Materials Simulation Techniques

Academic Year: (2023 / 2024) **Review date: 17-05-2023**

Department assigned to the subject: Materials Science and Engineering and Chemical Engineering Department

Coordinating teacher: JIMENEZ MORALES, ANTONIA

Type: Electives ECTS Credits : 3.0

Year : 1 Semester : 2

REQUIREMENTS (SUBJECTS THAT ARE ASSUMED TO BE KNOWN)

Solid mechanics; Algebra; Numerical methods.

OBJECTIVES

COMPETENCES:
CB6, Acquire and understand concepts that provide the foundation or opportunity to be original on the development and/or application of ideas, often in a research context.
CB7, Students will be able to apply the acquired knowledge and skills on problem resolution in new or hardly known environments in the context of wide (or multidisciplinary) contexts related to the area under study
CB8, Students will be able to integrate knowledge to face the complexity of making assessments based on limited or incomplete information, but considering the ethical and social responsibilities associated to the application of their knowledge and assessments.
CB9, Students will be able to communicate their conclusions and the knowledge and reasons that support them to specialized and the wide public in a clear and unambiguous manner
CB10, Students will acquire learning skills that allow them to continue studying in an autonomous and self-paced way.
CG1, Understand the challenges associated to Materials Science and Engineering in an industrial and research environment
CG3, Develop team working skills in a research environment
CG6, Acquire the required skills to defend a research project and its results.
CG7, Develop creative strategies for decision making to solve problems associated with materials, their design, processing and behaviour.
CE2, Be able to design new ways of optimizing the properties of different materials for specific applications, through the modification of their structure and composition.
CE9, Consolidate specific research skills in Materials Science and Engineering
CE10 Acquire knowledge and useful scientific and technical skills to solve specific problems associated with the work in a research laboratory in the field of material development and characterization

LEARNING RESULTS:
After the course, the students should have learned:

- To identify the most important simulation techniques and their ability to solve problems in Materials Science and Engineering
- The foundations of atomistic simulation techniques
- The foundations of finite element modelling.

DESCRIPTION OF CONTENTS: PROGRAMME

Program of the subject:

1. Introduction to simulation in materials science and engineering.
1.1. Principles of integrated computational materials engineering (ICME)
1.2 Scales in the structure and behavior of materials
1.3 Simulation techniques at the atomic scale
1.4 Simulation techniques at the mesoscale
1.5 Simulation techniques at the continuum scale
1.6 Multiscale simulations
1.7 Application examples in materials engineering

Part 1: Introduction to atomistic simulations , including Monte Carlo and Molecular Dynamics

2. Introduction to atomistic simulations
2.1 Computational methods
2.2 Quantum vs. Classical Mechanics.
2.3 QM/MM method.
2.3 Finite systems and periodic boundary conditions.

3. Monte Carlo methods and applications in materials engineering.

4. Molecular mechanics
4.1 Interatomic and molecular potentials
4.2 Geometry optimization

5. Molecular dynamics:
5.1 Integration of the equations of motion
5.2 Temperature and pressure control, neighbors, etc.
5.3 Determination of physical properties.

6. Introduction to computational thermodynamics
6.1. Thermodynamics. Gibbs free energy and models
6.2. Phase equilibrium in heterogenous media
6.3. Experimental data for thermodynamics modelling
6.4. CALPHAD method
6.5. Case study and examples

Part 2: Introduction to continuum micromechanics

7. Introduction.
7.1 Mean field approaches.
7.2 Bounding methods
7.3. Periodic microfield approaches
7.4. RVEs

8. Numerical solving methods.
8.1 Introduction to the finite element method. Principles. Spatial discretization and numerical integration. Time discretization. Boundary conditions.

LEARNING ACTIVITIES AND METHODOLOGY

LEARNING ACTIVITIES
AF1, Theoretical-practical classes.
AF2, Lab practices
AF3, Tutorials
AF4, Work in groups
AF5, Individual work from the student

METHODOLOGIES
MD1, Explanations in class, so the professor develops main concepts of the subject, practical examples or problems
MD2, Critical reading by students of textbooks and scientific publications recommended by the teacherMD3, Practical resolution of examples, problems or exercise, by the student (alone or in groups)
MD5, Obtaining experimental results in the lab, using research equipment and techniques, under professor supervision
MD6, Elaborating Works and reports, alone or in groups

ASSESSMENT SYSTEM

- Individual work (continuous evaluation) (SE2): 30%
- Team work on computer practices (SE3): 30%
- Final exam (SE4): 40%

% end-of-term-examination:	40
% of continuous assessment (assigments, laboratory, practicals…):	60

BASIC BIBLIOGRAPHY

- Daan Frenkel and Berend Smit Understanding Molecular Simulation, Elsevier.

- Introduction to Computational Materials Science. Fundamentals to Applications Richard Lesar, Cambridge University Press.

- O. C. Zienkiewicz amd R. L. Taylor. The Finite Element Method, Butterworth-Heinemann Editors.

ADDITIONAL BIBLIOGRAPHY

- Andrew Leach Molecular Modelling: Principles and Applications, Prentice Hall.

- J. M. Haile Molecular Dynamics Simulation: Elementary Methods , Wiley.