

Synchrotron & Neutron Scattering Methods Subcommittee Minutes
International Centre for Diffraction Data
19 March 2014

Attendance: List of attendees has been generated separately.

Next to:

1. The Call to Order by Dr. Matthew Suchomel at 3:00 pm
The BoD liaison was not present; report shown from J. Faber
2. The appointment of the Minutes secretary: R. Papoular
3. The approval of the Minutes of the previous 2013 Spring Meeting

The following topics were discussed:

4. User Facility news:
 - A. Europe/ESRF (Synchrotron)**

The High Resolution Powder Diffraction beamline is moving from station ID31 to station ID22. Stopped in December 2013, it is due to restart on the second quarter of 2014 with the following improvements: more photons on the sample (due to reduced horizontal divergence) and enhanced performance in the harder energy range (due to an in-vacuum undulator). <http://www.esrf.eu/id22>
 - B. USA:**
 - **APS (Synchrotron)**
 - [i] XRD & PDF beamlines both continue to be available for mail-in and on-site users
 - [ii] 11-BM was the “top” publishing beamline at the APS in 2013 (106 publications)
 - [iii] New APS upgrade plans for ‘MBA’ lattice (2014-2020)
[A **Multi-Bend Achromat** lattice is an assembly of dipolar, quadripolar and sextupolar magnets: <http://www.aps.anl.gov/Upgrade/Workshops/2013/MBA-Technology/>]
 - **LANL (Neutrons)**
 - [i] Proposed DOE budget will “cease their operational support” at LANSCE facility and the Lujan Neutron Scattering Center
 - [ii] Includes several Crystallography, Engineering and Disordered Materials beamlines
 - **NSLS (Synchrotron)**
 - [i] As of September 30th 2014, the NSLS will be shutting down its operations
 - [ii] New NSLS-II X-ray Powder XPD beamline will be open to users ~ summer 2015
 - **ORNL [SNS & HFIR] (Neutrons)**

Full and productive suite of instruments, looking for new users
(communication from A. Payzant)
5. ICDD Databases Updates related to S&N Subcommittee
 - A.** ICDD added a new tutorial in April 2014: “How to Analyze Synchrotron Data”
<http://www.icdd.com/resources/tutorials/pdf/Synchrotron-Applications.pdf>
 - B.** T. Fawcett: New feature for 2014: Instrument Parameter Files can now be uploaded and saved for both GSAS and FullProf
 - C.** J. Faber: Current analysis of TOF energy dispersive Neutron Diffraction Data usually involves a non-wavelength dependent transmission/extinction correction. To go beyond this approximation, measuring reference materials such as Corundum and Ceria as a function of energy is planned.
6. Update on efforts to include non-CW data in PDF-4 RDB [Relational Data Base] (constant wavelength): J. Faber

Great progress in this area for 2014: A task team of ICDD members and employees has worked on recalculating all single crystal data for neutron diffraction. J. Faber worked with ICDD editors and programmers to embed this capability into Release 2014 products. The latter capability will include neutron diffraction searches and indexes.

7. Top Pharmaceuticals Structure Update: Kai Zhong
 - A. 35 new structures are included in release 2014
 - B. Dozens of new PDF files
 - C. More are in progress for 2015, which may include solid excipient studies

8. DataQUACKER/GENIE & non-GiA [Grant-in-Aid] submissions
 - A. No published examples as yet of “Data Reports” in the Powder Diffraction Journal [where “Data Reports” are Short Abstracts with DOI [Digital Object Identifier] but not included in citation ranking]
 - B. Discussion related to how and when this will be realized resulted in the first motion listed below:
“The Synchrotron & Neutron Scattering Subcommittee recommends to the Technical Committee that it supports ongoing efforts to realize short ‘data report’ style entries with DOI [Digital Object Identifier] numbers in the PDJ [Powder Diffraction Journal], especially if this be used as an example to highlight the “fast track” route from GENIE to publications.”

The motion is seconded by Pete Wallace.

Votes in favor: 10 Yes, 0 No, 0 Abstained.

Motion passes and is forwarded to the Technical Committee.

9. The following second motion was dropped without any further consideration (obsolete?):
“The Synchrotron & Neutron Scattering Subcommittee recommends the efforts to incorporate CW NPD [Constant Wavelength Neutron Powder Diffraction] in the 2014 release and encourage the Technical Committee to continue considering long term strategies for handling TOF data.”

10. New Business:
Finally, the following point was briefly brought up by M. Suchomel and left open:
Would ICDD consider [as a service] to provide standardized instrument resolution functions which could be uploaded into the database for simulation and search/match? Could ICDD provide reference samples involving an extra fee?
Question from J. Cline: Which types of Instrument Profile Functions would be supported?

Meeting is adjourned at 3:40 pm.