COMMONWEALTH GRADUATE ENGINEERING PROGRAM
DISTANCE LEARNING COURSE PLANNING SHEET
UNIVERSITY OF VIRGINIA

Course MSE 623 – Thermodynamics of Materials Semester Fall 2006

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Textbook(s): (Student to purchase)

Thermodynamics in Materials Science, Second Edition

Robert DeHoff *University of Florida, Gainesville, USA*

List Price: $99.95
Cat. #: 4065
ISBN: 0849340659
Publication Date: 3/13/2006
Number of Pages: 624

Reference(s): Limit 4

none

Computer Needs:

Computer Capability _____

Software required? some version of matlab/mathematica/mathcad/etc Provided? no

Other _____

Attached are course syllabus and biographical sketch.

MSE 623 -Thermodynamics of Solids
Fall 2006

Proposed Course Content

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 selected 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 **understanding** and developing thermodynamics as a tool to help guide research and teaming in a variety of areas.

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)

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Dr. Shiflet has been a faculty member in SEAS since 1980. He has published 130+ papers in archival journals and an additional 60+ in conference proceedings. He holds six patents for alloy design, including several dealing with glassy metals. He has been awarded two creativity awards from the National Science Foundation, the ASM Research Award and has been elected as a Fellow of the American Society for Materials and the Japan Advancement of Science. He is a member of The Metallurgical Society of AIME and the American Society for Materials.

Research Interests: Dr. Shiflet's primary interests are in solid-state phase transformations of metal alloys. His research concerns thermodynamics, nucleation and the kinetics associated with growth of new phases. His work is sponsored by the National Science Foundation, Department of Energy, NASA and the Department of Defense.