UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Physical Chemistry of Materials

2122-2-E2701Q040

Aims

Objectives:
1) To present the thermodynamic behavior of binary mixtures;
2) To present the fundamental concepts related to symmetry in crystals,
3) To explain the consequences of defects in crystalline solids.

Knowledge and understanding.
At the end of the course the student knows:
- the thermodynamic behavior of binary mixtures, from ideal solutions to regular ones;
- the physical/mathematical concepts related to the symmetry in the crystals;
- the physical principles of diffraction techniques, in particular the use of X-ray analysis for determination of the structure;
- the compact structures;
- the consequences of the presence of defects in solids;
- the effect of defects on the functional properties of the materials.

Applying Knowledge and Understanding. At the end of the course the student is able to:
- read and interpret binary phase diagrams in the presence of solid and liquid phases;
- solve simple problems of geometry in solid state;
- solve simple structural problems;
- classify the defects based on their characteristics;

Making judgment. At the end of the course, the student is able to:
- determine the thermodynamic equilibrium conditions for the coexistence of various phases;
- choose the most appropriate analysis conditions to solve the structure of crystalline systems;
- correlate the structural properties of materials with functional ones.

Communication skills. At the end of the course the student is able to:

- explain the various zones of solid/liquid phase diagrams in binary mixtures;
- comment on the results of simple structural problems;
- illustrate the fundamental concepts of crystal diffraction;
- describe the effect of the presence of defects in crystalline systems.

Learning skills. At the end of the course the student is able to:
- understand any binary temperature/composition phase diagram;
- read the International Tables of Crystallography, including the most significant information;
- interpret some simple functional properties based on the structure of materials.

Contents

Thermodynamic of binary systems: from ideal solutions to phase diagrams

Simmetry crystal systems and space groups

X-ray diffraction: Bragg law and structure factor

Defects in solids

Detailed program

THERMODYNAMIC

Ideal solution, Rault's and Henry's laws. Thermodynamic equilibrium in heterogeneous systems, Gibbs phase rules. Phase diagram classification. Theory of regular solutions. Two components phase diagrams. Ternary phase diagrams

CRYSTAL STRUCTURE OF SOLIDS AND USE

Crystals: atomic structure and translational symmetry. Elementary cell and lattice. Symmetry, point group symmetry and group theory. Bravais lattices. Spatial point groups. Reciprocal lattice. X-ray, electron and neutron diffraction in crystals. Bragg and Von Laue laws, Ewald sphere. Single electron scattering, atomic form factor and form factor. Electron density. Effect of the atomic thermal motion. Effect of symmetry on the form factor and systematic absences. Experimental diffraction methods.Structure refinements. Lattices: Cubic Close Packing, Hexagonal Close Packing and Body Centered Cubic.

DEFECTS IN SOLIDS

Point defects: vacancies, interstitials, Frenkel and Shottky defects. Role of defects in ionic mobility and conductivity in solids. Extended defects: dislocations, grain boundary, stacking faults.

Prerequisites

Math: vectors and matrix, complex numbers.

Electromagnetic theory; wave functions.

Laws of Thermodynamic, single component phase diagrams, Gibbs free enegry of mixing (perfect gas)

Teaching form

Lectures (7 CFU) and exercises (1 CFU)

Textbook and teaching resource

Lecture slides,

Atkins de Paula "*Chimica Fisica*", 5a edizione (chapter 5)

Immirzi Tedesco "*La diffrazione nei cristalli*", libreriauniversitaria.it (chapters 1-7, 11, 15)

Semester

first semester

Assessment method

The course includes a written test and an oral exam. Passing the written test (vote> 18/30) is a prerequisite for the admission to the oral examination. The written exam must be passed in the same session of the oral exam. There are two written tests during the lessons cycle, one mid-term and one at the end. Those who positively pass the two tests (vote > 18/30 in both) are exempted from the written test for the corresponding session.

The written exam consists of:
- understanding of phase diagrams,
- resolution of problems of punctual and / or spatial symmetry,
- determination of geometric parameters (distances and bond angles) in solid state,
- use of the law of Bragg and deduction of structural factors.

The oral exam aims to verify the knowledge acquired concerning:
- the principles of the thermodynamic equilibrium of two-component systems,

- the physical principles of diffraction techniques, regarding to techniques related to X-ray analysis,
- the role and effects of the presence of defects in solids.

Office hours

on appointment