Course guide

295914 - FMF - Fundamentals of Functional Materials

Unit in charge: Barcelona East School of Engineering
Teaching unit: 748 - FIS - Department of Physics.

Degree: BACHELOR'S DEGREE IN CHEMICAL ENGINEERING (Syllabus 2009). (Optional subject).
BACHELOR'S DEGREE IN MECHANICAL ENGINEERING (Syllabus 2009). (Optional subject).
BACHELOR'S DEGREE IN MATERIALS ENGINEERING (Syllabus 2010). (Optional subject).

Academic year: 2023 ECTS Credits: 6.0 Languages: English

LECTURER

Coordinating lecturer: Lloveras Muntane, Pol Marcel
Cazorla Silva, Claudio

Others: Segon quadrimestre:
CLAUDIO CAZORLA SILVA - M10
POL MARCEL LLOVERAS MUNTANE - M10
ROBERTO MACOVEZ - M10

PRIOR SKILLS

It is recommended for students to have attended the courses of Physical Metallurgy, Electric and Magnetic Properties of Materials, Mechanical Properties of Materials, and Optical, Thermal and Acoustic Properties of Materials.

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Transversal:
02 SCS N3. SUSTAINABILITY AND SOCIAL COMMITMENT - Level 3. Taking social, economic and environmental factors into account in the application of solutions. Undertaking projects that tie in with human development and sustainability.
06 URI N3. EFFECTIVE USE OF INFORMATION RESOURCES - Level 3. Planning and using the information necessary for an academic assignment (a final thesis, for example) based on a critical appraisal of the information resources used.
07 AAT N2. SELF-DIRECTED LEARNING - Level 2: Completing set tasks based on the guidelines set by lecturers. Devoting the time needed to complete each task, including personal contributions and expanding on the recommended information sources.

TEACHING METHODOLOGY

Theory and case study lectures: the Lecturer introduces fundamental concepts and few proofs, complementing them with key examples and the discussion of some applications.

LEARNING OBJECTIVES OF THE SUBJECT

At the end of the course, the student must be able to:
- describe the fundamentals of functional properties of materials, in particular related to energy, chemistry and biomedicine, and their response to applied external fields.
- possess the capability to approach the conceptual problems underlying current challenges in material science and technology.
STUDY LOAD

<table>
<thead>
<tr>
<th>Type</th>
<th>Hours</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hours medium group</td>
<td>60.0</td>
<td>100.00</td>
</tr>
</tbody>
</table>

**Total learning time:** 60 h

CONTENTS

**Item 1. Physical foundations of the thermal properties of materials**

**Description:**
- Topic 1.1 Introduction to statistical physics
- Topic 1.2 Thermal properties of the ideal gas
- Topic 1.3 Thermal properties of crystals

**Specific objectives:**
- In completing Item 1 of the topic, the students should:
  - understand the basic principles of statistical physics that allow to explain the macroscopic theory of thermodynamics in terms of microscopic theories
  - recognize the main differences between the canonical and microcanonical ensembles and know how to deduce the fundamental thermodynamic properties of systems composed of non-interacting many particles in both ensembles
  - fully understand the concept of partition function and apply it to the estimation of thermodynamic properties
  - known the theory of ideal monoatomic and diatomic gases and being able to analytically deduce their thermodynamic properties
  - understand the basics of the vibrational and collective behaviour of atoms in monoatomic crystals
  - deduce the main thermodynamic properties of solids (e.g., free energy and heat capacity) within the harmonic approximation

**Related activities:**
Students should solve on their own a series of problems related to the Item contents and hand them over to the Lecturer.

**Related competencies:**
- 02 SCS N3. SUSTAINABILITY AND SOCIAL COMMITMENT - Level 3. Taking social, economic and environmental factors into account in the application of solutions. Undertaking projects that tie in with human development and sustainability.
- 06 URI N3. EFFECTIVE USE OF INFORMATION RESOURCES - Level 3. Planning and using the information necessary for an academic assignment (a final thesis, for example) based on a critical appraisal of the information resources used.
- 07 AAT N2. SELF-DIRECTED LEARNING - Level 2: Completing set tasks based on the guidelines set by lecturers. Devoting the time needed to complete each task, including personal contributions and expanding on the recommended information sources.

**Full-or-part-time:** 70h
- Theory classes: 28h
- Self study: 42h
Item 2: Solid-state phase transitions and microstructure

Description:
Topic 2.1 Magnetic domains.
Systems of magnetic ions: Classical and quantum paramagnetism. Ferromagnetism. Ising model and micromagnetic theory.

Topic 2.2 Structural phase transitions and microstructure.

