Universitat Autònoma de Barcelona

2023/2024

Synthesis and Structure of Crystalline and Amorphous Materials

Code: 103279
ECTS Credits: 7

Degree	Type	Year	Semester
2501922 Nanoscience and Nanotechnology	OB	3	1

Contact

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Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject. Please note that this information is provisional until 30 November 2023.

Teachers

Fernando Novio Vazquez

Prerequisites

It is highly recommended that in order to study this subject, the students have passed "Quimica dels Elements", "Química Orgànica" and "Laboratori de Microscòpies i Tècniques de Caracterització de Materials" from the 2nd year of the degree of Nanoscience and Nanotechnology, as many concepts of the 2nd year subjects will be used in the subject Synthesis and Structure of Crystalline and Amorphous Materials without previous explanation.

Objectives and Contextualisation

Synthesis and Structure of Crystalline and Amorphous Materials aims to provide a basic knowledge of materials and nanomaterials from their synthesis, structure and properties (mainly mechanical and chemical) point of view. Its content is based on aspects previously presented in subjects of the second year of the degree. In the part corresponding to the structure of the materials, it is based on the contents of the Chemistry of the Elements and the Microscopy Laboratory and Materials Characterization subjects, while the part of the polymeric materials is based on the contents of Organic Chemistry subject. This is a subject of Material Science in which an emphasis is placed on the structural and synthetic part, which is why Chemistry Bases subject for Nanoscience and Nanotechnology is in the field. Synthesis and Structure of Crystalline and Amorphous Materials is followed by a Solid State course where the Material Science topic is concentrated in its physical properties.

In a unified way the subject provides knowledge about the structure of crystalline materials, from the perfect crystals (reticular theory and crystalline lattices, infinite symmetry and X-ray diffraction) and following by real

crystals (crystalline defects). The study of crystalline materials is then completed with a presentation of the basics of the mechanical properties of the solids, of the phase transformation of metals and the most important ceramic structures. The synthesis of materials and nanomaterials is explained in two different topics where the different synthetic methodologies are exposed. The subject finishes with the study of the most important characteristics of polymeric materials. The subject consists of theory classes, exercises solving classes, classroom practices and laboratory practices.

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Competences

- Apply the concepts, principles, theories and fundamental facts of nanoscience and nanotechnology to solve problems of a quantitative or qualitative nature in the field of nanoscience and nanotechnology.
- Apply the general standards for safety and operations in a laboratory and the specific regulations for the use of chemical and biological instruments, products and materials in consideration of their properties and the risks.
- Be ethically committed.
- Communicate orally and in writing in one's own language.
- Demonstrate knowledge of the concepts, principles, theories and fundamental facts related with nanoscience and nanotechnology.
- Handle the standard instruments and materials of physical, chemical and biological testing laboratories for the study and analysis of phenomena on a nanoscale.
- Interpret the data obtained by means of experimental measures, including the use of computer tools, identify and understand their meanings in relation to appropriate chemical, physical or biological theories.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse physical, chemical and biological problems in the field of nanoscience and nanotechnology and propose answers or suitable studies for their resolution, including when necessary the use of bibliographic sources.
- Recognise the terms used in the fields of physics, chemistry, biology, nanoscience and nanotechnology in the English language and use English effectively in writing and orally in all areas of work.
- Resolve problems and make decisions.
- Show sensitivity for environmental issues.

- Work correctly with the formulas, chemical equations and magnitudes used in chemistry.
- Work on the synthesis, characterisation and study of the properties of materials on a nanoscale from previously established procedures.

