

# Fundamentals of crystallography

**MASTER'S DEGREE IN CRYSTALLOGRAPHY AND  
CRYSTALLIZATION**

***UNIVERSIDAD INTERNACIONAL MENÉNDEZ PELAYO***

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 cristalografia](#)

### 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 Ewald 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 de Química Física  
Universidad de Oviedo  
Presidente de la European Crystallographic Association*

**Giacovazzo , Carmelo**

*Full Professor  
University of Bari, Italy*

### Lecturers

**Albert de la Cruz, Armando Joaquín**

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

**Aroyo , Mois Ilia**

*Profesor Agregado  
Facultad de Ciencia y Tecnología  
Universidad del País Vasco*

**Gutiérrez Puebla, Enrique**

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



## 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

Workshop on Space Groups I

Carmelo Giacovazzo

Full Professor  
University of Bari, Italy

11:30 - 12:30

Workshop 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

Santiago García Granda

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

Armando Joaquín Albert de la Cruz

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