



# Crystallography School 2018

Organized by the Interdepartmental Centre for Crystallography (CrisDi)



Torino 28 May - 15 June 2018

## BASIC COURSES 28 May - 1 June 2018

**Prof. P. Benna**

**BC1: Introduction to Crystallography** (1½ CFU)

Crystalline State. Elements of symmetry. Point and spatial groups (examples). Direct and reciprocal lattice. International tables.

**Dr. A. Agostino**

**BC2: Instrumentation for X-Ray Diffraction** (1 CFU)

X-Rays sources. Filters and monochromator crystals. Detectors. Geometries.

**Dr. R. Cossio**

**BC3: Electron Diffraction** (1 CFU)

Electron sources: conventional and FEG. Magnetic lenses, aberrations and resolution of the electron beam: TEM, STEM, SEM. Types of electron diffraction: SAED, CBED, EBSD. Geometry, detectors and new instrumental developments.

**Prof. A. Pavese**

**BC4: X-Ray Diffraction** (1 CFU)

X-Rays interaction with matter. Kinematic theory. Ewald, Laue, Bragg. Atomic scattering factor. Structure factor and diffracted intensity. The temperature factor.

**Prof. M. Milanesio**

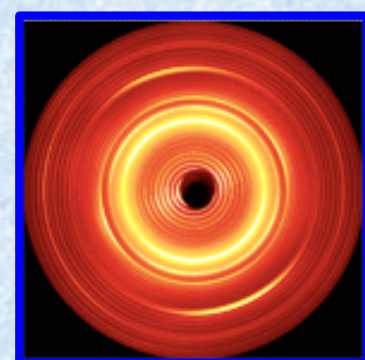
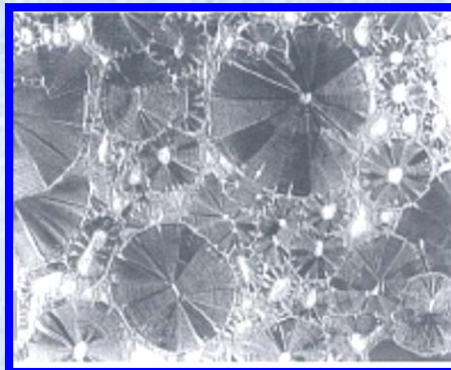
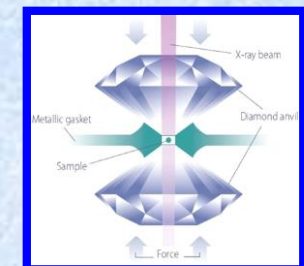
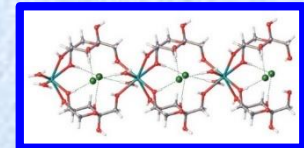
**BC5: X-Ray Diffraction Methods: Polycrystalline** (2½ CFU)

Powder diffraction: Principles. Experimental design. Sample preparation. Main instrumental aberrations. Peak profile function. Data analysis: Qualitative analysis. Data reduction. Quantitative analysis.

**Dr. D. Marabello**

**BC6: X-Ray Diffraction Methods: Single Crystal** (2½ CFU)

Definition and selection of crystals. Instrumentation. Determination of cell parameters. Data collection. Structure resolution and refinement. Critical evaluation of the results. **LAB - PART I**: Visit to the instrumental laboratory. **LAB - PART II**: Practice on structure resolution in a computer laboratory.



## SPECIALIZED COURSES

4-8 June 2018

**Prof. G. Di Nardo**

**SC1: Structural Study of Biological Macromolecules** (2 CFU)

Protein crystallization: requirements and strategies. Sample preparation. Protein crystallization methods and phase diagram. Screening of crystallization conditions. Optimization of protein crystals: seeding and additional screening. Co-crystallization with ligands: soaking. Protein X-Rays diffraction: Cryoprotectants and crystals preparation. Sample mounting. Structural solving methods: Molecular replacement. Anomalous diffraction and isomorphous replacement.

