Corso di Laurea in
SCIENZA E TECNOLOGIA DEI MATERIALI

Triennale – L30

General information		
Academic subject	***CRYSTALLOGRAPHY WITH LABORATORY***	
Degree course	*Material's science and technologies*	
Academic Year	*2021-2022*	
European Credit Transfer and Accumulation System (ECTS)		*6*
Language	*Italian*	
Academic calendar (starting and ending date)	*2nd semester, 2nd year*	
Attendance	*not required*	

Professor/ Lecturer	
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Tutoring (time and day)	Office hours, by appointment via email

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Syllabus	
Learning Objectives	*Acquiring fundamental knowledge about the crystalline solid state and single crystal X-ray scattering. Carry out an X-ray data collection from a single crystal of a material and determine its crystal structure.*
Course prerequisites	*Basic concepts of: chemistry, electromagnetism, matrices and vectors.*
Contents	***Crystallography and material's science*** *Introduction to the course. The contribution of the crystallography in several scientific fields such as: materials science, mineralogy, chemistry, earth sciences, solid state physics, cultural heritage and planetary studies. The correlation between the crystal structure and the properties of a material. Historical notes on the birth and development of crystallography: from Theophrastus to nowadays.* ***Crystals and crystallographic symmetry*** *Definition of crystal. Crystal lattice and unit cell. Mathematical description of a crystal. Symmetry operators working in the crystalline state. Center of symmetry. Rotation, inversion and screw axes. Symmetry and glide mirrors. Symmetry and Laue classes. Crystal systems. Bravais Unit Cells. Space group.* ***Diffraction of X-rays by crystals*** *Electromagnetic waves. X-rays. Wave-particle duality. Thompson and Compton Scattering. Analogy between the diffraction of X-rays and that of visible light. Laue's and Bragg's laws. Reciprocal lattice. Properties of a reciprocal lattice vector. Relationship between direct and reciprocal space. Ewald and limit sphere. Intensity of a diffraction effect. Interference between waves. Diffusion by a single atomic electron. Diffusion by an atom: atomic scattering factor. Thermal factor. Structure factor. Friedel's law and Laue's class. Effect of symmetry operators in reciprocal space: restricted phase and systematically extinguished reflections.*

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	The phase problem *Description of electron density through a Fourier series: Fourier synthesis. Origin of the phase problem. Wilson plot. Methods to solve the phase problem. Patterson synthesis and the heavy atom method. Sections of Harker. Direct methods: relations Σ1 and Σ2. Flipping charge method.* ***Structural refinements*** *Linear least squares method: Solution of the non-linear least squares problem using Taylor series approximation and the minimization of the refined parameter shifts. Refinable parameters in structural refinement. Constraints and restraints. Figures of merit of the refinement.*
Books and bibliography	*C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, M. Milanesio, G. Gilli, P. Gilli, G. Zanotti, G. Ferraris. Fundamentals of Crystallography, 3rd Edition, Oxford University Press, 2011.* *V. K. Pecharsky and P.Z. Zavalij. Fundamentals of powder diffraction and structural characterization of materials, 2nd Edition, Springer, New York, 2009 (Chs. 1- 3).* *C. Hammond. The basic of crystallography and diffraction, 3rd Edition, Oxford University Press, 2009.* *W. Massa. Crystal structure determination, 2nd Edition, Springer, Berlin, 2004.*
Additional materials	

Work schedule			
Total	Lectures	Hands on (Laboratory, working groups, seminars, field trips)	Out-of-class study hours/ Self-study hours
Hours			
150	*32*	*30*	*88*
ECTS			
6	*4*	*2*	

Teaching strategy	*Lectures and laboratory experiences.*
Expected learning outcomes	
Knowledge and understanding on:	Knowledge of the definition of crystalline state, of the symmetries operating in a crystal and of the fundamental aspects of X diffraction by single crystal. Knowledge of the structural parameters of a crystal structure.
Applying knowledge and understanding on:	Carry out structural determination on single crystals. Elaboration of single crystal X diffraction patterns.
Soft skills	• *Making informed judgments and choices* Critically assess the quality of a structural determination. Interpretation of a crystal structure. • *Communicating knowledge and understanding* Presentation and dissemination of the crystallographic knowledge with an appropriate scientific language.

	Presentation of the results obtained from a single crystal structural determination; ability to integrate quickly and effectively in the workplace and in scientific research laboratories. • *Capacities to continue learning* Learning and transfer of experimental diffraction protocol and of digital processing of single crystal diffraction patterns.

Assessment and feedback	
Methods of assessment	*Oral examination (100%)*
Evaluation criteria	• *Knowledge and understanding* ○ Minimum level: knowledge of the crystallographic symmetry, Laue's, Bragg's Law, Ewald's sphere and structure factor. ○ Intermediate level: Relationships between direct and reciprocal space. Intensity of a reflection. Influence of the symmetry operators in the reciprocal space. Experimental apparatus used to collect the diffraction patterns of a single crystal. Experimental steps necessary to perform a data collection. ○ Upper level: detailed knowledge of the structure factor. Data reduction. The phase problem and methods its solution. Nonlinear least squares method for structural refinement. • *Autonomy of judgment* ○ For the intermediate level: critical analysis of the quality of a structural determination. ○ For the upper level: correlate the parameters of the structure with some material properties. • *Communicating knowledge and understanding* ○ For all levels: the use of correct scientific terminology. Skills to discuss the topics of the course. • *Communication skills* ○ The student should properly discuss about the crystallographic concepts in an oral examination. Topics with an increasing degree of depth will be proposed in order to establish the student's level of knowledge
Criteria for assessment and attribution of the final mark	*Reaching the minimum level will result in a final grade between 18-20.* *Reaching the intermediate level will result in a final grade between 21-26.* *Reaching the higher level will result in a final grade between 27-30.*
Additional information	