

International Centre for Diffraction Data
ELECTRON DIFFRACTION Subcommittee Minutes
Wednesday, 19 March 2014
B. Wheaton, Chairman

1. Call to Order and Opening Remarks Bryan Wheaton
Roll Call and Attendance (See attendance sheet)
2. Appointment of Minutes Secretary
S. Gates was appointed to record minutes.
3. Approval of the 2013 Minutes
 - Motion moved by: T. Fawcett
 - Seconded by: C. Crowder
 - 5-YES, 0-NO, 0-ABSTAIN
4. Review of Mission Statement
Read through by B. Wheaton and no changes were suggested.
5. Report of Board Liaison John Anzelmo
No report to give.
 - B. Wheaton read comment from Liaison report left by Executive Director:
***General Comment:** The electron diffraction tutorials (2) and associated publication continue to be most frequent downloads on our website.*
6. Marketing Sales Information T. Fawcett
 - B. Wheaton indicated that he believes there is a need for education to the electron diffraction community about the ED based capabilities of PDF-4+.
 - Mention of upcoming (ED focused) technical bulletin that is being prepared by S. Gates
 - Opened discussion for possible workshops or training sessions
7. Electron Diffraction Software
 - Updates were given by K. Zhong about the new ED auto spot indexing features of PDF-4+.
 - P. Zavalij offered some insights into other possible methods that can be used to enhance the auto indexing feature issues addressed by K. Zhong during his presentation. C. Crowder will discuss these items with K. Zhong and P. Zavalij.

ACTION ITEM #1: T. Fawcett noticed a misprint in the ED auto indexing software. “Use strongest **peak**” instead of “Use strongest **pattern.**” (Science Department)
8. Discussion of Old Business
 - J. Friel provided an update on the EBSD ASTM standard. He indicated that a round robin study was carried out (by Andrew Deal) on samples sent to 12 laboratories, and the results have been published in a report (E41008) and a new EBSD standard defined (Z2627).
9. Discussion of New Business
 - B. Wheaton indicated that there are some upcoming electron diffraction based events:
 - Workshop at the Denver X-ray Conference by Stuart Wright (EDAX)
 - ED session at the Denver X-ray ConferenceB. Wheaton requested that every committee member help promote these events.
 - Responses were reviewed pertaining to where the focus of the ED Subcommittee should go now that the previous tasks have all been completed. Several subcommittee members submitted suggestions via email (*below*) and the topics were discussed.
 - Email Response I (*below*)
 - T. Fawcett – Indicated that there is an instructional presentation that could be used as a tutorial.

ACTION ITEM #2: Post new electron diffraction tutorial to the website (T. Fawcett)

- Email Response(s) II & III (*below*)
ICDD has already been discussing implementing a 2-D → 1-D data conversion feature, and the committee agrees it is a good idea. Some research needs to be done to determine the stipulations for doing this.

ACTION ITEM #3: Investigation into methods for generating a 2-D → 1-D data converter into PDF-4 (Science Department)

10. Suggestions?

- An email sent by J. Kaduk was discussed. He suggested we align with an electron microscopy school at Madison Area Technical College in some way to better market to the electron diffraction community.
 - H. McDonnell indicated that she has already contacted them and has offered our support in the form of demo database use.
 - Suggestion made to also contact San Joaquin College (California), who runs similar courses.

11. Adjournment

Subcommittee Member Responses to Electron Diffraction Needs

- I. I have been on this committee for many years. At meetings, we are often forced to discuss problems with making the relational database produce search/match output that fits our needs in electron diffraction. For example, most of us who identify small phases by electron diffraction in the TEM use the EDS X-ray spectrometer to determine the elements in the phase. In years past, ICDD produced a book of d-values organized by elements that could be detected with Be-window and atmospheric thin window X-ray detectors. That book was very convenient, even with the few errors that the community has identified over the years. It would be useful to have a search routine that simulated that type of look-up. With the relational database, it may even be possible to improve on the convenience of that book. I know that ICDD has made good strides in ED zone axis pattern simulation and orientation simulation. However, I believe there is value in finding a new way to tap into the PDF file to extract ED information for phase identification. Of course, one recent difficulty is the success of EBSD for phase ID in the SEM. EBSD search routines are quite different, and they may have taken our eyes off thin specimen analysis. Now there is interest in "transmission-EBSD", which may take our eyes even further off the ball.

Elemental and Interplanar Spacing Index: for phase identification by electron or x-ray diffraction, V. L. Himes, A. D. Mighell, J. K. Stalick, S. L. Young, M. J. Carr, C. E. Lyman, R. Anderson, M. A. Holomany, and R. Jenkins (eds.), NIST and ICDD, 1989.

- II. People are showing more interest in electron diffraction in last couple of years. As you know, it is possible to take powder ring patterns in electron diffraction routinely and quickly, then these ED ring patterns then can be integrated to get a pseudo powder pattern, and then these pseudo powder patterns can be used to identify compounds or polymorphs. There is software that can do this ED ring pattern integration; it would be really helpful if this can be streamlined.
- III. I'm sure you're aware that 2-dimensional X-ray detectors are becoming common, and that they produce much the same kinds of information about angular variations in intensity corresponding to the same d-spacing that one can obtain from TEM electron diffraction patterns. This information has historically been the basis for phase identification and diffraction pattern indexing in TEM patterns, but isn't used by the current ICDD search/match algorithms.

I've been wondering what (if anything) the ICDD plans to do to take advantage of the angular information available with a 2D detector. I think it's worth making sure they are aware of similarities between TEM diffraction patterns and data from 2-D XRD detectors, so that any changes they make for 2D XRD can be applied to data from both kinds of instruments.