UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Thermodynamics and Kinetics of Materials

2627-2-F5402Q027

Aims

The aim of the course is to provide students with the knowledge and skills necessary to master the complex mechanisms and processes that underlie the phase transformations of materials, both concerning the thermodynamic aspects and the kinetic ones. The knowledge and skills acquired will be applied to some case studies of technological relevance in the field of functional materials.

D1 - KNOWLEDGE AND UNDERSTANDING ABILITY

At the end of this training activity, the student must demonstrate that he/she is able to:
1 Describe the crystalline state and the main crystal structures
2 Describe the thermodynamic principles underlying equilibrium between condensed phases
3 Describe the thermodynamic principles underlying solid/solid phase transitions
4 Describe the kinetic processes underlying the formation of solid phases
5 Describe the physical principles underlying diffusion processes
6 Describe the physical principles underlying diffraction for the study of materials
7 Describe the physical principles underlying X-ray absorption spectroscopy
8 Describe the thermodynamic and kinetic principles underlying corrosion processes

D2 - CAPACITY TO APPLY KNOWLEDGE AND UNDERSTANDING
At the end of this training activity, the student must demonstrate that he/she is able to:
1 Obtain information on the crystalline state from diffraction techniques
2 Read and interpret multi-component phase diagrams
3 Predict the growth kinetics of materials and the methodologies to influence it
4 Interpret X-ray absorption spectra and correlate them with material properties
5 Predict the spontaneity of a corrosion process and evaluate its kinetics

D3 - JUDGMENT AUTONOMY
At the end of this training activity, the student must demonstrate that he/she is able to:
1 Correlate the various topics of the course, integrating them into a unified perspective

2 Apply the acquired knowledge to materials of technological importance
3 Select the techniques and experimental parameters useful for obtaining specific structural information in solids
4 Engage in a critical discussion on the relationships between structure and functional properties in a solid

D4- COMMUNICATION SKILLS
To be able to describe in a clear and concise form: i) the objectives, ii) the procedure and iiii) the results of the elaborations carried out.

D5 - LEARNING SKILLS
Expected results:
1 Collect and understand new information useful for rationalizing the structural properties of solids.
2 Collect and understand information about the technological evolution of some spectroscopic techniques.

Contents

Crystalline state and diffraction techniques. Thermodynamics of the solid state and phase diagrams. Phase transformation processes and crystal growth mechanisms. Diffusion and application examples. Fundamentals of selected spectroscopic techniques capable of investigating the correlations between structure, dynamics, and functional properties of certain classes of solids.

Detailed program

The crystalline state and the interpretation of the synoptic tables of the International Tables for Crystallography. Crystal systems, Bravais lattices, space groups. Diffraction techniques for the study of crystalline substances. Determination of lattice parameters and atomic positions.
Thermodynamics of materials, Gibbs approach and determination of equilibrium between condensed phases. Critical analysis of two-component temperature/composition phase diagrams. Substitutional and interstitial solid solutions. Phase diagrams and morphology: examples (steel). Brief overview and examples of three-component phase diagrams.
Thermodynamic classification of phase transformations and analysis of the behavior of state functions during transitions. Second-order transformations, Landau theory and order parameter. Application of Landau theory to order-disorder transformations.
Homogeneous and heterogeneous nucleation processes during solidification and solid-solid transformations. Crystal growth processes: case restricted to growth and general case of growth during nucleation.
Diffusion and solid-state diffusion. The concept of flux density, physical origin of diffusion and Fick's first law. Continuity equation and Fick's second law. Solutions to the second law and application to simple systems.
X-ray absorption spectroscopy (XAS): XANES EXAFS. Physical principles and application differences.
General principles of corrosion. Types of corrosion. Thermodynamics of corrosion and Pourbaix diagrams. Kinetics of corrosion and Evans diagrams.

Prerequisites

Basic knowledge of chemical systems and chemical interactions in condensed phases. Principles of interference between monochromatic waves.
Basic thermodynamics, Gibbs free energy and its derivatives. 1-component phase diagrams.
Knowledge of mathematical analysis and principles of differentiation. Differential equations, meaning and solutions.

Teaching form

24 two-hour lectures, in person, Delivered Didactics

Textbook and teaching resource

International Tables of Cristallagraphy,
Fundamentals of Crystallography (third Edition), Giacovazzo et al. Oxford.
Thermodynamics and Phase Diagrams, Arthur D. Pelton, in Physical Metallurgy, Elsevier, Ebook
B.S. Bokstein et al., Thermodynamics & Kinetics in Materials Science,
Teacher's slides and notes

Semester

First semester

Assessment method

Written and oral examination with a grade out of thirty.

The assessment of the learning outcomes expected by the D1-D5 descriptors is carried out in two phases.
Written exam featuring problems to solve (reading phase diagrams, thermodynamic calculations, and application of kinetic laws), open-ended questions (derivations), and multiple-choice questions. A passing grade (grade >18 out of 30) on the written exam allows access to the oral exam, which must be taken during the same session. During the oral interview, the student's critical analysis and communication skills, as well as their independent judgment, will be assessed.

Office hours

By appointment

Sustainable Development Goals

QUALITY EDUCATION | AFFORDABLE AND CLEAN ENERGY