

Crystallography workshop

Date: 08-09/12/2019

Venue: Nelson Mandela African Institution of Science and Technology (NMAIST)

Facilitators: Prof Abdelaziz El Jazouli and Prof Saida Krimi

University Hassan II, Casablanca, Morocco

Email: abdelaziz_eljazouli@yahoo.fr and krimisaida@yahoo.fr

Purpose of the workshop;

In order to understand and design new materials, the researchers need crystallographic information via X-ray and neutron diffraction experiments. Therefore education in crystallography, as well as strong contacts with crystallographers to build a network, are necessary. It is the reason why, during the 10th International Conference of the African Material Research Society (Arusha, Tanzania; December 10-13, 2019; africanmrs.net/tanzania-2019/), a two days workshop on crystallography is organized. The workshop consists of lectures and hands-on on basic X-ray diffraction and crystallography with applications to powder experiments and crystal structures of inorganic materials. Lectures will be followed by practical exercises. Participants must bring their own laptops to use for the practical sessions.

Outline

1) Introduction to Crystallography and X-Ray Diffraction (Abdelaziz El Jazouli, 4 hours):

- Notions of crystallography: direct lattice (direction, unit cell, plane, Miller indices, d_{hkl} -spacing); reciprocal lattice (definition, properties, application to the calculation of d_{hkl} -spacings), symmetry in crystallography, exercises.
- X-ray diffraction: production; absorption, diffraction, Bragg's law, intensities, XRD methods, exercises.

2) Crystallochemistry of Solids (Abdelaziz El Jazouli, 4 hours)

- Introduction to solid state.
- Classification of solids.
- Close-packed structures.
- Essential crystalline structures of solids: AX, AX₂, AX₃, A₂X₃, ABX₃, AB₂X₄.

3) XRD Rietveld Refinement (Saida Krimi, 8 hours)

- Analysis of powder diffraction data using the Fullprof Suite.
- General introduction to the programs.
- Analytical description of the powder diffraction pattern.
- Rietveld method: simulation of powder diffractograms, entering crystallographic data, refinement of crystal structure data from powder measurements and refinement strategies.

Workshop Agenda

<i>Sunday, December 8, 2019</i>		<i>Location: NM-AIST/Room X</i>
Time	Title / Instructor	
08:15.	Welcoming Remarks / Introduction to the Workshop - Prof Hulda Shaidi Swai, Nelson Mandela African Institution of Science and Technology, Arusha, Tanzania. - Prof Abdelaziz El Jazouli, University Hassan II, Casablanca, Morocco.	
08:30.	Introduction to Crystallography and X-Ray Diffraction	
	1) Notions of crystallography.	<i>(Prof Abdelaziz El Jazouli)</i>
10:00.	Break	
10:30.	2) Introduction to X-ray diffraction.	<i>(Prof Abdelaziz El Jazouli)</i>
12:30.	Lunch	
13:30.	XRD Rietveld Refinement	
	3) Presentation of Fullprof Suite program and use of Fullprof Suite Toolbar.	<i>(Prof Saida Krimi)</i>
15:30.	Break	
16:00.	4) Visualizing XRD spectra and exporting background using Winplotr program. Creating of parameter file using EdPCR program.	
		<i>(Prof Saida Krimi)</i>
18:00.	End of first day	
<i>Monday, December 9, 2019</i>		<i>Location: NM-AIST/Room X</i>
8:30.	Crystallochemistry of Solids.	
	5) Introduction to solid state. Classification of solids. Close-packed structures.	<i>(Prof Abdelaziz El Jazouli)</i>
10:00.	Break	
10:30.	6) Essential crystalline structures of solids: AX, AX ₂ , AX ₃ , A ₂ X ₃ , ABX ₃ , AB ₂ X ₄ .	<i>(Prof Abdelaziz El Jazouli)</i>
12:30.	Lunch	
13:30.	7) Refinement of spectra without structural model (Profile matching). Refinement of spectra with structural model (Rietveld method).	
		<i>(Prof Saida Krimi)</i>
15:30.	Break	
16:00.	8) Use and interpretation of the output files. Use of VESTA program to draw crystal structures.	
		<i>(Prof Saida Krimi)</i>
18:00.	Concluding remarks	