

XRD Subcommittee Meeting Minutes
25 March 2009
Jim Cline, Chairman
Minutes recorded by Scott Speakman

1. 2008 Meeting Minutes approved. (Motion by J. Faber.)
2. Nothing of significance reported from the Board (J. Faber)
3. B. He presented a report from the 1D/2D Detectors Task Group.

This was only a partial report from the task group since D. Balzar was absent. Topics of concern that the task group had discussed included:

 - a. Phase ID with linear/area detector
 - b. Factors in 2D data collection that produce systematic differences in relative peak intensity compared to conventional Bragg-Brentano geometry
 - c. Goals for 2D data (work in progress):
 - i. Ability to calculate 2D XRD pattern from PDF with corrected intensities
 - ii. Ability to convert 2D data into a reference useful for comparison to Bragg-Brentano data
 - d. Long term goal - direct phase ID from search/match of 2D data
 - e. B. He announced Upcoming Publication: Two-Dimensional X-ray Diffraction (J. Wiley)
 - f. Questions/Discussion Topics from audience included:
 - i. Statistical precision of photon counting with different area detectors
 - ii. Resolution possible with 2D
4. J. Cline started a follow-up discussion focusing on data from these detectors being submitted to ICDD.
 - a. Discussion/Question: What is ICDD's policy with respect to submission of data from these instruments?

Notes from the subsequent discussion:

 - i. There is currently no policy (S. Misture response).
 - ii. It was asked if some policy needs to be established.
 - iii. T. Blanton suggested that ICDD record, in experimental details, that data were collected with 2D detector.
 - iv. J. Cline suggested that submissions from 2D detector include calibration data (or verification of system) using SRM 676a.
 - v. S. Misture began a motion (not brought to vote): Recommend to the Board that we place a flag on 2D data to identify it in the database.
 1. S. Kabekkodu responded with modification to the motion: ICDD create a field for all data to indicate the type of detector used.
 2. Discussion considered that many different experimental details don't have flags too (incident beam optics, etc.).
 - vi. An informal suggestion was made that submissions from 2D detectors should include the original raw data.
 - vii. P. Whitfield suggested that it is important to note if multiple frames have been merged when submitting 1D data converted from 2D data.
 - viii. T. Blanton stated that long-term goal of ICDD is to have raw 2D data in database (ex., reference patterns for oriented polymers).

- ix. J. Faber's input was that there's value in recording 2D data and showing the picture; start with simple steps of storing and including the data.
- b. **CONCLUSION:** ICDD should note in the comments of the PDF reference, when data was collected with a 2D detector system.
 - i. This was not a formal motion, but rather a vocal recommendation from the body to ICDD headquarters.

Motion: S. Misture moved to close 1D and 2D Detector task group.
Motion passed.

- 5. J. Cline: The subcommittee requested that ICDD's editorial board (i.e., Kabekkodu) identify and submit a list of any requirements or additional developments necessary to accommodate 2D data in the database.
 - a. Subcommittee will reform task group to address any outstanding issues that are identified by the editorial board.
- 6. P. Zavalij gave a report of the Raw Data File Format task group.
 - a. Outcome was use of cif format.

Motion: P. Zavalij moved to close raw data file format task group.
Motion passed.

Meeting adjourned.