

Synchrotron & Neutron Scattering Methods Subcommittee

Meeting Minutes

25 March 2015

Matthew Suchomel, Chairman.

1. The session was co-chaired by Matthew Suchomel and Pamela Whitfield. The latter, currently at ORNL/SNS (Oak Ridge, Neutron Spallation Source), is stepping in as the new chair for the subcommittee.
2. R. Papoular is appointed Minute Secretary for the session.
The 2014 Minutes of the Subcommittee 2014 are approved.

3. Session started off with the Board of Director's Liaison's Report (BoD temp. Liaison: J. Faber)

The latter revolved around:

- [i] News about the GENIE software
- [ii] Recent additional work about Neutron Diffraction capabilities in the PDF-4+ Release 2014 (for CW measurements).
- [iii] Search and Identify features with Sieve/Sieve+.

In more details:

- [iv] D. Sagnella & E. Foster have written a paper about the GENIE software, with an emphasis on the new capability to Search and Identify neutron diffraction data and do quantitative analysis using the RIR method. [D. Sagnella & E. Foster Powder Diffraction/Volume 29/Supplement S2/December 2014, pp S31-S34.]
- [v] A large amount of work went into developing Neutron Diffraction Capabilities in PDF-4+ 2014 (CW neutron powder Diffraction). This effort is mentioned in part in the technical bulletin: [PDF-4 User's Guide to Synchrotron Data Analysis and Neutron Data Analysis (2014)]
- [vi] Additional comment by T. Fawcett
Any Tutorial(s) for GENIE? Yes, for X-rays; No, for Neutrons
- [vii] A lot of effort went into documenting the Sieve+ software, including technical bulletins and a 30-mn video by T. Fawcett, which are easily accessible from the ICDD webpage.

Most noticeably, a technical bulletin "Search and Identify with Sieve/Sieve+," can be freely retrieved from the ICDD website as a 22-page PDF file. This part of the session was concluded with information from M. Suchomel and a discussion on:

- [viii] "Rapid Communication [= RC]" papers published or in the press for the PDJ.
Briefly: - about 10 RC's in 2014
 - Most of them deal with the 'TOP 200' Pharma Project.
 - One RC is one page long:

- + The Top Half consists essentially of a title, an abstract and the list of authors.
 - + The bottom half typically consists of a figure featuring the diffraction pattern data and the solved or refined crystal structure (or part of it).
- [iv] Additional comment by M. Suchomel, and potential motion to the Technical Committee:

As they currently stand, RC's do not acknowledge, however briefly, the use of a large scale facility nor capture experimental facility details in the text. Should they not? The following suggested Motion, put forward by M. Suchomel, did not fly: "The Synchrotron & Neutron Scattering subcommittee recommends to the Technical Committee that Rapid Communication papers include appropriate brief user facility information and user agreement information" such as, in the case of the use of APS/11-BM beamline : "Use of the Advanced Photon Source at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract No. DE-AC02-06CH11357."

4. The next part of the session involved information about Synchrotron and Neutron Facilities in the world. The Synchrotron hemisphere was covered by M. Suchomel, while P. Whitfield covered the Neutron World.

4.A Synchrotrons around the World (M. Suchomel)

The following facilities were discussed in order:

4.A.1 ESRF (France)

- The High Resolution Powder Diffraction Beamline has moved and changed its name accordingly [from ID31 (previously) to ID22 (currently)].
- A facility upgrade (associated with a 12-24 month shutdown) will take place in 2019-2020.

4.A.2 ALBA (Spain)

- The dedicated Powder Diffraction beamline there is codenamed: BL04-MSPD. [BL = Beam Line; MSPD = Material Science and Powder Diffraction]. It is dedicated to high resolution but also high pressure experiments.
- It is now endowed with a MYTHEN strip detector and a MAD26 HR detector featuring 13 channels.
- The HP station makes use of a MarCCD plug-in for a RAYONIX SX165 Camera.

4.A.3 APS/ANL (USA)

- 11-BM HR Beamline: Continued (and busy) mail-in program. Saul Lapidus is taking the lead after the departure of M. Suchomel for CNRS, Bordeaux.

- 17-BM (Area Detector Beamline) is currently being upgraded. This beamline is mostly dedicated to Rapid Acquisition and High Pressure Work.

4.A.4 NSLS & NSLS-II (USA)

- The original NSLS was closed in the Fall 2014.
- New NSLS-II X-ray Powder Diffraction (XPD) beamline, is endowed with hard X-rays (in the 40-80 KeV range).
As of the date of the writing of these Minutes and as initially foreseen:
 - + First user experiments started in the Summer 2015.
 - + One Powder Diffraction beamline is operational and codenamed: XPD-1. The beamline itself is 28-ID-1. It operates with X-rays in the 30 - 70 KeV range. There is an emphasis on measuring PDF's (Pair Distribution Functions).
 - + This first beamline should be complemented later with the XPD-2 station, located at the 28-ID-2 beamline and nearly entirely dedicated to measuring Pair Distribution Functions [PDFs].

