Electron Diffraction Subcommittee Meeting Minutes
Tuesday, 9 March 2021
International Centre Headquarters
Virtual
10:30 am – 11:30 am
Alina Bruma, Chairman

1. Call to Order and Opening Remarks   A. Bruma
       Attendance tracked through Zoom.

2. Appointment of Minutes Secretary – J. Cannon appointed to record minutes.

3. Approval of 2019 Minutes
       ➢ Motion moved by: Alina Bruma   A. Bruma
       ➢ Second by: Tim Fawcett
       No objections, Motion passed with unanimous consent.

4. Review of Mission Statement -   A. Bruma

    The Electron Diffraction Subcommittee serves as a bridge between the electron diffraction
    community and the other parts of ICDD. It will communicate the needs of electron diffraction
    specialists to ICDD, so that ICDD may more effectively respond to those needs. It will assist in
    communicating to the electron diffraction community the way in which ICDD will serve them. To
    these ends, it will cooperate with other ICDD subcommittees and with the central organization of
    ICDD. Specifically, the subcommittee shall monitor the status of and suggest improvements to
    the databases and related products used in electron diffraction (those produced by other
    organizations, as well as those produced by ICDD).

5. Board of Directors' Liaison Report   (No motions or Report)   M. Leoni

6. ED Software suggested updates: work developed during 2020   A. Bruma

    User feedback and additional features implemented from last release and for next release:
       ➢ Alina Bruma Slideshow improvements suggested and implemented:
              ❖ Capability to perform measurements directly on the diffraction pattern
              ❖ Ability to drag and drop measurement tools (i.e. protractors, rulers, etc.) to measure
                 angles between diffraction spots in a pattern and distance between spots
              ❖ Tools to have a center transparency and drag and drop feature
              ❖ When a pattern was rotated the spots were rotating but the labels were not rotating or
                 fixed to the diffraction spots. This has been corrected
              ❖ Capability to move the label regarding the zone access to different parts of the
                 diffraction pattern
              ❖ To have scale bars directly placed on the diffraction pattern
              ❖ Including in software a table containing D spacing, HKL indices and Intensity of spots
              ❖ To have the ability to select specific diffraction spots
              ❖ To display a tooltip when user hovers at a specific reflection of interest
              ❖ Possibility to reset the view to the original zone access
              ❖ Diffraction pattern background color and modify color for specific spots
              ❖ Capability to overlay the diffraction pattern over another, have transparency feature
                 and a rotation capability
              ❖ Open .xrdml files following a drop down menu

       ➢ Conclusion:
              ❖ Second pilot testing completed: the software was very well received, found easy to
                 use, easy to install, has a good breadth of information available, quite powerful solving
                 problems of indexing diffraction patterns and fulfills common use cases

7. New Features Demonstration   J. Blanton / S. Webber

       ➢ Justin Blanton live demo of these features and changes:
              ❖ Zone access label can be dragged wherever the user wants

- ❖ Reset zone access with a Reset View button
- ❖ Background color is changeable
- ❖ Transparency setting slider to increase or decrease the transparency of the spots
- ❖ Interactive D spacing table
    - ▪ Clicking on a spot highlights those in the table (checked and bolded) and adds a label to the spot
    - ▪ Can change the units for the D spacing
    - ▪ Click on a row in table it will halo the spot selected
    - ▪ Customize labels of spot information
- ❖ Bug fixes
    - ▪ Rotation angle
- ❖ Looking to add the ability so that if you have a spot pattern open in the PDF and want to open it into a spot pattern module we'll implement a "File, open with feature" that will launch his advanced spot pattern simulator
    - ❖ Any features not implemented are on the to-do list for the next release
    - ❖ Suggested for overlaying to have both a foreground transparency and background transparency capability and rotation of the patterns as well

- ➢ Steffen Weber video on Electron Diffraction Tools
  (Not included in video but noted is that the module can overlay as many images or simulations as you want and each item has its own transparency controls)
    - ❖ Stand-alone application to be bundled with PDF-4+ database, launched from DDView SAED simulation window and DDView will provide XML file with info already entered by the user (camera constant, etc.)
    - ❖ Features of the application:
        - ▪ Image display & manipulation
        - ▪ SAED simulation (single or multiple)
        - ▪ Measurement tools (scalebar, ruler, protractor, grid)
        - ▪ Grid Indexing
        - ▪ Stereographic projection
        - ▪ Structure display
    - ❖ Modify file menu in the DDView SAED simulation window to add an item such as "Open in SAED Extension"
    - ❖ DDView provides XML file with info (ex. PDF number, camera constant, camera length, voltage, wavelength and image file name if specified)
    - ❖ Features for project - demo video SAED extension module:
        - ▪ If launched from DDView it will provide PDF number, one can add images and structure files, PDF entries from the installed PDF databases.
        - ▪ Elected files listed on the side with the image first and structural overlays below. It can be collapsed from thumbnail view to list view.
        - ▪ Main display in center with the image drawn first and structural overlays on top, wolf net projection to the right and below the hkl list with the reflections, atom list and unit cell atoms
        - ▪ Everything is synchronized so when the structure is rotated the simulated diffraction pattern also rotates
        - ▪ Orientation matrices can be saved in the list and recall them
        - ▪ Can rotate the simulation by a fixed amount
        - ▪ You can unlink the synchronization so you can move the structure separately
        - ▪ You can work on the simulation and rotate freely
        - ▪ Can change the color options, radii options and apply scaling factors to the size and apply thresholds
        - ▪ Can show labels and absences
        - ▪ When a structure phase selected there's panels where you can choose orientation and on the top there will be menus for structure, pattern simulation, stereogram and orientation
        - ▪ When an image is selected there's image manipulation options (can apply transfer functions for contrast, apply look up tables for color, etc.)
        - ▪ Can select reflection list using either X-Ray or Electron scattering factors
        - ▪ Can turn off the simulated overlay and work only with the image
        - ▪ Can then add a scale bar, rotate the image, use measurement tools (ruler, grid, etc.)
        - ▪ Can switch to dark theme in View menu

- Can show in the hkl list either all hkl or hkl with absences or only visible hkl or visible or visible hkl with absences
- Can hover over reflection for quick tool tip information
- When a reflection is clicked more extensive information appears
- You can click on reflection and show the planes, which is automatically desynchronized
- You can select a structural phase and then select rows of reflections changing the angle for the gridlines for grid indexing
  - Working on the list being shorter
  - Currently there is a rotation angle applied that's not correct so that the simulated pattern would match the image

➢ ~95% finished developing and debugging
➢ Finishing development and debugging to integrate into the next release
➢ Once finished then DDView integration will be worked on
➢ Considering if this should be a JADE Pro Toolkit item
➢ Stand-alone .exe can be bundled with anything

8. Suggestions   A. Bruma

➢ Next Steps:
  ❖ Priority and timeline of implementation of suggestions
  ❖ Tutorials will need to be put together
  ❖ Need larger new group testing program
  ❖ Users are not active ICDD members and membership needs to get information out to users about the software
  ❖ Need more new researchers using it and giving feedback

9. Adjournment   A. Bruma
  ➢ Motion moved by: Tom Blanton
  ➢ Second by: Andrew Payzant