in a 1-on-1 setting. I will provide info on the format, and on how to prep for this oral exam during the first few weeks of the semester. I will provide info on the format, and on how to prep for this oral exam during the first few weeks of the semester.

Exam 2 (written)
13 November (Friday)

Note that I've tried to link the assignments with the learning outcomes.

Project

For the course project you will utilize FactSage software to perform chemical equilibrium calculations on a complex system of your choosing. You will prepare a written report of your findings, and present those findings orally during finals period. Detailed information on the project will be provided later in the semester

Grading

Exam #1 (oral) 25%
Exam #2 (written) 25%
Problem Sets & In Class Problems/participation 20%
Project (written and oral components) 30%

Course Outline

This is a general outline - a more detailed description for each of the 3 main sections will be provided during the semester;

- I. The General Structure of Thermodynamics
 - I.1 Fundamental Equations (EN72 refresher)
 - I.2 Equilibrium
 - I.3 Alternate Thermodynamic Formulations
- II. Thermodynamics of Materials
 - **II.1** One Component Systems
 - II.2 Multicomponent, Single Phase Systems
 - II.3 Multiphase Equilibrium
 - **II.4 Chemically Reacting Systems**
- III. Complex Systems

FactSage Software – Dr. Besmann (week of Nov. 15, with extra class meetings) Class Project – Written Report and Oral Presentations

I *always* create very detailed lecture schedules as the course progresses.

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5.95J Teaching College-Level Science and Engineering Fall 2015

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