Practical Crystallography

Instructor: Prof. Michael Shatruk (Florida State University, USA)

Course Description: This course provides a concise practical introduction to crystallography and X-ray diffraction, with strong emphasis on the use of these methods to characterize crystal structures of materials. The course will cover the most important fundamental concepts in the light of their application to practical problems encountered in research projects related to chemistry and materials science.

Course Content:

Unit 1. Crystal structure: lattices, unit cell, symmetry elements, space groups.

Unit 2. General principles of diffraction. Miller planes. The Bragg law.

Unit 3. Powder diffraction: principles and applications. Profile fitting and the Rietveld method.

Unit 4. Laue's view of diffraction. Single-crystal diffraction experiments.

Unit 5. Solving and refining crystal structures. Introduction to SHELX.

Unit 6. Crystallographic disorder: its physical meaning and practical modeling.

Unit 7. Structure validation and publication. Crystallographic databases.

Unit 8. Introduction to neutron diffraction. Magnetic structures.