

## COURSE SYLLABUS

### Thermodynamics and Kinetics of Materials

2324-1-FSM01Q002

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#### 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 basic principles of solid state thermodynamics
- 2 Describe the kinetic processes in the solid state
- 3 Describe the solid state phase transition mechanisms
- 4 Describe the processes of diffusion and ion transport in the solid state
- 5 Describe the physical principles underlying diffraction and X-ray spectroscopy
- 6 Describe the physical principles underlying pulsed gradient NMR spectroscopy
- 7 Describe the properties of crystalline and amorphous states.

#### 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 Predict the results of a phase transformation process based on thermodynamic considerations
- 2 Obtain structural information from diffractometric techniques
- 3 Obtain dynamic and structural information from spectroscopic techniques
- 4 Correlate structure and functional properties in crystalline and amorphous systems.

#### D3 - JUDGMENT AUTONOMY

At the end of this training activity, the student must demonstrate that he/she is able to:

- 1 Choose the most useful techniques for the structural analysis of a solid
- 2 Select the experimental techniques and parameters to obtain specific structural information in solids
- 3 Select the experimental techniques and parameters to obtain specific dynamic information in solids

4 Addressing a critical discussion of 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 iii) 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**

Thermodynamics and kinetics of solids.

Phase transformation processes and the kinetic mechanisms (diffusion, transport) that are at their base.

Fundamentals of some spectroscopic techniques able to investigate the correlations between structure, dynamics and functional properties of some classes of solids.

### **Detailed program**

Thermodynamics and kinetics of phase transformations.

Fundamentals of Landau's theory. Order-disorder transitions.

Solid solutions. Polycrystalline systems and formation of grain boundary.

Homogeneous and heterogeneous nucleation during solidification and solid-solid transformations.

Kinetics in solid state. Processes of heat and matter transport.

Continuity equations. Principles of thermodynamics of irreversible processes. Onsager relations. Diffusion: Fick's law. Diffusion equation and solutions. Applications to diffusion processes in solids. Structural aspects of solid state transformations.

Radial distribution function, types of disorder. Structure of glasses and mechanisms of ion transport.

X-rays spectroscopy: EXAFS, XANES.

Diffusion coefficients measured by NMR.

### **Prerequisites**

Basic thermodynamics. Basic crystallography.

## **Teaching form**

Oral lessons.

## **Textbook and teaching resource**

B.S. Bokstein et al., Thermodynamics & Kinetics in Materials Science, Oxford University Press, Oxford, 2005.

A.R. West, Solid State Chemistry and its Applications, Wiley, Chichester, 2014.

Lecture notes of the teacher.

## **Semester**

First

## **Assessment method**

Oral exam with vote in thirtieths.

The verification of the learning of the results foreseen by the descriptors D1-D5 is carried out through an interview, during which at least two questions are asked the student on different parts of the program. The interview, in addition to ascertain the acquisition of knowledge and disciplinary skills, will tend to verify the critical analysis skills, the judgement level the and exposing capabilities acquired by the student.

## **Office hours**

By appointment

## **Sustainable Development Goals**

QUALITY EDUCATION | AFFORDABLE AND CLEAN ENERGY

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