Learning Outcomes

1. Appreciate the danger and risks of using samples and reagents and apply the right safety precautions for each case (goggles and/or special gloves, extractor hood, gas mask, etc.)
2. Be ethically committed.
3. Communicate orally and in writing in one's own language.
4. Correctly handle glass and another types of material usually found in a synthesis and characterisation laboratory.
5. Correctly handle the necessary material and instruments to prepare and characterise materials and nanomaterials.
6. Critically evaluate experimental results and deduce their meaning.
7. Describe the methods of synthesis and the properties of polymers.
8. Design simple experiments for the study of simple chemical and physical systems.
9. Differentiate the properties of amorphous crystalline materials.
10. Draft reports on the subject in English.
11. Employ information and communication technology in the documentation of cases and problems.
12. Enunciate and describe the crystalline structures of the most important materials and nanomaterials.
13. Graphically represent the structures of metals and ionic compounds
14. Identify and situate safety equipment in the laboratory.
15. Identify the standard methods for the synthesis of material, and describe their basics.
16. Identify the statistical methods for the treatment of the results of analyses to obtain information on their quality.
17. Interpret basic chemistry texts and bibliographies in English.
18. Interpret the data obtained from experimental measurements to characterise a chemical compound or a material.
19. Justify the results obtained in the laboratory from chemical compound synthesis, separation, purification and characterisation processes on the basis of knowledge of their structure and properties.
20. Justify the results obtained in the laboratory from material and nanomaterial synthesis and characterisation processes in accordance with knowledge of their structure and properties.
21. Learn autonomously.
22. Make adequate use of laboratory materials and instruments.
23. Make correct calculations of the properties of crystalline and amorphous materials, and of nanomaterials.
24. Manage the organisation and planning of tasks.
25. Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
26. Perform basic synthesis, separation and purification procedures in a chemistry laboratory
27. Perform basic synthesis, separation and purification procedures in a synthesis and characterisation laboratory.
28. Perform calculations with the structural parameters of metal cells and ionic solids.
29. Present brief reports on the subject in English.
30. Propose creative ideas and solutions.
31. Reason in a critical manner
32. Recognise the relationship between structure, bond characteristics, and properties of solids.
33. Recognise the structures of crystalline materials through cell parameters.
34. Recognise the terms relative to physics and materials.
35. Relate experimental data with the physical and chemical properties and/or analysis of the systems that are the object of study.
36. Resolve problems and make decisions.
37. Safely handle chemical and material reagents.
38. Show sensitivity for environmental issues.
39. Understand the properties of solids with structural imperfections.
40. Use basic instruments to characterise chemical and material compounds.
41. Use data processors to produce reports.

42. Use suitable strategies for the safe elimination of reagents.
43. Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

Content

Synthesis and structure of crystalline and amorphous materials

Lecturing hours: 40h theory, 10 h problems and 8 h laboratory

0. INTRODUCTION TO THE SUBJECT

1. RETICULAR THEORY AND CRYSTAL LATTICE

The crystalline state. Basic and defining properties of the crystalline state. Abstraction of the crystalline state. Direct (or real) lattices. The crystalline lattice as a basis of R^3. Reticular rows. Crystallographic planes. Miller indexes. Interplanar spacing. Reticular densities. Metric and Reciprocal lattice (dual space). Relationships between the reciprocal lattice and the direct lattice. Reticular calculations. Reference systems transformation of. Primitive and multiple lattices. Two-dimensional lattices. Two-dimensional lattices' punctual symmetry. Bravais lattices. Punctual symmetry of Bravais lattices and relationship with crystal systems.

2.- INFINITE SIMETRY

Finite and infinite symmetry. Reminder of punctual symmetry. Symmetry in a periodical medium. The 32 punctual groups. Elements of symmetry with translation. Beams of symmetry elements. The 17 symmetry planar groups. The 230 space symmetry groups. The Hermann-Mauguin notation. Order and multiplicity. Equivalent positions. General and special positions. Wyckoff letters. The international tables for crystallography.

3.-. X-RAY DIFFRACTION

Introduction. Diffraction geometrical conditions. Laue equation, Ewald construction, Bragg's law. Intensity of diffraction. Structure factor, systematic extinctions. Friedel's law. Laue groups. Diffraction symbols. Space group symmetry determination. Concept of crystal structure determination. Structure Factor and electronic density. The structure factor as a Fourier transform of electronic density. The phase problem. Crystal structure determination utility. Crystal structure databases. Powder diffraction. The Debye Scherrer method. The powder diffractometer. Powder Diffraction as a technique forthe identification of crystal phases. The Powder Diffraction File.

