Fundamentals of crystallography

MASTER'S DEGREE IN CRYSTALLOGRAPHY AND CRYSTALLIZATION

UNIVERSIDAD INTERNACIONAL MENÉNDEZ PELAYO

Másteres Universitarios

This document can be used as reference documentation of this subject for the application for recognition of credits in other study programmes. For its full effect, it should be stamped by UIMP Student's Office.

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

2012-13

Degree

MASTER'S DEGREE IN CRYSTALLOGRAPHY AND CRYSTALLIZATION
Curso de Postgrado en fundamentos de cristalografía

ECTS Credits

4

Type

OBLIGATORIAMANDATORY

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

García Granda, Santiago

Catedrático Universidad de Oviedo

Giacovazzo , Carmelo

Director de Instituto de Cristalografía, CNR

Lecturers

Gutiérrez Puebla, Enrique

Instituto de Ciecias de los Materiales de Madrid, CSIC

Albert de la Cruz, Armando Joaquín

Doctor en Ciencias Químicas

Investigador Científico (Área de Química)

IQFR-CSIC

Aroyo , Mois Ilia

Profesor Asociado Extranjero Universidad del País Vasco

SCHEDULE

Timetable

22/10/2012

10:00 - 11:00

General Introduction to the course

Santiago García Granda

Catedrático de Química Física
Universidad de Oviedo
Presidente de la European Crystallographic Association

11:30 - 12:30

2-dimensions periodicity

Enrique Gutiérrez Puebla

Profesor de Investigación
Instituto de Ciencia de Materiales de Madrid (ICMM)
Consejo Superior de Investigaciones Científicas (CSIC)

12:30 - 13:30

Workshop on 2-D periodicity I

Enrique Gutiérrez Puebla

Profesor de Investigación
Instituto de Ciencia de Materiales de Madrid (ICMM)
Consejo Superior de Investigaciones Científicas (CSIC)

15:30 - 16:30

Workshop on 2-D periodicity II

Enrique Gutiérrez Puebla

Profesor de Investigación
Instituto de Ciencia de Materiales de Madrid (ICMM)
Consejo Superior de Investigaciones Científicas (CSIC)

16:30 - 17:30

Open discussion

Enrique Gutiérrez Puebla

Profesor de Investigación
Instituto de Ciencia de Materiales de Madrid (ICMM)
Consejo Superior de Investigaciones Científicas (CSIC)

Santiago García Granda

Catedrático de Química Física
Universidad de Oviedo
Presidente de la European Crystallographic Association

23/10/2012

9:00 - 11:00

3-dimensions periodicity I

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

11:30 - 12:30

3-dimensions periodicity II

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

12:30 - 13:30

Workshop on 3-D periodicity I

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

15:30 - 16:30

Workshop on 3-D periodicity II

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

16:30 - 17:30

Open discussion

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

24/10/2012

9:00 - 11:00

Worshop on Space Groups I

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

11:30 - 12:30

Worshop on Space Groups II

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

12:30 - 13:30

Crystal lattices I

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

15:30 - 16:30

Crystal lattices II

Carmelo Giacovazzo

Full Professor

University of Bari, Italy

16:30 - 17:30

Open discussion

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

25/10/2012

9:00 - 10:00

Crystal lattices III

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

10:00 - 11:00

Workshop on Crystal lattices I

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

11:30 - 13:30

Workshop on Crystal lattices II

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

15:30 - 16:30

Personal or Group Tutorials

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

16:30 - 17:30

Open discussion

Carmelo Giacovazzo

Full Professor
University of Bari, Italy

26/10/2012

9:00 - 11:00

Math Review

Mois Ilia Aroyo

Profesor Agregado
Facultad de Ciencia y Tecnología
Universidad del País Vasco

11:30 - 13:30

International Tables for Crystallography

Mois Ilia Aroyo

Profesor Agregado
Facultad de Ciencia y Tecnología
Universidad del País Vasco

15:30 - 17:30

Workshop on Symmetry. International Tables I

Mois Ilia Aroyo

Profesor Agregado
Facultad de Ciencia y Tecnología
Universidad del País Vasco

29/10/2012

9:00 - 10:00

Workshop on Symmetry. International Tables II

Mois Ilia Aroyo

Profesor Agregado
Facultad de Ciencia y Tecnología
Universidad del País Vasco

10:00 - 11:00

Group-subgroup relations and lattice transformations I

Mois Ilia Aroyo

Profesor Agregado
Facultad de Ciencia y Tecnología
Universidad del País Vasco

11:30 - 13:30

Group-subgroup relations and lattice transformations II

Mois Ilia Aroyo

Profesor Agregado
Facultad de Ciencia y Tecnología
Universidad del País Vasco

15:30 - 16:30

Introduction to Reciprocal Space

Santiago García Granda

Catedrático de Química Física
Universidad de Oviedo
Presidente de la European Crystallographic Association

16:30 - 17:30

Open discussion

Santiago García Granda

Catedrático de Química Física
Universidad de Oviedo
Presidente de la European Crystallographic Association

Mois Ilia Aroyo

Profesor Agregado
Facultad de Ciencia y Tecnología
Universidad del País Vasco

30/10/2012

9:00 - 10:00

Single Crystal, Powder and Twins

Santiago García Granda

Catedrático de Química Física
Universidad de Oviedo
Presidente de la European Crystallographic Association

10:00 - 11:00

Atoms, ions, molecules and macromolecules

Santiago García Granda

Catedrático de Química Física
Universidad de Oviedo
Presidente de la European Crystallographic Association

11:30 - 12:30

Bonds and interactions in the solid state

Santiago García Granda

Catedrático de Química Física
Universidad de Oviedo
Presidente de la European Crystallographic Association

12:30 - 13:30

Conformations and chirality: Natural products and Macromolecules

Armando Joaquín Albert de la Cruz

Investigador Científico
Instituto de Química-Física Rocasolano (IQFR)
Consejo Superior de Investigaciones Científicas (CSIC)

15:30 - 17:30

Personal or Group Tutorials

Armando Joaquín Albert de la Cruz

Investigador Científico
Instituto de Química-Física Rocasolano (IQFR)
Consejo Superior de Investigaciones Científicas (CSIC)

Santiago García Granda

Catedrático de Química Física
Universidad de Oviedo
Presidente de la European Crystallographic Association