



Course guide

295914 - FMF - Fundamentals of Functional Materials

Last modified: 12/04/2022

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: 2021 **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

Students should 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 classes: the teacher introduces fundamental concepts and few proofs, complementing them with key examples and demonstrations, as well as with the discussion of some applications.

Problem solving and guided activities: the teacher carries out the resolution of representative problems; students review fundamental concepts and solve some problems under the teacher's supervision.

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.



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.

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.

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

Oriental 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.

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 guided and autonomous exercises proposed by the instructors during the course. Percentages are:

Resolution of exercises of Item 1: 40%

Resolution of exercises of Item 2: 30%

Resolution of exercises of Item 3: 30%

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.).
- Marder, Michael P. Condensed matter physics. 2nd ed. John Wiley & Sons, 2010. ISBN 9780470617984.
- Strobl, Gert. The Physics of Polymers [on line]. Berlin Heidelberg New York: Springer, 2007 Available on: bibliotècnica UPC.

Complementary:

- 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 at the Benasque center for Science in the Pyrenees mountains, February, 9-13, 2004. Berlin: Springer, 2005. ISBN 9783540236726.



RESOURCES

Other resources:

During the course, the teachers will provide students with study material and sometimes recommend material available online, both from general sources such as Wikipedia or from specific websites such as that of the research group of the instructors (<https://gcm.upc.edu/en>).