Course guide
295914 - FMF - Fundamentals of Functional Materials

Last modified: 02/10/2025

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

Degree: BACHELOR'S DEGREE IN BIOMEDICAL ENGINEERING (Syllabus 2009). (Optional subject).
BACHELOR'S DEGREE IN CHEMICAL ENGINEERING (Syllabus 2009). (Optional subject).
BACHELOR'S DEGREE IN ELECTRICAL ENGINEERING (Syllabus 2009). (Optional subject).
BACHELOR'S DEGREE IN ENERGY ENGINEERING (Syllabus 2009). (Optional subject).
BACHELOR'S DEGREE IN INDUSTRIAL ELECTRONICS AND AUTOMATIC CONTROL 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: 2025 **ECTS Credits:** 6.0 **Languages:** English

LECTURER

Coordinating lecturer:

Others:

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 INFORMATI0N 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 should be able to:
- Understand the functional properties of materials and their applications, particularly those related to energy, chemistry, biomedicine, sensors, and actuators, as well as their behavior under the influence of external fields.
- Have the ability to address conceptual problems related to the challenges of current and future technologies in various engineering domains related to functional materials.

STUDY LOAD

Type	Hours	Percentage
Hours large group	60,0	40.00
Self study	90,0	60.00

Total learning time: 150 h

CONTENTS

Item 1: Phase transitions and ferroic materials: fundamentals and applications

Description:
Topic 1.1 Introduction to phase transitions: thermodynamic, mechanistic, and kinetic classification. Phase stability and application to pharmaceutical drugs.
Topic 1.2 Ferroelastic phase transitions: Introduction to elasticity. Introduction to Landau's theory. Self-accommodation and microstructure. Functional properties: Shape memory effect and superelasticity.
Topic 1.3 Micromagnetism. Magnetoelastic coupling and magnetic shape memory effect. Magnetostructural systems and magnetic superelasticity.
Topic 1.4 Caloric effects in the solid state. Applications for refrigeration and heat pumps.

Specific objectives:
At the end of block 1, students will be able to:
- identify and characterize the different phases of a material, its stability and thermodynamic properties.
- Identify and characterize the ferroelastic behavior of a material and its microstructure.
- Identify and characterize the magnetostructural coupling.
- Identify applications derived from the previous properties.

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 INFORMATI0N 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: 50h
Theory classes: 20h
Self study : 30h

Block 2: Energy materials: fundamentals and applications

Description:
Topic 2.1: Introduction to heat and charge transport.
Heat carriers, Fourier’s law, Boltzman transport equation, Lattice phonons, Semiconductors and metals, Superconductivity

Topic 2.2: Thermoelectric materials
The Seebeck effect, Thermoelectric figure of merit, Examples and applications

Topic 2.3: Energy storage materials
Superionicity and solid-state electrolytes, Cathode and anode electrochemical battery materials, Hydrogen storage compounds, Fuel cell materials and catalysts

Topic 2.4: Photovoltaic and photocatalytic materials
Solar cell devices, Light absorbent and selective contact materials, Electrolysis and photoinduced hydrogen production, Photocatalytic materials

Topic 2.5: Ferroelectric materials
Crystal symmetry and ferroelectric polarization, Ferroelectric domains and P-E loops, Nanoscale domains: Ferroelectric skyrmions, Pyroelectricity and piezoelectricity, Flexoelectricity

Specific objectives:
1. Understand Fundamentals of Heat and Charge Transport
Describe heat carriers and their behavior under Fourier’s law.
Explain the Boltzmann transport equation and its application to lattice phonons.
Differentiate between heat and charge transport in semiconductors, metals, and superconductors.

2. Analyze Thermoelectric Materials and Their Applications
Understand the Seebeck effect and its role in thermoelectricity.
Evaluate the thermoelectric figure of merit and its impact on material efficiency.
Identify examples and applications of thermoelectric materials.

3. Explore Materials for Energy Storage
Explain superionicity and the role of solid-state electrolytes.
Describe key materials for cathodes, anodes, and hydrogen storage.
Understand the principles of fuel cells and the materials used as catalysts.

4. Investigate Photovoltaic and Photocatalytic Materials
Understand the structure and operation of solar cell devices.
Describe light-absorbing materials and their role in energy conversion.
Analyze the processes of photoinduced hydrogen production and photocatalysis.

