**Thermodynamics of Solids (~20 h)**

Prof. Sean Li

School of Materials Science and Engineering

The University of New South Wales, Australia

<http://www.materials.unsw.edu.au/profile/sean-li>

This is an advanced course built on the knowledge gained in the introductory classes in Thermodynamics & Phase Transformations. This course is designed for senior year students and aims to provide an in-depth understanding on the principles of thermodynamics of solids and its applications to production of inorganic materials, selection of materials for hostile environments, adsorption and chemisorption processes, energy conversion devices, surfaces and interfaces, defects in solids, reaction kinetics, phase equilibria and phase transformations etc.

On completion of this course the student should be able to:

1. Understand the use of the Ellingham and Pourbaix–Ellingham diagrams for the production of inorganic materials in various atmospheres and pressures.

2. Understand the use of the Ellingham and Pourbaix – Ellingham diagram for the selection and application of materials in high temperature, hostile and corrosive environments.

3. Understand the thermodynamics of adsorption on surfaces and interfaces.

4. Understand the application of thermodynamics to energy conversion devices such as fuel cells, heat pumps, heat pipes, batteries, solar cells etc.

5. Understand the application of thermodynamics to defects, phase equilibria, phase diagrams, and phase transformations in metals in metallic and non metallic systems.

6. Understand the concepts of nonequilibrium thermodynamics and its implications

**Laws of Thermodynamics and Equilibrium**

Introduction, The first law of thermodynamics (System and Surroundings, Heat and Work, Reversibility, Internal Energy, State Functions, The First Law, Enthalpy, Intensive and Extensive, Properties and Notation, Heat Capacities, Ideal Gas, Enthalpy of Formation), Entropy and the Second Law (Entropy not Conserved, Entropy Changes, Entropy Changes in Chemical Reaction and the Third Law), Property Relations (Free Energies, Maxwell Relations, Chemical Potentials, Partial Molar Quantities, Other Definitions), Equilibrium, Thermodynamic Activities, Chemical Equilibrium

**Diffusion**

Atomic Mechanisms of Diffusion, Interstitial Diffusion (Interstitial Diffusion as a Random Jump Process, Effect of Temperature – Thermal Activation, Steady – State Diffusion, Nonsteady - State Diffusion, Solution to the Diffusion Equation), Substitutionally Diffusion (Self- Diffusion, Vacancy Diffusion, Diffusion in Substitutional Alloys, Diffusion in Dilute Substitutional Alloys), Atomic Mobility, High Diffusivity Paths (Diffusion along Grain Boundaries and Free Surface, Diffusion along Dislocations)

**Surfaces and Interfaces**

Interfacial Free Energy, Solid/Vapour Interfaces, Boundaries in Single-Phase Solids (Low-Angle and High Angle Boundaries, Special High-Angle Grain Boundaries, Equilibrium in Polycrystalline Boundaries, Thermally Activated Migration of Grain Boundaries, The kinetics of Grain Growth), Interphase Interfaces in Solids: (1) Interface Coherence (Fully Coherent Interface, Semicoherent Interfaces, Incoherent Interfaces, Complex Semicoherent Interfaces), (2) Interphase Interfaces in Solids (Fully Coherent Precipitates, Partially Coherent Precipitates, In coherent Precipitates, Precipitates on Grain Boundaries), (3) Second-Phase shape: Misfit Strain Effects (Fully Coherent Precipitates, Incoherent Loss, Plate-like Precipitates, Coherency Loss, Solid/Liquid Interfaces), (4) Interface Migration (Diffusion-Controlled and Interface-Controlled Growth)

**Solidification**

Nucleation Pure Metals (Homogeneous Nucleation, the Homogeneous Nucleation Rate, Heterogeneous Nucleation, Nucleation of Melting, Growth of a Pure Solid: (1) Continuous Growth, (2) Lateral Growth (Surface Nucleation, Spiral Growth, Growth from Twin Intersections), Heat Flow and Interface Stability

**Defects in Solids**

Structural Point Defects in Elemental Crystals, Vacancies: Experimental Verification, Interactions between Vacancies and Impurities, Interaction between Imperfections and Impurities, Electronic Defects, Defects in Ionic Compounds, Frankle Defects, Schottky-Wagner Defects, Interactions Among Defects, Intrinsic and Extrinsic Defects in Ionic Crystals, Experimental Determination of Defect Type, Nonstochiometry