**Name of the module:** Themodynamics 2

**Number of module: 365-1-2121**

BGU Credits: 4

ECTS credits: 6

Academic year: 2013- 2014

Semester: Fall

Hours of instruction: 3 lecture hours + 1exercise class hour per week

Location of instruction: room

bulding

Language of instruction: Hebrew

Cycle: First cycle

Position: a mandatory module for 2nd year undergraduate students in the Department of Materials Engineering to be taken on Fall semester

Field of Education: Materials Engineering

Responsible department: Materials Engineering

General prerequisites: students should complete modules mathematical analysis. Highly recommended thermodynamics 1

Grading scale: the grading scale would be determined on a scale of 0 – 100 (0 would indicate failure and 100 complete success 0 to 100), passing grade is 56*.*

Lecturer: Prof. Roni Shneck

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Office hours: Tuesday, from 11 to 13AM.

Module evaluation: at the end of the semester the students will evaluate the module, in order to draw conclusions, and for the university's internal needs.

Course Description

A course on three applications of classical thermodynamics in materials science and engineering: theory of solutions, phase diagrams and chemical reactions.

We begin with the definition of two new thermodynamic potentials – the free energies of Helmholtz and Gibbs. We show that the free energy of closed systems decreases toward a minimum in natural isothermal isochoric or isobaric processes respectively. We demonstrate that the use of the new potentials is more convenient than using the statement of the second law that the entropy of the universe increases.

The Gibbs free energy is used to explain and predict the shape of the phase diagram of pure materials and to derive the Clausius-Clapeyron equation of the equilibrium boundary lines between phases.

The main part of the course is devoted to the theory of solutions. Partial thermodynamic properties of the individual constituents of a solution and the activity are defined. Their variation with the composition in solution of attracting and of repealing constituents is learnt, including the Henri and Raoult laws. The inter-relations between partial properties and properties of the whole solution are studied, the Gibbs-Duhem equation, the tangent construction and the weighted average sum of partial quantities. The approximation of the excess properties or the activity coefficient by Margules series is used to derive the properties of regular solutions as the simplest extension beyond ideal solutions.

The model of regular solution is used to introduce eutectic binary phase diagrams and the conditions for phase separation in a system of repealing constituents. It is shown that the minimum free energy of the whole system that contains multiple phases coincides with the state of equal partial free energy of each component in each phase. Derivation of different binary phase diagrams by minimizing the free energy of mixing of solutions by the common tangent construction is learnt and used to classify phase diagrams according to the type of relations between the constituents.

The central role of thermodynamics in understanding and controlling chemical reactions is studied in the last part of the course. Like any system, all chemical reactions tend to equilibrium. The condition for equilibrium is the equality of the sum of free energies of the products and the energy of the reactants. It is shown to be identical to the state of minimum of the total free energy. This is a required extension of the conditions of equilibrium between phases, learnt in the previous chapter. These conditions are generalized to establish the Gibbs phase rule that determines the number of degrees of freedom available to maintain a set of reacting phases at equilibrium. It is shown that the free energy difference of the reaction determines the composition of the system at equilibrium by the equilibrium constant and is a measure of the driving force of the reaction.

Confirmation: the syllabus was confirmed by the faculty academic advisory committee to be valid on 2013-2014.

Last update:

The effect of pressure, temperature and initial composition on the yield of the reaction is an outcome of the equilibrium conditions and can be qualitatively deduced from Le-Chatelier's principle. Three type of reaction are discussed: (a) Reactions between gases and pure solids, which are applied for extractions of pure elements from ores and for protecting metals from oxidation, (b) Reactions with more degrees of freedom, involving condensed-phase solutions and (c) reactions between gases with maximum degrees of freedom.

Objectives 1. Learn the skills for thermodynamic analysis of phase diagrams, properties of solutions and chemical reactions. 2. Gain the knowledge to calculate equilibrium compositions of multiphase systems and chemical reaction. 3. Understand tendencies and effect of external variables on processes in materials Aims Develop understanding of the conditions for equilibrium in multiphase systems and chemical reactions, the role of external variables (the phase rule) and internal properties and understand the role of thermodynamics in processes in materials.