5. Develop a Comprehensive Understanding of Ferroelectric Materials
Define crystal symmetry and its connection to ferroelectric polarization.
Explain the properties of ferroelectric domains, including P-E loops and nanoscale features like skyrmions.
Explore related phenomena such as pyroelectricity, piezoelectricity, and flexoelectricity.

6. Apply Knowledge Through Problem-Solving
Solve practical problems related to heat transport, energy storage, and material properties.
Apply theoretical concepts to real-world examples in energy and material science.

Related activities:
Students will have to independently solve and submit to the teaching staff a set of problems related to the topic content.

Full-or-part-time: 50h
Theory classes: 20h
Self study : 30h

Block 3. Disordered & polymeric functional materials: fundamentals and applications

Description:
Topic 3.1 - Introduction to (dynamically) disordered materials
1.1 Molecular & macromolecular constituents and dynamics; glasses and mesophases
1.2 Entropy & the Boltzmann distribution, application to orientationally disordered crystals
1.3 Plastic crystals for energy applications
1.4 Electrical and mechanical properties of disordered materials: ion conductors and viscoelasticity

Topic 3.2 - Glasses
2.1 Crystallization vs glass transition and ageing
2.2 Adam-Gibbs theory and dynamic-thermodynamic correlation
2.3 Variety of amorphous solids and their mechanical, solid-state chemistry and optical applications
2.4 Single-component vs multi-component glasses, pharmaceutical relevance

Topic 3.3 - Polymeric materials and their applications
3.1 Amorphous & semicrystalline polymer materials; conformation of linear polymers: Miller theory & Kuhn ideal chains
3.2 Mechanical properties: normal (Rouse) & segmental relaxations; viscoelasticity of polymer melts
3.3 Rubbers and hydrogels: entropic elasticity, mechanical and energy applications
3.4 Liquid crystal polymers and fibres, block-copolymers, composite materials and amorphous polymer dispersions, and their applications

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;
- 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.
- 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
- describe the main technological applications of glasses and of synthetic 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 INFORMATI0N 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.
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Full-or-part-time: 50h
Theory classes: 20h
Self study : 30h

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: 33%
Resolution of exercises Item 2: 33%
Resolution of exercises Item 3: 33%

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:
- Sears, Francis Weston; Salinger, Gerhard L. Termodinámica, teoría cinética y termodinámica estadística. 2ª ed. Barcelona [etc.]: Reverté, DL 1978. ISBN 9788429141610.
- White, Mary Anne. Physical properties of materials. 2nd ed. Boca Raton (Florida): CRC Press, cop. 2012. ISBN 9781439866511 (CART.).
- Wadhawan, Vinod. Introduction to ferroic materials. CRC Press, 2000. ISBN 9789056992866.
- Jones, Richard A. L. Soft condensed matter. Oxford [etc.]: Oxford University Press, 2002. ISBN 9780198505891.
- Doi, Masao. Soft matter physics. Oxford: Oxford University Press, 2013. ISBN 9780199652952.
- Strobl, Gert. The Physics of Polymers : concepts for understanding their structures and behavior [on line]. Berlin Heidelberg New York: Springer Verlag, 2007 [Consultation: 14/09/2022]. Available on: https://ebookcentral-proquest-com.recursos.biblioteca.upc.edu/lib/upcatalunya-ebooks/detail.action?pq-origsite=primo&docID=3062750. ISBN 9783540252788.

Complementary:
- Marder, Michael P. Condensed matter physics. 2nd ed. John Wiley & Sons, 2010. ISBN 9780470617984.
- Salje, Ekhard K. H. Phase transitions in ferroelastic and co-elastic crystals : an introduction for mineralogists, material scientists, and physicists. Cambridge [etc.]: Cambridge University Press, 1993. ISBN 0521384494.
- Planes, Antoni; Mañosa, Lluís; Saxena, Avadh. Magnetism and structure in functional materials : workshop of the Interplay of Magnetism and Structure in Functional Materials, held al the Benasque center for Science in the Pyrenees mountainsm, February, 9-13, 2004. Berlin: Springer, 2005. ISBN 9783540236726.

RESOURCES

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