Diffraction methods

MASTER'S DEGREE IN CRYSTALLOGRAPHY AND CRYSTALLIZATION

UNIVERSIDAD INTERNACIONAL MENÉNDEZ PELAYO

GENERAL DATA

Brief description

The course teaches the fundamentals of diffraction and imaging, focusing on the common nature of both phenomena, the universality of the processes of diffraction of photons, neutrons and electrons and the practical use of these methods in crystallography.

Name

Diffraction methods

Code

101160

Academic year

2016-17

Degree

MASTER'S DEGREE IN CRYSTALLOGRAPHY AND CRYSTALLIZATION

ECTS Credits

7

Type

MANDATORY

Duration

Duracion A

Language

English

CONTENTS

Contents

The course introduces these fundamental concepts:

*Radiations used in crystallography: Photons, neutrons and electrons. Properties and production of the different radiations. Interactions with matter. Differences that make each of them useful for each particular problem alone or in combination.

* Mathematical model of the lattice and the interaction matter/radiation. Scattering from atoms, molecules and crystals. Structure factors, systematic absences, extinction, anomalous scattering. Laws of Laue and Bragg. Fourier synthesis of the structure.

* The Phase Problem.

This block of lessons is accompanied by practical contents, essentially solved and proposed exercises and problems, to enable students to get acquainted with the quantitative practical aspects of diffraction. The concepts of structure factor and Fourier synthesis, as well as other quantitative aspects are practiced intensively using computer simulation and database mining.

Once the most fundamental aspects are acquired, the course continues with an in depth description of the practical details associated with diffraction experiments:

* X-ray, neutrons and electron sources. Generation, Optics and detection of the different radiations. Large Facilities for the generation of synchrotron radiation and neutron beams.

* Experimental methods. Geometry of the diffraction experiment. Experimental stations. Radiation safety.

* Diffraction data collection. Design and optimization of the data collection experiment. Data processing and reduction.

During this block of lectures, practical work will be done on defining diffraction data collection experiments and selecting the beamlines best suited for a given experiment in Large Facilities. Two practical sessions are devoted to getting hands-on experience with X-ray diffraction data analysis and reduction.

The contents of the course are completed with an introduction to the most relevant crystallographic imaging techniques and to other techniques used as an alternative or a complement to diffraction methods in crystallography:

* X-ray and electrons imaging.
* Absorption Spectroscopies (EXAFS, XANES...)
* Particle scattering.

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

ET1. Designing optimal diffraction experiment depending on the problem and the compound, defining the instruments and the most appropriate and the data acquisition strategy that maximizes their usefulness.

ET2. Keep under control the acquisition and processing of data in each time knowing the physical and experimental characteristics that determine the validity and accuracy of the diffraction data.

ET3. Using imaging techniques (direct space) as a complement to diffraction experiment (reciprocal space) or as a single instrument for solving problems.

ET4. Develop a critical assessment capability of diffraction experiments and data allowing it to be independent of the methods of "black box computing" common in environments where data analysis methods are complex.

ET5. Develop the intellectual tools and techniques for the implementation of new experiments and unorthodox and novel experimental techniques at the border of the currently available that allows you to explore new problems.

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

This course aims to provide students with fundamental knowledge, both theoretical and applied since, about:

- Understand the nature and properties of radiation used in crystallography (X-rays, neutrons and electrons), the properties that make them suitable as "experimental probes" and the proper and safe use during experimentation.

- The phenomenon of diffraction, depending on its origin and characteristics of the radiation type and the properties thereof, the relationship between diffraction crystalline periodicity.

- Know the methods used in crystallography to obtain diffraction data, selecting the most appropriate method for each problem and the optimization of the equipment needed to implement each experimental technique (generators, goniometers, detectors).

- Methods of direct space (image) used both as crystalline materials bracket as diffraction experiments for isolation and crystallization crystallography studies

- Unorthodox and novel experimental techniques at the frontier of the currently available that allows you to explore new problems.

EVALUATION

Evaluation system

Evaluation of the practical exercises and final exam

FACULTY

Coordinator/s

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SCHEDULE

Schedule

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