Learning outcomes of the module:

On successful completion of the course the students should

1. Knowledge of analyzing natural tendencies by the second law and by free energy approaches.
2. Read P-V-T phase diagrams of single components and T-X binary phase diagrams. Understand the meaning of phase equilibrium and tendencies upon deviation from equilibrium.
3. Understand the construction of unary and binary phase diagrams by minimization of the free energy including the common tangent construction.
4. Application of Clausius-Clapeyron equation to determine saturation vapor pressure and lines of phase equilibrium.
5. Definition of partial quantities, activity, activity coefficient and their variation with the composition of the solution.]
6. Knowledge of the properties of ideal, regular and general solutions.
7. Familiarity with the relations between partial properties and total properties of solutions, Gibbs-Duhem equation, tangent rule and weighted average of the partial quantities.
8. Understand and apply the conditions for equilibrium between phases in phase diagrams to determine their composition.
9. Understand and apply the conditions for equilibrium in chemical reactions to determine the equilibrium composition. Analyze the effect of external variables by the Le-Chatelier's principle.
10. Understand and apply the phase rule to determine the degrees of freedom in multiphase systems and the conditions required to maintain the phases at equilibrium. Understand the outcomes of deviations from equilibrium.

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Attendance regulation: attendance and participation in class is recommended.

Teaching arrangement and method of instruction: The module consists of lectures and exercises.

Assessment:

1. Exam 65% (or 85% for the student who has lower grade in the quiz)
2. Quiz 20% (not mandatory)
3. Homeworks 15%

100%

Work and assignments: Student will conduct 6 home works related to the exercises in the class.

Quiz: midterm, open questions.

Exam: at the end of semester, open questions.

Time required for individual work: in addition to attendance in class, the students are expected to do their assignment and individual work: at least two hours per week, 10 hours before the quiz and 24 hours before exam.

Module Content\ schedule and outlines:

Lectures:

Introduction to materials processing 2h

Extractive metallurgy of metals 5h

Extraction of Mg and Al by electrolysis 4h

Introduction to casting technologies 2h

Advantageous and disadvantageous of various casting technologies 4h

Defects originated from casting process 4h

Introduction to powder metallurgy 2h

Fabrication of metal and ceramic powders 2h

Compaction and shaping of powders 2h

Compaction and shaping of powders 2h

Sintering of metal and ceramic powders 2h

Cold working processes. Advantageous and disadvantageous 4h

The effect of cold working on mechanical and physical properties of metals 2h

Post deformation heat treatment (recovery, recrystallization and grain growth) 4h

Multistage cold working 2h

Module Content / schedule and outlines

Definition of the Helmholtz and Gibbs and free energies and their properties 4h

Phase diagram of a single component, derivation from the free energy, nature of equilibrium between vapor phase and condensed phase, triple and critical points on the phase diagram 5h

The Clausius-Clapeyron equation 2h

Equivalence of the entropy and free energy approaches 1h

*Theory of solutions*

Definition of partial quantities, activity and activity coefficient, ideal and real solutions, excess quantities 3h

Typical variation of the activity with composition, Henri and Raoult laws, relations with the energy of the whole solution 3h

The Gibbs Duhem equation, derivation of partial properties of one component from the properties of the other and from properties of the whole solution 3h

Margules series and properties of regular solutions, the microscopic quasi-chemical model of a regular solution 3h

The phase diagram of regular solutions, conditions for equilibrium of two multicomponent phases 3h

General binary phase diagrams, variation of activity with composition in multiphase systems 3h

*Chemical reactions*

Chemical reactions between gases 3h

Chemical reactions between gases and pure condensed phases 4h

Chemical reactions with solutions, the Gibbs phase rule 2h

Exercises:

Free energy changes in simple systems

Phase diagram of single component, Clausius-Clapeyron equation

Partial free energy, activity and activity coefficient.

