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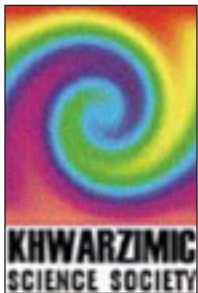
XXI Congress of the International
Union of Crystallography

23-31 August 2008



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Workshop on Structure Determination using Powder X-ray Diffraction

Lahore, Pakistan, August 2007

Crystallography is taught in Pakistan as a part of the solid state physics curriculum at the undergraduate and post-graduate levels. However, the treatment is superficial, teacher training is often inadequate, concepts such as symmetry, point and space groups are neglected and crystal structure determination is generally limited to the simplest structures. Furthermore, there are few diffraction facilities, computational resources are severely limited, and crystallographic software is generally unavailable.

With this background in mind, the Khwarzmic Science Society (KSS) (www.khwarzmic.org) decided to organize a national workshop dealing with different aspects of crystal structure determination. The workshop on powder diffraction (XRD) was the first of its kind in the country. It was hosted at the Centre for Solid State Physics in Lahore where one of the organizers (S.A.Siddiqi) is a professor. The workshop was partially sponsored by Bana International and Bruker-AXS, Germany.

The opening lecture "Diffraction Studies of Nanostructures" was given by N.M. Butt (Chairman of the Pakistan Science Foundation). As president of KSS and Chair of the Advisory and Organizing Committees, S.A. Siddiqi presented an overview of the KSS, which was established in 1997 and is arguably Pakistan's most active society for the popularization of science.



N.M. Butt in his inaugural address.

On the first day of the workshop the basics of crystallography were covered including symmetry, point and space groups, crystal lattices and the seven crystal systems. Special emphasis was placed on crystallographic notation problems students routinely face. Miller indices, planes, directions and fractional coordinates and the difference between lattices and structures were carefully described. An exercise worksheet was distributed. The second day dealt with diffraction and crystal structure determination. It featured marathon lectures by Falak Sher (Pakistan Inst. of Engineering and Allied Sciences) who methodically covered peak indexing, space group determination using systematic absences and the phase



Menges Goetz, Nazma Ikram, Ijaz M. Ghauri, Saadat A. Siddiqi, Falak Sher and Jamil Khan.

problem. M. S. Anwar (Lahore) covered the physical basis of diffraction focusing on the duality between real and reciprocal space, the Fourier and the convolution connections to crystal structure determination. On the final day, Falak Sher discussed the Rietveld method of refining trial crystal structures and demonstrated computer-based refinement methods, using the freely available program, GSAS with real examples. Menges Goetz (Bruker-AXS) described the instrumental, sample and background contributions to peak profiles and the "fundamental parameters" approach to analyzing peak profiles as it relates to refining crystal structures.

The meeting was enhanced by lectures on related topics. Ar-



Falak Sher describing the diffraction from body-centred iron



shad Bhatti (Islamabad) lectured on "microscopic characterization of nanostructures" and Umair Manzoor from the same institute discussed "Electron microscopy and electron diffraction". Speakers also made reference to neutron diffraction and synchrotron radiation throughout the lectures, adding to the value of the workshops.

Participants assessment forms indicated that the workshop was an overall success. Only 50 of more than a hundred individuals who applied could be accommodated. These were either users of XRD equipment, indi-



Participants during one of the lecture.

individuals who planned to buy new instruments under funding acquired from the Higher Education Commission (H.E.C.) of Pakistan or materials science students who were interested in learning about crystal structures. There were also a few H.E.C. Ph.D. scholars who were proceeding abroad to undertake research in the same subject. The attendees represented three (out of the four) provinces of the country and came from, for example: Sindh U (Jamshoro), Karachi U, U.E.T. Lahore, the Punjab U (School of Biological Sciences, Physics and Chemistry Dept, Centre of Excellence in Molecular Biology, Centre for Solid State Physics), Bahauddin Zakarriya U (Multan), PIEAS, Quaid-e-Azam U, Islamia U Bahawalpur, Government College of Technology (Bahawalpur), Dyal Singh College Lahore, PCSIR Labs Lahore, Pakistan Atomic Ener-

gy Commission, U of Peshawar, U of Agriculture (Faisalabad), NIBGE (Faisalabad), COMSATS (Islamabad), Vienna U (Austria).

The participants were of varied backgrounds including physics, chemistry, biology, soil and environmental sciences, materials science, agriculture, engineering and geology. More details of the events, lecture notes and photographs can be accessed from the KSS website (www.khwarzimidc.org).

The KSS is planning an International Winter School on Crystallography in the year 2008 and formation of a Pakistan Union for Crystallography Research (PUCAR – literally meaning “a loud call for attention” in the Urdu language!) is envisioned in the very near future. This will definitely consolidate crystallographic research and teaching in the country and bring our standards in line

with international practices.

M. Sabieh Anwar and S.A. Siddiqi

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