UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Physical Chemistry of Materials

2021-2-F5401Q040

Aims

Objectives:
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 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:
- 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:
- 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:
- 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:
- read the International Tables of Crystallography, including the most significant information;
- interpret some simple functional properties based on the structure of materials.

Contents

Simmetry crystal systems and space groups

X-ray diffraction: Bragg law and structure factor

Defects in solids

Detailed program

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. X-ray, electron and neutron diffraction in crystals. Bragg and Von Laue laws, Ewald sphere. Reciprocal lattice. 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.

Teaching form

Lectures (5 CFU) and exercises (1 CFU)

In the Covid-19 emergency period, lessons will be held remotely asynchronously with synchronous videoconferencing events.

Textbook and teaching resource

Lecture slides,

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

Semester

second 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:
- 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 physical principles of diffraction techniques, regarding to techniques related to X-ray analysis,

- the role and effects of the presence of defects in solids.

During the Covid-19 emergency period, oral exams will only be online. They will be carried out using the WebEx platform and on the e-learning page of the course there will be a public link for access to the examination of possible virtual spectators.

Office hours

on appointment