Thermodynamics of Materials

3.00 Fall 2000

Department of Materials Science and Engineering
Massachusetts Institute of Technology
77 Massachusetts Institute of Technology
Cambridge, MA 02139

1 Course Description

Thermodynamics of Materials, MIT 3.00, is designed as course that will give students a necessary foundation for a comprehensive understanding of materials science and engineering. As virtually every subsequent materials science course has a working knowledge of thermodynamics and its applications as a prerequisite, this course must be structured so that each student can obtain this necessary foundation if they apply themselves to its study.

There are three major aspects to this course.

1.1 Understanding of Thermodynamic Principles

Thermodynamics as an isolated discipline is an abstraction of natural processes and equilibrium states that follow from a few postulates that are un-controverted by physical observation. Without application, thermodynamics can be developed as a mathematical deduction of these few postulates and subsequently used to derive profound statements about probable and improbable natural processes.

Because materials scientists and engineers should be expected to apply thermodynamics to systems and processes for which rote formulations have not been developed, the development of this philosophical approach to thermodynamics is necessary for a solid foundation.

1.2 Applications of Thermodynamic Principles to Material Properties

A materials science and engineering student with a sufficient background in thermodynamics should be able to apply thermodynamic reasoning and mathematics to materials problems of interest. This requires that a student should be able to accurately manipulate the mathematics of thermodynamics to derive symbolic representations of material behavior and equilibrium as well as utilize thermodynamic data to calculate corporeal numbers. As described below, there are a set of canonical examples of materials applications of thermodynamics that are traditionally considered to be endemic to materials science—a student should have working familiarity with the canonical examples.

1.3 Articulation and Communication of Thermodynamic Reasoning

A particular utility and germane topic of materials thermodynamics is as a vehicle for the efficient communication of complex concepts and the effective refutation of meretricious assertion. Students should be able to communicate thermodynamic reasoning by composition and public discourse.

2 Course Objectives

A broad objective is that the students should have a working familiarity with each of the topics provided in the Syllabus.

The following objectives are more specific and separated into three tables that should be compared to the aspects in Sections 1.1, 1.2, and 1.3.

2.1 Thermodynamic Principles

Educational Objectives *Understanding Thermodynamic Principles*		
Objective		Specific Examples
P-I	Understanding the first law of thermodynamics.	Recognizing the difference between state functions like the internal energy and path-dependent quantities like work and heat. Understanding that work and heat represent forms of energy transfer, and that the effect on the state of body depends only on the sum of work and heat transfered. Recognition and distinction the different means that a solid can store internal energy. Understanding the concept of reversibility or quasi-static processes. Recognizing and understanding of different types of thermodynamic systems and processes.
P-II	Understanding the second law of thermodynamics.	Understanding that entropy is a state function. Understanding the conditions and processes by which entropy of a system can change. Recognition that entropy of the universe increases in spontaneous processes. Understanding that maximization of entropy of an isolated system; or, equivalently, the minimization of internal energy in a quasi-static adiabatic system leads to a definition of equilibrium.
P-III	Understanding the uses of auxiliary thermodynamic functions.	Understanding of how to construct an energy function that is minimal at equilibrium for a given set of constraints. Understanding of the mathematical relations that follow from the definitions of the auxiliary functions. Understanding that an appropriate thermodynamic potential is uniform in a system at equilibrium.
P-IV	Understanding the distinction between thermodynamic requirements and material properties.	Understand the difference between thermodynamic relationships, models for material behavior, and the idealization of models as approximations to real materials.
P-V	Understanding the construction of a phase diagram.	Understanding relation between molar free energy curves of solutions, common tangents and phase diagrams. Understanding the meaning of multiphase equilibrium portions of a phase diagram and how the Gibbs phase rule applies to them. Understanding how the lever rule is applied and the compositions of multiples phases in equilibrium. Understand relation between stability and curvature of a molar free energy of solution.
P-VI	Understanding the microscopic origins of thermodynamic quantities.	Understanding of relation of entropy to the number of accessible states. Understanding of the relation of the partition function to the probability of finding a system in a particular state.