Topic 2.3 Magnetostructural coupling.

Topic 2.4 Phase stability.
Phase equilibrium. Topological phase diagrams. Applications to pharmaceutical drugs.

Specific objectives:
At the end of item 2, students will be able to:
- identify and classify the materials according to the magnetic behavior.
- identify the relevant physical quantities (order parameters) and the thermodynamic properties at phase transitions.
- identify and characterize the ferroelastic behavior of a material, the microstructure and their origin.
- identify and characterize the magnetostructural behavior in materials with strong coupling.
- identify applications related to the properties discussed above.

Related activities:
Students should solve on their own a series of problems related to the Item contents and hand them over to the Lecturer.

Related competencies:
02 SCS N3. SUSTAINABILITY AND SOCIAL COMMITMENT - Level 3. Taking social, economic and environmental factors into account in the application of solutions. Undertaking projects that tie in with human development and sustainability.
06 URI N3. EFFECTIVE USE OF INFORMATION RESOURCES - Level 3. Planning and using the information necessary for an academic assignment (a final thesis, for example) based on a critical appraisal of the information resources used.
07 AAT N2. SELF-DIRECTED LEARNING - Level 2: Completing set tasks based on the guidelines set by lecturers. Devoting the time needed to complete each task, including personal contributions and expanding on the recommended information sources.

Full-or-part-time: 28h
Theory classes: 16h
Self study: 12h
Item 3. Microscopic and macroscopic properties of soft matter

Description:
Topic 3.1 Introduction to disorder and molecular degrees of freedom
Orientational and conformational degrees of freedom. Introduction to mesophases. Charge transport, applications to electrochemical devices. Dynamic mechanical analysis and dielectric spectroscopy.

Topic 3.2 Structural and orientational glasses

Topic 3.3 Polymeric materials

Topic 3.4 Liquid crystals and self-assembled phases
Thermotropic liquid crystals, liquid crystal polymers and fibers. Introduction to binary systems. Polymer gels, amphiphilic molecules and block-copolymers: self-assembly, lyotropic liquid crystals. Applications (liquid crystal displays, bulletproof vests, supercapacitors, OLEDs, drug delivery) and biological relevance of organic materials.

Specific objectives:
After taking the item 3 of this course, the students will be able to:
- describe the types of condensed phases that can be displayed by a single-component system based on the shape and size of its microscopic constituents, and ascertain which phases are observed at lower or higher temperature;
- describe the main experimental techniques available to identify phases and study molecular dynamics and phase transitions, and explain linear response theory and its main implications;
- discuss the degree of disorder inherent to a condensed phase, and its main characteristic microscopic dynamic processes; discuss the role of disorder and dynamics for rheological and mechanical properties;
- express the degree of orientational order of liquid crystals through the nematic order parameter, and be able to relate it with the anisotropy of rheological, dielectric and optical properties of nematic phases;
- use random walk models, self-similarity, affine deformation and entropic elasticity theory to describe the properties of linear polymers and of polymer networks (elastomers);
- classify phase transitions, and describe the phenomenology of the glass transition in a number of systems ranging from atomic and molecular structural glasses to plastic crystals, and from liquid crystals to polymers.

Related activities:
Students should solve on their own a series of problems related to the Item contents and hand them over to the Lecturer.

Related competencies:
02 SCS N3. SUSTAINABILITY AND SOCIAL COMMITMENT - Level 3. Taking social, economic and environmental factors into account in the application of solutions. Undertaking projects that tie in with human development and sustainability.
06 URI N3. EFFECTIVE USE OF INFORMATION RESOURCES - Level 3. Planning and using the information necessary for an academic assignment (a final thesis, for example) based on a critical appraisal of the information resources used.
07 AAT N2. SELF-DIRECTED LEARNING - Level 2: Completing set tasks based on the guidelines set by lecturers. Devoting the time needed to complete each task, including personal contributions and expanding on the recommended information sources.

Full-or-part-time: 40h
Theory classes: 16h
Self study : 24h
GRADING SYSTEM

The student's final mark will be calculated as a weighted average of the marks obtained from the resolution of exercises proposed by the instructors during the course. Percentages are:

Resolution of exercises Item 1: 40%
Resolution of exercises Item 2: 30%
Resolution of exercises Item 3: 30%

Reevaluation tasks will not be performed.

EXAMINATION RULES.

Students should work out the exercises individually and autonomously out of the Lecture hours and deliver them before the deadline set by the instructors.

BIBLIOGRAPHY

Basic:

Complementary:

RESOURCES

Other resources:
During the course, lecture notes will be available through Atenea.