Synchrotron & Neutron Scattering Methods
Wednesday March 16th, 2016
Chair – Pamela Whitfield

Called to order by P. Whitfield
Minutes approved as written. T. Blanton motioned; C. Segre seconded

Amy Gindhart was appointed minutes' secretary.

Reviewed mission statement – no changes suggested
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.

Board of Directors' Liaison Report – V. Peterson
Motion has been implemented for TOF data in the database.
Further optimization is needed and that will appear in 2017 product.
Grants are in place collecting data to get magnetic structures, still in process since grant cycles are still open.

S. Kabekkodu – TOF Developments
Data has been tested using 1005 entries with TOF integrated intensities.
Database was tested with ICDD validation process.
Successfully processed all the entries and the template database is now available for program development.

J. Blanton – TOF developments in the software
2014 – Constant wavelength neutron simulation/phase identification in PDF4+ products for entries with atomic coordinates or structure factors
2016 – TOF simulations using a Fortran program coded by J. Faber
- only works for patterns with atomic coordinates or structure factors
- TOF profile function 1 or 3 from GSAS.
- Tested files from ORLN-POWGEN and ISIS-Polaris
- Fullprof format is supported
- X-axis now allows d-spacing, time-of-flight, 1/d and Q

He provided a quick demonstration of the usage in the newest PDF-4+.
Isotopic Substitution for Neutron Diffraction Patterns – applied to both CW and TOF.
2017 release – TOF Phase ID being prepared within SIeve+

J. Faber – For the first time, we are dealing with I/Ic for TOF data and CW data.

P. Whitfield provided a brief update on User Facilities-

Synchrotron:
ESRF (France) – ID22 new goniometer to be installed later in 2016
Australian Synchrotron – now run by ANSTO. 10 years funding in place. Powder diffractometer goniometer just refurbished.
APS (USA) – 11 BM mail-in program close to being oversubscribed.
NSLS-2 (USA) – XPD now in the user program with 2D detectors
Diamond (UK) – I15-1 will enter user program in April. I11 operating for 6 months

Neutron:
SNS & HFIR (USA) – HFIR now running 7 cycles per year, up from 6; POWGEN rebuild will be started at the same time as replacement of inner reflector plug, so it is expected to be out of user program until after commissioning
NCNR-NIST (USA) – BT-8 new monochromator being installed in 2016
Chalk River (Canada) – NRU now run by Canadian Nuclear Laboratories; scheduled to close in 2018
ISIS (UK) – Hoping to continue upgrade of HRPD 90 degree detectors; IMAT being commissioned with imaging detector; diffraction detectors will follow when funding permits. GEM next in line for upgrade.
ANSTO- V. Peterson- Facility has been taking on a lot of work from J-PARC reactor that has been down and has been a very active site in general this past year.

T. Fawcett – wants a copy of the slides of user facilities to make sure we are sending information to the right people from ICDD headquarters.

P. Whitfield – trying to dig up data from NOMAD for use in TOF search match.
V. Peterson said she can get some J-PARC data to contribute to help with the TOF search match.

J. Faber – really wants more experimental data into the PDF products, so definitely need to drive the organizations to help contribute data.

C. Hubbard- Tell collectors that submitting through PDJ would help get more publications on materials using neutron and synchrotron data, as well as get more data into the databases.

No new business to discuss.

No Motions