

Synchrotron Diffraction Methods Subcommittee Meeting

3 – 4 pm, Wednesday, March 17, 2010

The meeting was chaired by Matthew Suchomel from the Advanced Photon Source.

J. Reid took the meeting minutes.

Minutes from last year's meeting were reviewed and approved with no comments.

John Faber was asked about recommendations at the Board of Directors and suggested that no recommendations came to the Board from the Subcommittee.

Matthew gave some brief updates from multiple synchrotron sources around the world:

- Advanced Photon Source (APS), 11-BM beamline
 - The mail-in service has been expanded: users can specify more scan protocols and temperatures & receive additional data formats. Hot gas blower added for on-site measurements up to 950 °C.
- Australian Synchrotron Powder Diffraction Beamline
 - Added an analyzer-crystal detector and high pressure diamond anvil cell
- Nagoya University Small Synchrotron Radiation Facility (NUSRF)
 - New synchrotron with 2 powder XRD lines currently under construction.
- Shanghai Synchrotron Radiation Facility (SSRF)
 - New 3rd generation source, powder diffraction line now operational.
- HASYLAB
 - The B2 beamline at DORIS III will be closing in the next two years, to be replaced by new high resolution powder diffraction beamline at PETRA III
- Swiss Light Source (SLS), Materials Science Beamline
 - They have recently added a robotic sample changer for industrial users.
- Diamond Light Source (UK), beamline I11
 - Added PSD Mython detector (90°), starting new trial-mail in program
- National Synchrotron Light Source II (NSLS II)
 - Under construction, with high-energy powder diffraction beamline planned.

It was suggested that the ICDD should be encouraging Grant-in-Aid submissions to 11-BM specifically, and mail-in synchrotron powder diffraction beamlines in general, and a motion was proposed by Suchomel:

Motion #1

The Synchrotron Diffraction Methods Subcommittee strongly recommends that the Technical Committee encourage Grant-in-Aid recipients to utilize increasingly available mail-in synchrotron powder diffraction resources to complement in-house lab based measurements, especially for complicated patterns or patterns prone to preferred orientation and related effects.

The motion was voted on and passed with 10 votes for, 0 votes against and 0 abstentions.

Diane Sagnella (ICDD) made a brief presentation demonstrating the potential for using her program DataQuacker (DQ) for the preparation and submission of new synchrotron patterns to the ICDD.

Diane's presentation led to discussion about the feasibility of modifying DataQuacker to facilitate web-based submissions.

Brian Toby and Mark Rodriguez would like to see a direct, web-based pipeline for new diffraction data to the ICDD, and Frank Rotella indicated that a web-based, streamlined system is currently in place for the Protein Data Bank (PDB).

Mark proposed a motion to which Mike Bennett added a qualifying statement regarding ICDD correspondence with the data submitter:

Motion #2

The Synchrotron Diffraction Methods Subcommittee recommends that DataQuacker be modified to support web based powder diffraction submissions, with corresponding communications to the data submitter to ensure that the data has been transmitted properly.

The motion was voted on and passed with 12 votes for, 0 votes against and 0 abstentions.

Matthew and Scott Misture initiated discussion about the pros and cons of considering high resolution multiphase sample patterns for inclusion in the PDF, and how these types of data should be handled.

Suri Kabekkodu mentioned that some of these phases will be captured as calculated patterns after the publication of their atomic coordinates.

Jim Kaduk mentioned the value associated, in some cases, with getting phases faster than they can be abstracted and supplied by single crystal databases, and the value of proprietary powder diffraction data content that is exclusively the ICDD's.

Tim Fawcett mentioned some possible pitfalls associated with accepting multiphase patterns, and issues with lattice parameters taken from multiphase samples.

Brain made the point that there are important technological materials that can't be prepared as a single phase yet, and it is important to consider some of these multiphase patterns until better data becomes available.

Once this discussion was completed, with no new business, the meeting was adjourned.