Calculation of the activity of one component from the activity of the other

Properties of regular solutions

Binary phase diagrams, application of the equilibrium condition between phases

Chemical reactions between gases

Chemical reactions between gasesand condensed phases, the Gibbs phase rule

Chemical reactions with solutions.

Required reading:

1. D.R. Gaskell, Introduction to the thermodynamics of materials (formerly: Introduction to metallurgical thermodynamics) W[ashington, D.C. Taylor & Francis, c1995.](javascript:open_window(%22https://lib20.bgu.ac.il/F/PDXG3X8DEAKLFV2T8Q65AAD73LLJ2BSF2RGKLQ68NF5G6MPG1M-58387?func=service&doc_number=001409409&line_number=0014&service_type=TAG%22);) (TN 673.G33 1995) (TN 673.G33 1981)
2. Lecture notes (in Hebrew): (a) The thermodynamic potentials (b) Phase diagram of a single component (c) Solution theory (d) Binary phase diagrams (e) Chemical reactions (f) The phase rule.

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| Additional literature:   1. M. Hillert, [Phase equilibria, phase diagrams, and phase transformations :  their thermodynamic basis,](javascript:open_window(%22https://lib20.bgu.ac.il/F/PDXG3X8DEAKLFV2T8Q65AAD73LLJ2BSF2RGKLQ68NF5G6MPG1M-51810?func=service&doc_number=002088665&line_number=0008&service_type=TAG%22);)  [Cambridge University Press, 20](javascript:open_window(%22https://lib20.bgu.ac.il/F/PDXG3X8DEAKLFV2T8Q65AAD73LLJ2BSF2RGKLQ68NF5G6MPG1M-51811?func=service&doc_number=002088665&line_number=0010&service_type=TAG%22);)08 (QD 503.H554 2008)  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | | |  |  |  |  | | --- | --- | --- | --- | |  | 1. J. B. Hudson, [Thermodynamics of materials :  a classical and statistical synthesis](javascript:open_window(%22https://lib20.bgu.ac.il/F/PDXG3X8DEAKLFV2T8Q65AAD73LLJ2BSF2RGKLQ68NF5G6MPG1M-58365?func=service&doc_number=001337738&line_number=0009&service_type=TAG%22);) [New York : Wiley, C1996](javascript:open_window(%22https://lib20.bgu.ac.il/F/PDXG3X8DEAKLFV2T8Q65AAD73LLJ2BSF2RGKLQ68NF5G6MPG1M-58366?func=service&doc_number=001337738&line_number=0010&service_type=TAG%22);) (TA 418.52.H83 1996) 2. O. F. Devereu, Topics in metallurgical thermodynamics ,  [New York : Wiley, 1983](javascript:open_window(%22https://lib20.bgu.ac.il/F/PDXG3X8DEAKLFV2T8Q65AAD73LLJ2BSF2RGKLQ68NF5G6MPG1M-05639?func=service&doc_number=000025034&line_number=0009&service_type=TAG%22);) (TN 690.D47) |  | TA 418.52.H83 1996 | |  |  |  | [Hudson, John B.](javascript:open_window(%22https://lib20.bgu.ac.il/F/PDXG3X8DEAKLFV2T8Q65AAD73LLJ2BSF2RGKLQ68NF5G6MPG1M-58364?func=service&doc_number=001337738&line_number=0008&service_type=TAG%22);) | |  |  |  |  | |  |  |  | [New York : Wiley, C1996](javascript:open_window(%22https://lib20.bgu.ac.il/F/PDXG3X8DEAKLFV2T8Q65AAD73LLJ2BSF2RGKLQ68NF5G6MPG1M-58366?func=service&doc_number=001337738&line_number=0010&service_type=TAG%22);) | |  |  |  | xvii, 365 p. | |  |  |  | | | | |  |  | 2nd ed. |
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