**Name of the module: Calculations of phase diagrams**

**Number of module: 365-2-6191**

BGU Credits: 3

ECTS credits: 4

Academic year: 2013-2014

Semester: Autumn semester

Hours of instruction:3 hours per week

Location of instruction: will be defined

Language of instruction: Hebrew

Cycle: Second cycle

Position: An advanced course for graduate students in Materials Engineering Department

Field of Education: Materials Engineering: Modeling of thermodynamic functions that are necessary for the description of phase competition in materials, Computational methods used for construction of phase diagrams, analysis of the equilibrium states in binary and ternary solid solutions. Critical analysis of experimental data that is necessary to compute the binary phase diagrams.

Responsible department: Materials Engineering

General prerequisites: none

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 65.

Lecturer: Prof. David Fuks

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Office hours:

Monday, from 9 to 11 AM

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:

The course is devoted to advanced description of phase diagrams for binary and ternary systems, modeling of thermodynamic functions to describe the phase competition in solid solutions. In the framework of the course the students will learn the different physical models and their application to the study of phase equilibrium as well as approximations used in definition of important thermodynamic functions for solids.

The first part of the course is related to definition of thermodynamic parameters and functions that are important in analysis of the phase competition in mono-component materials, and application to the analysis of the phase equilibrium in such systems. The links of thermodynamic and elastic properties of solids are also considered.

The second part describes the different types of binary phase diagrams and the analytical models that are used to approximate the temperature and composition dependence of the corresponding free energies. The ways to link these functions to the available experimental data are also discussed.

The third part is devoted to determination of the competition of phases in ternary solid solutions and describes the link of stability of binary alloys with the equilibrium states in ternary systems. The specific features of the topology of ternary phase diagrams are discussed.

In all parts of the course the results of the theory and the experimental data on the phase diagrams for concrete binary and ternary systems are discussed.

Aims of the module:

To introduce students to the main principles of the computer calculations of phase diagrams for mono-atomic materials and binary and ternary alloys. To provide a general explanation of the differences in construction the phase diagram and the main data that may be accessed from the diagrams.

Students will learn the mandatory fundamental aspects of the modeling of thermodynamic functions to analysis of phase competition in materials. The course will focus also on the link of available experimental data with the parameters of the functions to reproduce the phase stability, mixing, and decomposition on the phase diagrams.

Objectives of the module:

Students would understand the ways of modeling the thermodynamic functions that are necessary to construct the phase diagrams for the mono-atomic materials as well as for binary and ternary solid solutions. The basic principles of construction of binary phase diagrams would be supported by practical work. The students will collect the knowledge about specific features of topology of ternary phase diagrams. Students will create the computer program for calculations of phase diagram.

 Learning outcomes of the module:

On successful completion of the course the students should be able to:

1. Define and describe the ways of modeling thermodynamic functions on the basis of the main physical concepts of thermodynamics of solid and liquid phases.
2. Discuss and explain the models that describe the mixing of components in binary and ternary solid solutions.
3. Relate the specific features of the phase diagrams with the experimental data that should be available to reproduce the phase equilibrium between different phases.
4. Calculate the phase diagram for binary solid solution on the basis of given thermodynamic data.
5. Summarize the main differences in the calculations of the phase diagrams for binary and ternary systems.

Attendance regulation: attendance and participation in class is mandatory (at least 80%).

Confirmation: the syllabus was confirmed by the faculty academic advisory committee to be valid on 2012-2013.

Last update: 05.09.2012

Teaching arrangement and method of instruction: lectures, which include the examples for solving problems linked to the thermal properties of materials.

Assessment:

Final work: 100%

Work and assignments: Final work is devoted to the modeling of thermodynamic functions that reproduce the given phase diagram for binary system. Construction of the phase diagram with the obtained functions is the obligatory result of the final work.

Time required for individual work: in addition to attendance in class, the students are expected to do their assignment and individual work: at least 2 hours per week.

Module Content\ schedule and outlines:

1. Parameters that describe the phase competition between the phases for

pure elements and binary systems. Phase competition as a basis for the problem

of relative stability of phases. (3 hours)

2. Gibbs free energies and Clausius–Clapeyron relation. (3 hours)

3. P-T phase diagrams for pure elements. Melting. Polymorphic

 transformations. Entropy and volume changes in phase transformations

and their relation to the type of phase diagram. (3 hours)

4. Moments of phonon spectra in solids. Structure and thermodynamic functions

for liquid metals. Calculation of thermodynamic functions from the

data on elasic properties of solids. Application to melting problem. (3 hours)

5. Mixing energy and mixing entropy in binary alloys. Models of ideal and regular

solid solutions. Application of lever rule to phase diagrams for the systems with the decomposition in two disordered solid solutions. Approximations beyond regular solid solution. Phase diagrams that are non-symmetric with respect to equiatomic composition (3 hours)

6. Competition of the free energies and solid-liquid transformations

in binary alloys. Phase diagrams of type "sigar". Phase diagram with azeotropic

point. (3 hours)

7. Modeling of thermodynamic functions for the eutectic and peritectic systems.

 (3 hours)

8. Total immissibility in solid state. Degenerated two-phase region. Phase diagrams

with
congruent transformation. (3 hours)

9. Phase diagrams with ordering phases. Thermodynamic functions that include

long range order parameters, definition, temperature dependence, homogeneity

region. Phase diagrams with intermetallic compounds. (3 hours)

10. Ternary phase diagrams. Definition of composition of the phase

 in ternary systems. Isothermic cross-sections. Construction of ternary phase

diagram on the basis of binary diagrams. (3 hours)

11. Decomposition in ternary solid solutions. Missibility gap on the ternary phase

diagram. (3 hours)

12. Three-phase and four-phase equilibrium, change of the topology of the

ternary phase diagram with temperature. (3 hours)

13. Ternary phase diagrams with intermetallic compounds

temperature dependence. Thermodynamic functions in liquids. Melting

 (3 hours)

Required reading:

Computer calculations of phase diagrams, L. Kaufman, H. Bernstein, Academic Press, New York-London, 1970.

CALPHAD (Calculations of Phase Diagrams): A Comprehensive Guide, vol. 1,

N. Saunders, A.P. Miodownik, Pergamon, NY-Oxford-Tokyo, 1998.

Additional literature:

# Phase Equilibria, Phase Diagrams and Phase Transformations,

Their Thermodynamic Basis, 2nd Edition, Mats Hillert, KTH, Stockholm, 2007.

Statistical Thermodynamics of Alloys, N.A. Gocken, Plenum Press, NY-London, 1986.