**Prof. F. Cámara**

**SC2: In situ non-ambient conditions by Single-Crystal XR Diffraction** (2 CFU)

High Temperature: Heating devices, mounting of the crystal and temperature calibration. Effects of temperature. Cell parameters and thermal expansion. Structures. High Pressure: Background & technical problems. Cell parameters & equations of state EoS. Structures. Examples of distortive phase transitions studied by in-situ SCXRD: Expansion of Landau.

**Prof. A. Ferrari**

**SC3: Solid State Properties: Modelization** (2 CFU)

Introduction to the "CRYSTAL09" code. Dielectric and electronic properties in solids. Fundamental equations. Simulation of XRD spectra. Study cases.

**Dr. E. Costa**

**SC4: Introduction to Crystal Growth** (1½ CFU)

Basic of growth mechanism: Nucleation processes. Heterogeneous and homogeneous nucleation. Growth of a crystal. Equilibrium shape. Interface and roughening. Growth technologies: Main growth mechanism. Melt grown. Solution grown. Floating zone growth. Other methods. Characterization of crystals: Crystal defects. Twins. Crystal surfaces. Inclusions and precipitates. Selected method of characterization. Etching. X-ray topography. Optical microscopy. SEM. TEM.

**Dr. N. Curetti**

**SC5: Practical course for HP in situ Experiment - Diamond Anvil Cell** (1 CFU)

DAC cell: components and assembly for HP experiment. Use of the standard-crystals for monitoring the internal P. Application of the DAC in XRD experiment.

**Dr. F. Bertolotti**

**SC6: The Debye Scattering Equation: a Total Scattering approach for characterizing Nanomaterials** (1 CFU)

Fundamentals of Debye Scattering Equation (DSE). Data collection and reduction for total scattering experiments. Characterization of structure, microstructure and morphology of nanocrystals through the DSE. DSE applications. The DebUsSy program suite: an overview. Tutorial session on the DebUsSy program suite.

11-15 June 2018

**Dr. A. Agostino**

**SC7: The Rietveld Method** (2 CFU)

Basic theory. Problems with the Rietveld method: Indexing. Peak-shape function (PSF). Background. Preferred orientation and texture.

**Prof. R. Arletti**

**SC8: Inorganic Crystallochemistry** (1 CFU)

Basis of the Crystallochemistry. Compact Packing of Sphere. Coordination Polyhedra. Crystalline Structure: examples. Polymorphism and Isomorphism: examples. Different kind of Silicates: Chain, Layered, Framework. Zeolites: structural features and properties.

**Prof. E. Belluso - Dr. S. Capella**

**SC9: Use of TEM-EDS for the characterization of Natural or Synthetic sub-micrometric Inorganic Phases** (2 CFU)

Sample preparation. Data acquisition: Morphology. Electron diffraction. Semi-quantitative composition. Structure. Refinement of acquired data.

**Prof. R. Giustetto**

**SC10: Causes of Colour in Minerals** (2 CFU)

Crystal Field Theory (in octahedron and tetrahedron); Jahn-Teller Effect. Intervale charge transitions, transitions between valence orbitals and conduction band. Colour Centres; artificial procedures to colour minerals and gems. Iridescence, Luminescence and Fluorescence.

**Prof. R. Arletti**

**SC11: In situ/operando X-Ray Powder Diffraction** (1 CFU)

High pressure X-Ray powder diffraction (cell, geometries, conventional and non conventional sources). High temperature XR powder diffraction. In situ/in operando X-Ray powder diffraction on porous materials: experiments and data analysis.

**Prof. M. Dapiaggi**

**SC12: Pair Distribution Function Analysis of Complex, Disorder and Amorphous Materials from Total Scattering Data** (1 CFU)

Total scattering data: why? How to evaluate the structure-properties relationship of complex and disorder material. Basic theoretical needs and experimental setup. Amorphous 'on the go'... very short range order. How to obtain a PDF and how to refine it to a model (practical).

**Dr. L. Pastoro**

**SC13: Crystal growth for beginners** (1 CFU)

Ideal crystal vs real crystal. How to nucleate, grow and modify crystals in lab. Surfaces and interfaces. Surface analysis by SPM technique.s

