Synchrotron & Neutron Scattering Methods Subcommittee
Wednesday, 14 March 2018
International Centre Headquarters
Conference Room D
3:00 p.m. – 4:00 p.m.
P. Whitfield, Chairperson

1. Call to Order ***P. Whitfield***

2. Appointment of Minutes Secretary ***D. DelCasale***

3. Approval of Minutes from March 2017 ***J. Faber, A. Payzant***

4. Review of Mission Statement

> The Synchrotron & Neutron Scattering Methods Subcommittee of the International Centre for Diffraction Data (ICDD) will connect the ICDD's Technical Committee with the international synchrotron and neutron scattering community. It will educate ICDD members about advances within the community, and help identity new opportunities to enhance ICDD databases. The subcommittee will provide recommendations to address unique aspects associated with these experimental methods, and will assist the technical staff of the ICDD to integrate information obtained at synchrotron and neutron scattering facilities into the ICDD databases.

5. Board of Directors' Liaison Report ***R. Papoular***

No motions to report

6. TOF Developments in PDF-4 ***S. Kabekkodu (absent)/J. Blanton***

J. Blanton reported that in the 2018 Release, developments implemented for TOF data included d-spacing and intensities to allow users to import TOF neutron diffraction patterns, whether in .cif or .xye format, to get the peak positions of the pattern and then perform a phase identification. In 2019, nothing additional was added in terms of functionality, but we will now begin calculating TOF data for new entries in future releases.

7. ICDD requests TOF data files ***J. Blanton***

Discussion and questions about how to submit TOF data to ICDD. Should there be guidelines in order to submit TOF data? Genie is not suitable for this type of submission.

Motion: The Synchrotron and Neutron Scattering Methods Subcommittee recommends to the Board of Directors that clarification and submission requirements are needed for TOF data submissions. A user Guide for submission of TOF data is requested.
Scott Misture moved the motion. John Faber seconded the motion, 5 yes, 0 No, 0 Abstain

8. User Facility News-update ***Pam Whitfield***

ORNL
SNS-Currently on shutdown for inner reflector plug replacement. Planned startup in May 2018.

POWGEN
Rebuild is complete, and redistribution of some detectors to second side. Ten additional detectors and new radial collimator added. The Tzero chopper is being replaced of which is a vital component to maintain low background.

HFIR
A new detector on WAND. The delivery of the new detector for NRSF2 beamline is expected soon.

CANADA

The NRU reactor shuts down for decommissioning in March 2018 after 60 years of operation. A proposal was made to upgrade the MNR reactor at McMaster University and move some smaller instruments (not C2) from Chalk River.

Argonne- APS
11-BM-Continuing the successful the mail-in program. Data used by Jim Kaduk for ICDD Pharmaceutical Project.

ESRF
The upgrade project consists of one-year shutdown from mid-2018 for the ring upgrade. Increase in brilliance by an order of magnitude. There are no planned instrument upgrades for the high-resolution beamline (ID22). The required upgrades were completed during the move from the previous location at ID31.

SLS
There will be a few months downtime planned in early 2019 due to nearby construction work, which will cause vibration. The planning is also underway for a future ring upgrade. MS beamline – Eiger2D detector to replace Pilatus and long-term replacement for the Mythen PSD.

SwissFEL
There is instrument commissioning underway. This is only relevant for macromolecular applications

ISIS
HRPD is next instrument in line for an upgrade.

Diamond
ID15-2 PDF beamline will be offering mail-in access this year.

ANSTO ***Vanessa Peterson***
The new China Spallation Neutron Source (CSNS) in Dongguan, about 60 miles north of Hong Kong, produced its first neutrons at the end of August 2017 and recently its first neutron powder diffraction pattern.

9. Magnetic contribution(s) to PDF entries?

   A. Payzant mentioned that the comments section should be used to indicate magnetic structures but it is rarely noted.

Motion: The Synchrotron and Neutron Scattering Methods Subcommittee recommends to the Board of Directors that headquarters explore the flagging of the elements that pose issues for neutron simulation and known magnetic structures.

J. Faber moved the motion, R. Papoular seconded, 5 Yes, 0 No, 0 Abstain

10. New & Other Business

Pair Distribution Function generation? Any benefit in having a PDF generation? Atom-atom pair distance. This would be useful for pharmaceuticals, polymers, etc.

Motion: The Synchrotron and Neutron Scattering Subcommittee recommends to the Board of Directors to explore:
Pair Distribution Function to be generated from PDF.
John Faber moved the motion, S. Misture seconded, 4 Yes, O No, 1 Abstain

11. Adjournment
The Meeting adjourned at 4:00 p.m. ***S. Misture***