Fundamentals of crystallography

MASTER'S DEGREE IN CRYSTALLOGRAPHY AND CRYSTALLIZATION

UNIVERSIDAD INTERNACIONAL MENÉNDEZ PELAYO

GENERAL DATA

Brief description

The course aims to provide the general basis of crystallography and crystallographic methods. From an homogenization of the initial basis of all students of the master we will proceeded to deeply develop all basic concepts required to progress in the study of the actual crystallographic methods both in advanced research and professional skills. Theories and methods developed in the last hundred years by many crystallographers, including more than 25 Nobel Prize winners, will be extracted and transmitted in this module To achieve that we will follow, as backbone, the book Fundamentals of Crystallography and a selected group of very active scientists working on the field of crystallography, senior outstanding crystallographers. The course is based on the experience of three former editions, allowing consider the inputs of three generations of students, to have more elaborated materials and tuning the time schedules. All concepts will be develop by scientists with a solid background on crystallography working for many years directly on crystallography and using and developing new methodologies in crystallography and related fields.

Name

Fundamentals of crystallography

Code

101159

Academic year

2016-17

Degree

MASTER'S DEGREE IN CRYSTALLOGRAPHY AND CRYSTALLIZATION

ECTS Credits

4

Type

MANDATORY

Duration

Duracion A

Language

English

CONTENTS

Contents

The aim of Fundamentals of Crystallography is to provide an advanced background on the historical, mathematical, methodological and practical aspects of crystallography. That will be essential tools to develop all following matters and subjects.

One fundamental concept to develop is symmetry, with special emphasis to 1-D, 2-D and 3-D periodic systems, introducing the special symmetry aspects of aperiodic structures, modulated systems, and non crystallographic symmetries. Particular attention will be paid to the mathematical formulation of symmetry and the use of the International Tables for Crystallography. Concepts of crystallographic point groups, crystal lattices and space groups will be deeply investigated from both theoretical and practical points of view.

Next, the concept to introduce is the Reciprocal Space, dual with the Real Space and the basis of the Diffraction experiment, the Ewal Sphere, and directly related to the Fourier Transform operation.
The twinning observed in many crystalline materials will be addressed explaining the twin laws and studying the methods for detect and handle all different kinds of twinned materials.

The importance of the chemical contents of the crystals, and all atomic and molecular interactions within the crystal lattices will be fully introduced. These atomic and molecular contents have full influence on the crystal growth, the crystal habits and the physical and functional properties of these materials. Particular attention will be paid to the anomalous dispersion and the relation with the determination of the absolute structure, and its importance on drug development, and the multiple applications of the absorption edges in the field of macromolecular crystallography and materials sciences.

At the end of this course the students will be able to fully understand the symmetries of the Real and Reciprocal Spaces and its relationships, in particular those related with the diffraction experiments. The students should be able to use all existing mathematical tools to describe spatial symmetry and symmetry transformations. Understand the role of atoms and molecules and their interactions in building the crystal and giving the properties to a particular crystalline material.

COMPETENCES

General competences

CG1. Capacity for analysis and synthesis
CG2. Troubleshooting
CG3. Working in an interdisciplinary team
CG4. Working in an international context
CG5. Learning and work independently
CG6. Ability to apply theoretical knowledge in practice
CG7. Capacity to development and transmission of ideas, projects, reports, solutions and problems
CG8. Ability to organize and plan
CG9. Ability to understand the language and proposals of other specialists

Specific competences

CE1. Knowing what a crystal and its differences with other states of matter: gases, liquids, amorphous materials, polymers, etc..
CE2. Analyze the existing symmetry in any periodic distribution (crystalline or macroscopic).
CE3. Determine the network descriptor vectors and the cell correctly defining the periodic distribution.
CE4. Assign the symmetry group distribution.
CE5. Handling Tables of Crystallography and deduction of the topological properties of the distribution.
CE6. Understand the impact position entails the constituents of the distribution and the interactions between them.

LEARNING PLAN

Training activities

- Active Classes
- Problem-solving workshops.
- Workshops and experimental demonstrations in the classroom.
- Practices computing and databases
- Individual or group tutoring
- Seminars.
- Visits to company or research center
- Evaluation
- Team work

Learning outcomes

At the end of the matter, the student, using these fundamental theoretical knowledge / practical about:

- Translations periodicals. Conventional analysis of periodic structures. Reference systems and description.
- Symmetry of solids and crystals. Tools to facilitate the description of the periodic structures.
- Description of crystal structures. Reference systems. Systematization, and naming conventions. International Tables for Crystallography.
- Constituents of the crystals and their interactions.

EVALUATION

Evaluation system

The evaluation system will be based on a personal and continuous interaction at expositive classes and workshops. The individual or group contributions to solve the problems given in the workshops and the personal initiatives of work on widen particular aspects of interest will be taken in account.

Control test examinations will be performed along the course to check the level of understanding.

Considering all these inputs a final mark will be given to each student, after a joint discussion of all professors.

FACULTY

Coordinator/s

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Catedrático de Química Física
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Presidente de la European Crystallographic Association

Lecturers

Giacovazzo , Carmelo

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SCHEDULE

Schedule

From 9:00 to 17:30 from Monday to Friday