MSE 3001: Chemical Thermodynamics of Materials

Credit hours and contact hours: 3-0-0-3

Instructor: Robert Speyer

Textbook: No textbook used. Instructor notes used.

Specific course information

Catalog description: Principles and applications of thermodynamics to materials science and engineering. Phase equilibria and the concepts necessary to interpret phase diagrams.

Prerequisites: MSE 2001 - Principles &Applications of Engineering Materials and Math 2403/2552 - Differential Equations or MATH 2602 - Linear and Discrete Math

Course: Required

Specific goals for the course

Outcomes of instruction:

Outcome 1: The student will develop a fundamental understanding of the properties of gases, and the first and second laws of thermodynamics.

1.1 The student will demonstrate an understanding of how gases exert pressure; have an energy, and the causes of deviation from ideal behavior.
1.2 The student will demonstrate an understanding of heat, work, and reversibility.
1.3 The student will demonstrate an understanding of a Carnot cycle, encompassing isothermal and adiabatic processes, and how through the concept of efficiency, the Clausius inequality is developed.
1.4 The student will be able to derive Maxwell relations from definitions of Gibbs and Helmholtz energies and enthalpies, and to apply them to practical applications in Debye heat capacity theory and isoenthalpic throttling to form cryogenic fluids.
1.5 The student will demonstrate an understanding of the competition between energy and entropy in the Areas of vacancy formation, aqueous dissolution, and equilibrium vapor pressure.

Outcome 2: The student will be able to apply thermodynamic fundamentals to phase and reaction equilibria.

2.1 The student will demonstrate an understanding of the merits of auxiliary functions and intensive variables in predicting equilibrium under varying experimental conditions.

2.2 The student will demonstrate an understanding of how equality of the chemical potential can be used as the basis for developing coexistence curves in unary phase equilibria.
2.3 The student will demonstrate an ability to translate and manipulate tabulated thermodynamic data.
2.4 The student will be able to calculate adiabatic flame temperatures, and equilibrium constants for reactions among gases, and between gases and pure condensed phases.
2.5 The student will demonstrate knowledge of industrial processes such as extractive metallurgy, the operation of a blast furnace, a basic oxygen furnace, and matt smelting. The the student will be able to derive the Gibbs-Helmholtz relation and correlate it to LeChatlier's principle.
2.6 The student will demonstrate an understanding of solution theory, vapor pressure measurements, and manipulations using the Gibbs-Duhem relation.
2.7 The student will be able to calculate binary phase diagrams of fully miscible solid and liquids from solution theory.
2.8 The student will understand fractional distillation and crystallization.
2.9 The student will be able to apply regular solution theory to explain more complex binary phase diagrams.
2.10 The student will be able to derive the phase rule and apply it to all concepts developed in the course.
2.11 The student will be able to read and interpret binary and ternary phase diagrams, both with and without solid solution.

Student Outcomes:

(1) An ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics.

Topics covered:

1. Empirical properties of gases – Molecular view, energy and velocity, real versus ideal gases.
2. The first law of thermodynamics – Temperature, work, and heat. Reversibility, special conditions, constant volume/pressure heat capacities.
3. The second law of thermodynamics – Carnot engine and the Clausius inequality. Entropy and statistical thermodynamics, configurational and thermal entropy.
4. Auxiliary functions – Combined first and second laws, Maxwell relations and examples: Debye heat capacity, forming cryogenic fluids. Competing entropic and energetic forces: vapor pressure, vacancy formation, aqueous solutions.
5. Chemical thermodynamics – Equilibrium indicated by intensive and extensive functions. Clapeyron equation and unary phase equilibria. LeChatelier's principle.
6. Temperature dependence of thermodynamic functions – Sensible and latent heats. The third law and using tabulated thermodynamic data. Experimental calormetric methods.
7. Reaction equilibria – Combustion and adiabatic flame temperatures. Standard Gibbs energy of reaction and gaseous equilibria. Condensed phase equilibria with gases and the reduction of metals. Extractive metallurgy. Gibbs-Helmholtz relation.

8. Solutions – Raoult's and Henry's laws. Vapor pressure measurement. Gibbs energy of mixing and integration of the Gibbs-Duhem relation.
9. Binary phase equilibria – Fully miscible solids and liquids. Refining and fractional crystallization. Regular solutions and intermediate compounds.
10. The phase rule – Foundations and applications to unary equilibria, reaction equilibria, and binary phase equilibria.
11. Ternary phase equilibria – Phase rule analysis with pure solids; the CaO-Al_2O_3-SiO_2 system. Solid solutions.

Correlation between Outcomes of Instruction and Student Outcomes:

Outcomes of Instruction	Student Outcomes						
	1	**2**	**3**	**4**	**5**	**6**	**7**
1.1 The student will demonstrate an understanding of how gases exert pressure; have an energy, and the causes of deviation from ideal behavior.	X						
1.2 The student will demonstrate an understanding of heat, work, and reversibility.	X						
1.3 The student will demonstrate an understanding of a Carnot cycle, encompassing isothermal and adiabatic processes, and how through the concept of efficiency, the Clausius inequality is developed.	X						
1.4 The student will be able to derive Maxwell relations from definitions of Gibbs and Helmholtz energies and enthalpies, and to apply them to practical applications in Debye heat capacity theory and isoenthalpic throttling to form cryogenic fluids.	X						
1.5 The student will demonstrate an understanding of the competition between energy and entropy in the Areas of vacancy formation, aqueous dissolution, and equilibrium vapor pressure.	X						
2.1 The student will demonstrate an understanding of the merits of auxiliary functions and intensive variables in predicting equilibrium under varying experimental conditions.	X						
2.2 The student will demonstrate an understanding of how equality of the chemical potential can be used as the basis for developing coexistence curves in unary phase equilibria.	X						
2.3 The student will demonstrate an ability to translate and manipulate tabulated thermodynamic data.	X						
2.4 The student will be able to calculate adiabatic flame temperatures, and equilibrium constants for	X						

reactions among gases, and between gases and pure condensed phases.							
2.5 The student will demonstrate knowledge of industrial processes such as extractive metallurgy, the operation of a blast furnace, a basic oxygen furnace, and matt smelting. The the student will be able to derive the Gibbs-Helmholtz relation and correlate it to LeChatlier's principle.	X						
2.6 The student will demonstrate an understanding of solution theory, vapor pressure measurements, and manipulations using the Gibbs-Duhem relation.	X						
2.7 The student will be able to calculate binary phase diagrams of fully miscible solid and liquids from solution theory.	X						
2.8 The student will understand fractional distillation and crystallization.	X						
2.9 The student will be able to apply regular solution theory to explain more complex binary phase diagrams.	X						
2.10 The student will be able to derive the phase rule and apply it to all concepts developed in the course.	X						
2.11 The student will be able to read and interpret binary and ternary phase diagrams, both with and without solid solution.	X						

School of Materials Science and Engineering Student Outcomes:

(1) An ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics.
(2) An ability to apply engineering design to produce solutions that meet specified needs with consideration for public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors.
(3) An ability to communicate effectively with a range of audiences.
(4) An ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts.
(5) An ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.
(6) An ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions.
(7) An ability to acquire and apply new knowledge as needed, using appropriate learning strategies.