2.2 Thermodynamic Applications

Educational Objectives *Application of Materials Thermodynamics*		
Objective		Specific Examples
A-I	Conversion of work to heat	Calculate rise in temperature in system with known materials properties. Calculate states of materials systems for specific processes. Integrate temperature dependent heat capacities.
A-II	Entropy calculations	Calculate the change in entropy in systems for specific materials systems and processes. Calculate entropy changes for phase changes near equilibrium temperatures.
A-III	Entropy calculations	Calculate the change in entropy in systems for specific materials systems and processes. Calculate entropy changes for phase changes near equilibrium temperatures.
A-IV	Stored energy calculations	Calculate stored energy is elastic systems. Calculate stored energy is polarizable media. Calculate stored energy is magnetic media. Calculate stored energy is electrochemical systems.
A-V	Equilibrium Calculations	Calculate constraints of the relations between material properties of homogeneous materials at equilibrium. Calculate the conditions and restrictions of equilibrium for single phase systems. Apply the chemical potential equality to systems of chemical equilibrium. Calculations of equilibrium from equilibrium constant expressions. Calculate equilibrium partial pressures of gas phases in equilibrium with solids. Apply the Gibbs phase rule. Apply and calculate potentials from the Nernst equation.
A-VI	Geometric constructions	Construct and apply common tangents. Apply constructions to obtain the chemical potential of species in solution. Apply and calculate phase fractions according to the lever rule. Apply and calculate wetting angles from Young's equation.

2.3 Thermodynamic Articulation

Educational Objectives

Articulation of Thermodynamic Concepts

Objective		Specific Examples
C-I	The production of concise and accurate written statements about materials thermodynamics.	Ability to write a concise, true statement using thermodynamic language.
C-II	Demonstrated ability to verbally communicate thermodynamic ideas	Construct a well-thought-out question about thermodynamic behavior. Answer a question with confidence and accuracy.

3 Assessment Criteria

The nature of this course as a fundamental prerequisite lends itself to a two-step assessment process.

The first is to assess whether the students have successfully mastered the syllabus. As described below, this assessment will include traditional methods of examination and graded problem sets, and also direct assessment through class participation.

The second assessment determines whether the student has gained sufficient thermodynamic fundamentals to proceed in her upper division courses. This requires self-evaluation questionnaires of fourth-year students.

3.1 Concurrent

In class participation in the form of random “cold calls” will take place about three times per lecture. Students’ responses will be recorded and will form approximately 1/5 of their final grade. Cold calls will test thermodynamic concepts and will allow the instructor to gauge his effectiveness immediately. Students also receive credit towards their grade by volunteering an excellent comment or a particularly clarifying question. This assessment method is consistent with the goals stated in sections 2.1 and 2.3.

Homeworks will be given out every week and graded. These grades will constitute about 1/5 of the grade. Homework questions are constructed to test and hone the students’ skills of manipulating thermodynamic relations, calculating real numbers, and performing geometric constructions. This assessment method is consistent with the goals stated in sections 2.2. Students are encouraged to work in groups and an entire group can receive credit for joint submission of a single assignment. Group cooperation is consistent with goals stated in section 2.3.

Three exams will be given. Questions on the exams will test the students familiarity with thermodynamic principles as they apply to materials. Answers on the exams will typically require concise descriptions or thermodynamic refutation of practical problems. Exams will test understanding of principles and communication of their understanding rather than computational applications.

3.2 Subsequent

The true assessment of a fundamental prerequisite course is a determination whether it achieved its goals of preparing the student for advanced study. This may only be ascertained after sufficient time has passed.

Students in DMSE will be given a questionnaire at the end of their first semester of their fourth year. This evaluation method will commence in December, 2002.

The questionnaire will be as follows:

Course 3 Senior Questionnaire on Thermodynamics of Materials		
	Yes	No, because...
Did your course in thermodynamics (3.00) give you an appropriate preparation for your upper division courses in course 3?		
Do you understand where phase diagrams come from and how to read them?		
To you understand the difference between thermodynamic driving forces and kinetic processes?		
Do you feel that you have developed an ability to use thermodynamics to "think on your feet" when discussing topics about materials phenomena?		
Do you understand how to use thermodynamic constructions to answer practical problems (i.e., common tangent construction, lever rule, chemical potential by intercept)		