4. REAL CRYSTAL

Short and long distance order. Punctual defects:vacancies, interstitials, substitutions. Linear defects: dislocations. Surface defects: grain boundaries. Crystal defects' observation.

CLASSROOM PROBLEMS

1) Reticular theory

2) Symmetry (plane groups)

3) Symmetry (space groups), structural types

4) X-ray diffraction (1)

5) X-ray diffraction (2)

5.- MECHANICAL PROPERTIES OF SOLIDS

Introductory concepts . Stress-Strain diagrams. Mechanical properties of metals. Elastic deformation. Plastic deformation. Dislocations and mechanisms of metal hardening. (4h)

6.- PHASE TRANSFORMATIONS IN METALS

Phases, microstructures and microconstituents. Two components phase diagrams. Eutectic systems. Microstructures in diagrams with eutèctic points. Solid solutions and intermediate phases. Eutectoids and peritectics. Phase transformations and microstructural changes. Nucleation and growth. Transformation diagrams. Changes in mechanical properties. (4h)

7.- STRUCTURE AND PROPERTIES OF CERAMICS

Electrostatic bonding energy. Compact sphere model. Eutectic structures. Structures based on ion packaging. Related structures. Defects in ceramics. Solid solutions Diagrams of ceramic phases. Mechanical properties. Types of ceramic materials according to their applications. Glasses. Glass-ceramics. Other materials (7h)

8-. SYNTHESIS OF MATERIALS

Thermodynamic and kinetic considerations of solids reactions. Solid-gas reactions. General aspects. Thin layers synthesis. Physical Vapour Deposition. Chemical Vapour Deposition. Molecular Beam Epitaxy. Solid-liquid reactions. Crystallization, precipitation and solidification. Sol-Gel method. Solvothermal and hydrothermal techniques. Electrochemical synthesis. Solid-solidreactions. Ceramic method. Synthesis by combustion. Microwave synthesis. (7h)

9.- SYNTHESIS OF NANOMATERIALS

Top-down methods. Thin layered nanostructures. Bottom-up methods. Synthesis of nanoparticles. Precipitation Hydrothermal techniques. Synthesis assisted by micelles. Thermal methods. Sol-gel methods. Polyol method. (4h)

10-. SYNTHESIS AND STRUCTURE OF POLYMERS

Basics. Molecular weight. Types of polymers. Synthetic methods. Addition polymers. Condensation polymers. Other reactions. Structures and stereoisomery. Crystallinity in polymers. Mechanical and thermomechanical properties. Applications. Composite materials (4h)

SYNTHESIS OF MATERIALS LABORATORY (2 SESSIONS OF 4H)

1) SYNTHESIS AND STRUCTURAL STUDY OF MAGNETIC MATERIALS

2) SYNTHESIS OF INORGANIC NANOPARTICLES

Methodology

Methodology:

The student will carry out three types of activities: directed, autonomous and supervised.

1.- Guided activities: Attendance is compulsory and carried out in the presence of a teacher.

1. Theoretical classes: The teacher exposes the contents of the subject and answer to the possible doubts that the student has.

2. Solving of problems classes: The knowledge acquired in the master classes and in the autonomous activities of the student, mainly through the study, are applied to the resolution of problems and exercises related to the contents of the subject.

3. Classroom practices / Laboratory practices: By carrying out of practical work related to the contents of the subject (work with PC programs and synthesis work in the laboratory).

2.- Autonomous activities: With these activities, the student alone, or in group, must achieve the competencies of the subject. Within these activities, we have studying, problems resolution, documents writing, texts reading and bibliographic research.

