Course guide
295914 - FMF - Fundamentals of Functional Materials

Last modified: 14/06/2023

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 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 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

Type	Hours	Percentage
Hours medium group	60,0	100.00

Total learning time: 60 h

CONTENTS

Item 1. Physical foundations of the thermal properties of materials

Description:
Topic 1.1 Introduction to statistical physics
Macrostates and microstates. Entropy and thermodynamic probability. Distribution functions: Fermi-Dirac, Bose-Einstein, and Maxwell-Boltzmann. Partition function and thermodynamic properties.

Topic 1.2 Thermal properties of the ideal gas
Ideal monoatomic gas. Statistical interpretation of work and heat. Equipartition of energy. Quantum linear oscillator. Diatomic ideal gases: partition functions for vibrational and rotational degrees of freedom.

Topic 1.3 Thermal properties of crystals
Phonons and vibrational density of states. Heat capacity of crystals: Einstein's and Debye's models. Thermal expansion. Thermal conductivity. Ionic conductivity
Metallic crystals: electron gas, Fermi level, and work function. Electronic contribution to the heat capacity of crystals. Electronic contribution to the thermal conductivity of crystals. Electrical conductivity.

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 cristals
- 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 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: 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.
Thermodynamic signature of phase transitions. Ehrenfest classification. Landau theory. Long-range interactions. Self-accommodation and microstructure. Shape memory effect and superelasticity.

Topic 2.3 Magnetostructural coupling.
Magnetocrystalline anisotropy and magnetoelastic coupling. Magnetostriction. Metamagnetism. Caloric and multicaloric effects. Magnetic shape memory and magnetic superelasticity.

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 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: 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
Glass-forming liquids, orientationally disordered solids, plastic crystals. Glass transition, primary and secondary relaxation dynamics. Ageing and stable glasses.

Topic 3.3 Polymeric materials
Phases of linear polymers. Conducting polymers and polymer fibers. Rotational isomeric state model. Kuhn equivalent chain. Relaxations and glass transition in amorphous and semicrystalline polymers, relation to viscoelasticity. Rubbers and entropic elasticity.

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 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: 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:
- 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.
- Wadhawan, Vinod. Introduction to ferroic materials. CRC Press, 2000. ISBN 9789056992866.
- 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.).
- 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.