

MATSE 401: THERMODYNAMICS OF MATERIALS

Course Designation: MatSE401; a required junior-level undergraduate course for students in Ceramic Science and Engineering and Metals Science and Engineering, and an elective course for the Polymer Science option.

Catalog Description: Discussion of three fundamental laws of thermodynamics and their applications to materials systems, particularly phase transformations and phase equilibria in single and binary systems.

Course Description: The course starts with the first law of thermodynamics and its applications to the calculations of heat involved in various materials processes such as chemical reactions and phase transformations. Second law of thermodynamics and the concept of entropy are then introduced. The application of maximum work theorem to engine efficiency is briefly discussed. Various thermodynamic potentials are defined to determine the equilibrium of a system under various thermodynamic conditions, with an emphasis on the Gibbs free energy functions at constant temperature and pressure conditions. The relationships among thermodynamic properties are derived using the Maxwell relations. Phase diagrams of single-component systems are constructed from the Gibbs free energy function, and the Clapeyron equation is applied to describe the phase boundaries. Applications of thermodynamics to the determination of chemical equilibrium and to the calculation of the voltages of electrochemical reactions are also discussed. The last part of the course is focused on the solution thermodynamics and its application to binary phase-diagrams.

Prerequisites: Chem 15

Textbook: David V. Ragone, Thermodynamics of Materials, Volume I, J. W. Wiley 1995

Course Objectives:

1. To provide students with an elementary understanding of three laws of thermodynamics, and their applications as well as limitations.
2. To teach students to perform simple thermodynamic calculations for basic materials processes such as chemical reactions and phase transformations and the concept of thermodynamic equilibrium.
3. To provide a student the ability to determine the possibility or impossibility that a given thermodynamic process will take place under certain thermodynamic conditions.
4. To teach students how to understand relations between free energies and single-component and binary phase diagrams.

Topics Covered

1. Introduction to classical equilibrium thermodynamics and its relation to non-equilibrium thermodynamics and statistical thermodynamics.
2. First law of thermodynamics and its applications to constant pressure processes: calculation of enthalpy as a function of temperature; calculation of heat of reactions including chemical reactions and first-order phase transformations such as melting and solidification; calculation of adiabatic flame temperature.
3. Second law of thermodynamics and introduction of entropy: reversible processes and maximum work theorem. Carnot cycles and engine efficiencies.
4. Third law of thermodynamics; calculation of entropy.
5. Combined first and second law of thermodynamics; equilibrium conditions; introduction of Helmholtz and Gibbs free energy functions.
6. Relation of thermal properties; Maxwell relations and property relationship.
7. Introduction of chemical potential and phase equilibria in one component systems; pressure-temperature phase diagrams of single-component systems; Clapeyron equation.
8. Equilibrium of chemical reactions: definition of standard states; gas reactions; gas-solid reactions; oxidation reactions and the Ellingham diagram.
9. Solution thermodynamics: activity and activity coefficient; free energy of formation of solutions; chemical potentials of species in a binary system; Gibbs-Duhem relation.
10. Relation between free energies and phase equilibria in binary systems; binary phase diagrams; Level rule and Gibbs phase rule.
11. Electrochemistry: half-cell reactions; cell voltage; concentration cells.

Class Schedule: 3 credit course offered annually and meeting 3 times per week for 50 minutes

Course Outcomes:

1. Given the data on standard enthalpies and heat capacities, a student should be able to perform simple thermodynamic calculations such as heat of chemical reactions and phase transformations.
2. With available thermodynamic data from tables, a student should be able to calculate the free energy of chemical reactions and phase transformations and able to determine whether a phase transformation or chemical reaction is thermodynamically possible.
3. With an Ellingham diagram, a student should be able to determine whether oxidation or reduction reactions will take place at a given temperature and oxygen partial pressure.
4. With a pressure-temperature phase diagram, a student should be able to determine which phase is thermodynamically stable at a given temperature and pressure and whether the volume change is positive or negative across the phase boundaries.
5. A student should be able to calculate simple binary phase diagrams using simple models.
6. With a binary phase diagram, a student should be able to determine the equilibrium phases, their compositions and volume fractions, as well as heating and cooling curves.
7. A student should be able to write simple half-cell reactions and calculate cell voltages of electrochemical cells based on the free energy of reactions.

Assessment Tools:

1. Two mid-term evening exams and one final exam.
2. Homework problem sets and in-class quizzes.

Professional Component:

This course addresses the scientific and engineering principles regarding to the relationship between materials chemistry and microstructure, and the design of materials processes.

Prepared by: L. Q. Chen, March 2002

MAP TO DEPARTMENTAL OUTCOMES (For further detail, see coursebook)											
a	b	c	d	e	f	g	h	i	j	k	l
1	2	1	3	1	2	3	2	2	1	1	1

MAP TO DEPARTMENTAL OBJECTIVES (For further detail, see coursebook)						
(1)	(2)	(3)	(4)	(5)	(6)	(7)
2,3,4	1,2,3,4			2,3,4		