3.- Supervised activities: The student may ask the teachers of the subject supported tutorials for the assimilation of the subjects exposed in theory and problem solving classes, and for the solving of follow-up work.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Class problems	11	0.44	21, 6, 3, 8, 11, 12, 29, 23, 24, 16, 18, 17, 2, 38, 25, 30, 31, 28, 34, 32, 33, 35, 39, 13, 36, 43
Laboratory and class practices	13	0.52	6, 3, 7, 9, 8, 26, 27, 11, 12, 29, 23, 24, 16, 15, 14, 18, 17, 20, 19, 4, 5, 37, 2, 25, 31, 28, 34, 32, 33, 10, 35, 39, 13, 36, 43, 22, 40, 42, 41, 1
Text reading	2	0.08	21, 7, 9, 12, 16, 15, 17, 2, 31, 34, 32, 33, 39
Thoretical classes	40	1.6	6, 3, 7, 9, 8, 11, 12, 16, 15, 17, 2, 38, 31, 34, 32, 33, 39
Type: Supervised			
Supervised sessions	5	0.2	6, 3, 7, 9, 8, 12, 23, 24, 16, 15, 18, 17, 20, 19, 2, 38, 25, 30, 31, 28, 34, 32, 33, 35, 39, 13, 36
Type: Autonomous			
Bibliographic Research	7	0.28	21, 7, 9, 12, 24, 16, 15, 17, 25, 31, 34, 32, 33, 35, 39
Problem resolutions	16	0.64	21, 6, 11, 23, 18, 17, 19, 2, 38, 25, 30, 31, 28, 34, 35, 13, 36, 43, 41
Studying	60.75	2.43	21, 6, 7, 9, 8, 11, 12, 23, 24, 16, 15, 18, 38, 25, 30, 31, 28, 34, 32, 33, 10, 35, 39, 13
Work reports	10.25	0.41	21, 6, 7, 9, 11, 12, 24, 16, 15, 18, 17, 2, 38, 25, 30, 31, 34, 32, 33, 10, 35, 39, 13, 36, 43, 41

Assessment

Evaluation

Assessment of the subject:

The subject will be evaluated continuously and will consist of the following evaluation activities:

Theoretical part

Represents 70% of the final mark. The student can chose for two ways of evaluating this part:

1) The continuous evaluation in which 2 mid-term tests will be carried out, and

2) The final evaluation where a final test will be carried out.

Continous evaluation:

First mid-term text: The contents of chapters 1 to 5 will be evaluated (35% of the final grade)

Part Two: The contents of chapters 6 to 10 will be evaluated (35% of the final grade)

If these tests are successfully passed with an average grade higher than 5.0 (provided that the mark of one of the partials is not less than 4), the final test will not be required.

If the average is less than 5, or any of the mid-term marks is less than 4, the student must pass the second-chance recovery test to pass the subject.

Final test:

The students will do a final test that will be divided into two exams corresponding to each part of the subject. Each exam will have a weight of 35% of the overall grade. Students may attend one or both parts of the final exam. To pass the subject, the average mark of the two parts (mid-term or final exam) must be equal to or greater than 5.0 (each part mark must be greater than 4).

Delivered exercises:

It will represent 15% of the final mark.

First mid-term exam: Students will have to resolve autonomously problems related to the contents of the subject that will be delivered in class.

Second mid-term exam: Class attendance is mandatory. Therefore, when the teacher considers it appropriate, and without prior notice, it will be able to collect exercises of the continuous work: problems solved in class or at home, tests written in class, or online questionnaires. In the case of justified absence in the day when the exercise is delivered, this exercise will not be considered in the calculation of the final mark. The justification will require the presentation of medical justification (it is not valid overlapping with other subjects, trips, work ...).

Classroom practices and laboratory practices:

They represent 15% of the final mark. The mark will be the average between the evaluation of the work done by the student in the classroom practices (50%) and in the laboratory practices (50%).

Attendance at laboratory practical sessions is mandatory

Improve mark in the final exam

The students who have passed the subject by mid-term exams but wish to improve the mark of one or both partial exams, they may attend the final exam under the following conditions:

1) If the student improves the mark, the best mark will be used.