4.A.5 MAX-IV (Lund, Sweden)

- As of today (21 Jan 2016), MAX-IV is the planned next-generation synchrotron radiation facility in Lund and should be inaugurated next June 21, 2016.
- The first beamlines should start operation soon after, making use of a 3 GeV ring.
- Although a station dedicated to macromolecular crystallography is due to start operation shortly, there is no plan there for a dedicated powder diffraction beamline going into operation before 2019.

4.B Neutrons around the World (P. Whitfield)

4.B.1 LANL / LANSCE (Los Alamos, USA)

- The user program is now effectively closed.
- Most of Personnel have moved to Oak Ridge (ORNL).

4.B.2 ORNL = SNS + HFIR (Oak Ridge, USA)

SNS = Spallation Neutron Source

HFIR = High-Flux Reactor

P. Whitfield praises the friendly staff there, and advocates the use of the new POWGEN and NOMAD Powder Diffraction Beamlines. POWGEN is the High Resolution powder diffraction beamline, whereas NOMAD [for Nano Materials Diffraction] is a medium-resolution beamline geared towards the measurement of Pair Distribution Functions. Limited Mail-in options exist for both POWGEN and NOMAD.

POWGEN has started a new partnership with beamline 11A at the Advanced Photon Source where users can get X-ray data if they have

an approved proposal at POWGEN. [GEN for General purpose beamline].

4.B.3 NRU (Chalk River, Canada)

NRU = National Research Universal.

Should close down on March 31, 2018.

4.B.4 OPAL Research Reactor (Australia)

The Open Pool Australian Lightwater (OPAL) reactor is a state-of-the-art 20 Megawatt reactor and it is a very productive one.

High-Flux Neutron Powder Diffractometer: Wombat High-Resolution Neutron Powder Diffractometer: Echidna

4.B.5 ILL (France) is now back up and running.

This first review was completed with information regarding other facilities, such as ISIS (UK) and J-Parc (Asia) without forgetting the planned European Spallation Source [ESS] foreseen to start operation in 2019 with its first neutrons and followed with a Users' program scheduled for 2023.

4.B Comment by T. Fawcett about the Russian Dubna reactor: JINR/Frank Laboratory for Neutron Physics which produces neutrons but mostly for Partner Member Nations (from the former Eastern Bloc).

4.C 18th-Joint Synchrotron/Neutron School in 2016 P. Whitfield draws this part of the session to a close by advertising the three-week long Joint APS/ORNL Synchrotron X-ray/Neutron School, of which ICDD Fellow member B. Toby is the Co-director.

More about this school can be found at the following website:

<http://neutrons.ornl.gov/nxs>

50 attendees were selected out of 200 applicants. Mostly 2nd-3rd year grad-students. The school consists of lectures in the morning(s) and tutorials and experiments in the afternoon(s).

5. Update on the TOF & CW Neutron Developments within PDF-4+ (by J. Faber). It is followed by a solid discussion, involving among others: P. Whitfield, J. Faber, C. Hubbard, and A. Payzant.

Most noticeably:

- Search match is now functioning for constant wavelength [CW] neutron data.
- Next step is to get it to work with TOF neutron data. The requirement for the inclusion of information regarding various line shapes and instrument response functions for various TOF instruments is emphasized.

6. Two Motions for 2015 (M. Suchomel):

Proposed Motion #1:

"The Synchrotron & Neutron Scattering Subcommittee recommends to the Technical Committee that funding be provided for J. Faber to continue his efforts in implementing search-match capabilities for neutron time-of-flight [TOF] data."

6.1 Additional Comment from T. Fawcett: Nice motion, but money is already in the budget for it.

Motion passed. 10 YES, 0 NO, 1 ABS

Proposed Motion #2

"The Synchrotron & Neutron Scattering Subcommittee recommends to the Technical Committee that the ICDD support efforts to capture additional information such as magnetic structures (including transition temperatures) from neutron-derived structures and experimental data."

6.2 Additional comment from S. Kabekkodu: What about Experimental Neutron datasets?

6.3 Additional comment from P. Whitfield: A Magnetic CIF-format is not as yet well and uniquely defined.

6.4 Additional comment from T. Fawcett: We do need as much as possible neutron data (magnetic and otherwise) irrespective of a non-definitive CIF format.

6.5 Additional comment from S. Kabekkodu: It is so far possible to calculate magnetic neutron spectra using the JANA software.

6.6 Conclusion comment from T. Fawcett: Carry this plan as a two-step process:

[i] First, start to work with experimental magnetic data as soon as possible.

[ii] Second, take care of calculated data as well, but only as a second step.

Motion passed. 10 YES, 0 NO, 0 ABS

7. Meeting is adjourned at 4:00 pm.

Respectfully submitted by R. Papoular on January 21, 2016