MSE 623 - Thermodynamics of Solids
Fall 2000

Proposed Course Content

TEXT: "Thermodynamics in Materials Science" by Robert DeHoff

The goal of this course is to teach basic materials science thermodynamics. It is also designed to prepare students to take advanced coursework in areas such as phase transformations, surface science, crystallography, and electrochemistry. The content is designed to teach the material at a level for understanding free energy curves, phase diagrams, Ellingham diagrams and Pourbaix diagrams, all based on activities and chemical potential. Emphasis will be on developing thermodynamics as a tool to help guide research and teaming in a variety of areas. Some numerical techniques will be introduced and coordinated with William Johnson (e.g., calculation of phase diagrams).

1 Lecture:

1. Structure of Thermodynamics (classification of thermodynamic systems, variables: state functions, process variables, extensive and intensive properties)
2. Laws of Thermodynamics

3 Lectures:

3. General Strategy for Deriving Thermodynamic Relations (entropy and volume relations to T and P; energy functions expressed in terms of T and P; a general procedure for deriving relations applied to ideal gas, solids and liquids).

3 Lectures:

4. Equilibrium in Thermodynamic Systems (formulation of general criterion for equilibrium; mathematical formulation of general criterion for equilibrium; application to finding equilibrium in a unary two phase system)

2 Lectures:

5. Unary Heterogeneous Systems (structure of unary phase diagram in (P,T) space; chemical potential and Gibbs free energy; chemical potential surfaces; Clausius-Clapeyron equation)

3 Lectures:

6. Multicomponent, Homogeneous Nonreacting Systems: Solutions (partial molar properties; chemical potential in multi-component systems; fugacities, activities, and activity coefficients, behavior of dilute solutions, solution models: ideal, regular, atomistic models/quasi-chemical)

4 Lectures:

7. Multicomponent Heterogeneous Systems (conditions for equilibrium; Gibbs phase rule; the structure of phase diagrams; interpretation of phase diagrams; application of phase diagrams in materials science; introduction to Thermo-Calc version of CALPHAD)

3 Lectures:

8. Thermodynamics of Phase Diagrams (free energy-composition (G-x) diagrams; models for binary phase diagrams: ideal & regular solution)

3 Lectures:

9. Multicomponent, Multiphase Reacting Systems (reactions in the gas phase; reactions in multiphase systems; Richardson-Ellingham diagrams for oxidation; predominance diagrams and multivariant equilibria: Pourbaix high temperature oxidation diagrams)

2 Lectures:

10. Electrochemistry (equilibrium within an electrolyte solution; equilibrium in two phase system involving an electrolyte; equilibrium in an electrochemical cell; Pourbaix diagrams)

3 Lectures:

11. Surfaces and Curvature (geometry of surfaces; surface excess properties; equilibrium in systems with curved surfaces; surface tension; capillarity effects on phase diagrams; Gibbs-Wulff construction; adsorption at surfaces)