2) If the student does not improve the mark, the average of the two marks will be made.

Unique assessment

In the case of students who take the unique assessment:

- They will have to attend the laboratory practices under the same conditions as the rest of the students.
- They will have to take an exam of the whole subject on day of the second mid-term exam of the continuous evaluation.
- The same day of the exam, they will have to deliver several exercises and/or assignments corresponding to evidences and practices (classroom and laboratory).

The grade will be = Exam grade (70%) + Evidence grade (15%) + Practices grade (15%)

If the final grade does not reach 5 and/or the exam grade does not reach 4, the student has another opportunity to pass the subject by means of the recovery exam, which will coincide with the recovery exam of continuous assessment students. The grade of the recovery exam replaces the grade of the previous exam only, not the evidences or practical works.

Others

Any copy action or ethically reprehensible actions in the assessment activities will suppose a zero mark in the subject, regardless of other disciplinary implications.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Problem resolutions (Evidences)	15%	3	0.12	21, 6, 3, 7, 8, 26, 11, 29, 23, 24, 15, 18, 17, 20, 19, 5, 25, 30, 31, 28, 34, 10, 35, 13, 36, 43, 40, 42, 41, 1
laboratory and classaroom practices	15%	1	0.04	21, 6, 3, 8, 26, 27, 11, 29, 24, 14, 18, 17, 20, 19, 4, 5, 37, 2, 38, 25, 30, 31, 34, 10, 35, 36, 43, 22, 40, 42, 41, 1
written exams	70%	6	0.24	21, 6, 7, 9, 8, 12, 23, 16, 15, 18, 17, 2, 30, 31, 28, 34, 32, 33, 35, 39, 13

Bibliography

Bibliography:

Chapters 1-5:

C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, M. Milaneso, G. Ferraris, G. Gilli, P. Gilli, G. Zanotti and M. Catti. "Fundamentals of Crystallography" Edited by C. Giacovazzo. 3rd edition, IUCr Texts on Crystallography No. 15, IUCr/Oxford University Press, 2011. ISBN 978-0-19-957365-3.

C. Pico, M.L. López García, M.L. Veiga "Cristaloquímica de materiales" Editorial Síntesis, 2007. ISBN 978-84-975650-7-3.

X. Solans "Introducció a la cristal·lografia", Edicions de la Universitat de Barcelona, 1999. ISBN 84-8338-124-9.

U. Müller "Relaciones de simetría entre estructuras cristalinas", Ediciones Síntesis, ISBN 978-84-9955897-6-3.

Unió Internacional de Cristal·lografia http://www.iucr.org/

Departament de Cristal·lografia del Instituto de Química-Física Rocasolano del CSIC

http://www.xtal.iqfr.csic.es/Cristalografia/index2.html

Chapters 6-10:

W.D. Callister, D.G. Rethwisch "Materials Science and Engineering", Wiley, 6th Ed. ISBN-13:

978-0470505861

W.D. Callister, Jr., D. G. Rethwisch "Fundamentals of Materials Science and Engineering", Wiley, 4th Ed. ISBN 978-1-118-32269-7

D. R. Askeland, P.P Fulay, W.J. Wright "The Science and Engineering of Materials", C.L. Engineering, 6th Ed. ISBN-13: 978-0495296027

A.R. West "Solid State Chemistry and Applications", J. Wiley & Sons (1989) ISBN-13: 978-0471917977

J. N. Lalena, D.A. Cleary, E. E. Carpenter, N. F. Dean "Inorganic Materials. Synthesis and Fabrication", J. Wiley & Sons (2008) ISBN-13: 978-0471740049

A. Rudin, P. Choi "The Elements of Polymer Science and Engineering" Academic Press, 3rd. Ed. ISBN

978-0-12-382178-2 8

Software

1) VESTA

1) Microsoft programs (mainly Word, Excel and Power Point)

2) MAXIMA