

Synchrotron & Neutron Scattering Methods Subcommittee
International Centre for Diffraction Data
Minutes of the Meeting of March 13th, 2013

Attendance: List of attendees has been generated separately and on record at ICDD.

1. Call to Order by Dr. Matthew Suchomel at 3:00 pm
The BoD liaison officer Dr. Vanessa Peterson was excused. Dr. John Faber filled in instead.
2. Appointed Minutes secretary: Robert Papoular
3. The Minutes of the previous 2012 Spring Meeting are approved.
4. Dr. John Faber reported on the current Neutron Scattering Project. The latter involves J. Faber, C. Crowder, O. Gourdon and S. Kabekkodu.

A first purpose of this project is to expand the PDF-4 RDB [Relational Database] format to include CW [Constant Wavelength] and TOF [Time-of-Flight] neutron as well as EDS [Energy Dispersive] X-ray information.

A second goal is to modify the POWD12++ interface, which generates calculated diffraction patterns from PDF cards, in order to include Neutron Scattering.

A. What has been completed so far?

POWD12++ has been modified to obtain neutron calculated diffraction patterns from X-ray PDF cards by:

- [i] incorporating elemental neutron cross-sections into the software [e.g., neutron absorption, energy-dependence, new isotope table ...]
- [ii] Modifying the LP [Lorentz-Polarization] correction factors, since the latter are different for neutrons and X-rays.
- [iii] computing I / I_c [relative intensities] for neutron data.

B. What remains to be done:

...is to compute [d (d-space), I (intensity)] pairs for the 172,000 entries that have atomic coordinates in the 2012 PDF-4 RDB for the PDF card.

A most important point emphasized by Dr. J. Faber is the establishing of a composite (effective) resolution for a representative neutron powder diffractometer obtained by averaging the [U,V,W] Caglioti parameters over the triplet values obtained at various Neutron Scattering Centers in the USA.

Another implementation yet to be carried out relates to TOF neutron diffraction data measured at a fixed angle [LANSCE, Los Alamos]. The latter implementation requires the use of calibration and taking into account the associated complex Instrument Response Function.

C. More efforts in progress include:

- the Test Refinement by Prof. E. Antipov of neutron calculated data
- The acquisition and the subsequent Le Bail fitting of EDS X-ray data obtained at the NSLS light source [Brookhaven, NY].

5. Comments are then made on the two motions submitted to the Technical Committee in 2012:

The first 2012 motion recommended short citations in the journal "Powder Diffraction" as an incentive for the "submission of timely and high-quality database entries" using the web-based DATAQUACKER [Genie] devised and implemented by ICDD staff Dr. Diane Sagnella.

Diane gave a short update on the great DATAQUACKER [Genie] web interface progress.

ICDD's Executive Director Dr. Tim Fawcett's feedback suggested two types of fast track publications:

- [i] rapid communications that would be cited in "Powder Diffraction"
- [ii] short reports that would not.

After some discussion it was established that all published reports would get DOI [Digital Object Identifier] numbers that can be cited, but only the longer "rapid communications" are counted against the PD journal's impact factor.

- The second 2012 motion recommended that "neutron data be added to the database". In view of the update by Dr. John Faber on "NON-CW Patterns in the ICDD Database", it was suggested to include in the motion that ... ongoing efforts to incorporate non-CW diffraction [let it be either NPD TOF (Neutron Powder Diffraction Time-of-Flight) or X-ray EDS (Energy Dispersive diffraction)] be continued, and that the Technical Committee and ICDD staff are encouraged to contact members regarding possible submissions to the ICDD PDF databank.

6. Miscellaneous topics briefly mentioned upon closing session:

- [i] Can any use be made of the Rietveld Users' list archive [maintained and moderated by Dr. Alan Hewat, ILL / Grenoble, France]?
- [ii] Is there any way the ICDD databases may be turned into databases adaptable to each user's instrument profile [specific resolution function]?

7. New motion in 2013: None Meeting is adjourned at 4:00 pm.

Respectfully submitted by Robert Papoular on April 5th, 2013.