Manual of ElectronDiffraction Tools

In order to meet the needs of the phase analysis and unit cell determination based on the electron diffraction pattern of diffractograms of HRTEM images, we developed an image processing and analysis package for the SAED patterns and HRTEM images based on the DigitalMicrograph scripting: (a) pattern indexing for a known phase online, (b) extraction of the d-spacing for unit cell determination in Mdi Jade, (c) phase analysis based on the intensity profile, the linear image and its surface plot.

If you have any question or suggestions, please contact me:

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1. How to install ElectronDiffraction Tools

- Make sure DigitalMicrograph software (DM, Gatan Microscopy Suite Software) has been installed on your PC. It can be available at http://www.gatan.com/products/tem-analysis/gatan-microscopy-suite-software.
- Download the package of ElectronDiffraction tools (Install files.rar) from: https://github.com/hlshi527214/ElectronDiffraction-tools/tree/master/Installer files
- Unzip it and copy ElectronDiffraction Tools.gtk to ...\Gatan\DigitalMicrograph\PlugIns
- Run DM, a new menu ED Tools will be built on the menu bar. Click the item ED Tools/ElectronDiffraction tools to enter the graphical user interface, as shown in Figure 1b.

2. Overview of ElectronDiffraction Tools

ElectronDiffraction tools, as a package of DigitalMicrograph software, can process electron diffraction patterns or HRTEM images included native DigitalMicrograph files (dm3), as well as all common greyscale images (JPG, GIF, TIF, BMP etc.).

- Lattice box: define a crystal.
- Indexing box: perform the pattern indexing for a known phase.
- Profile box: make a profile processing and analysis.
- Lattice calculator box: make some crystallographic calculations.

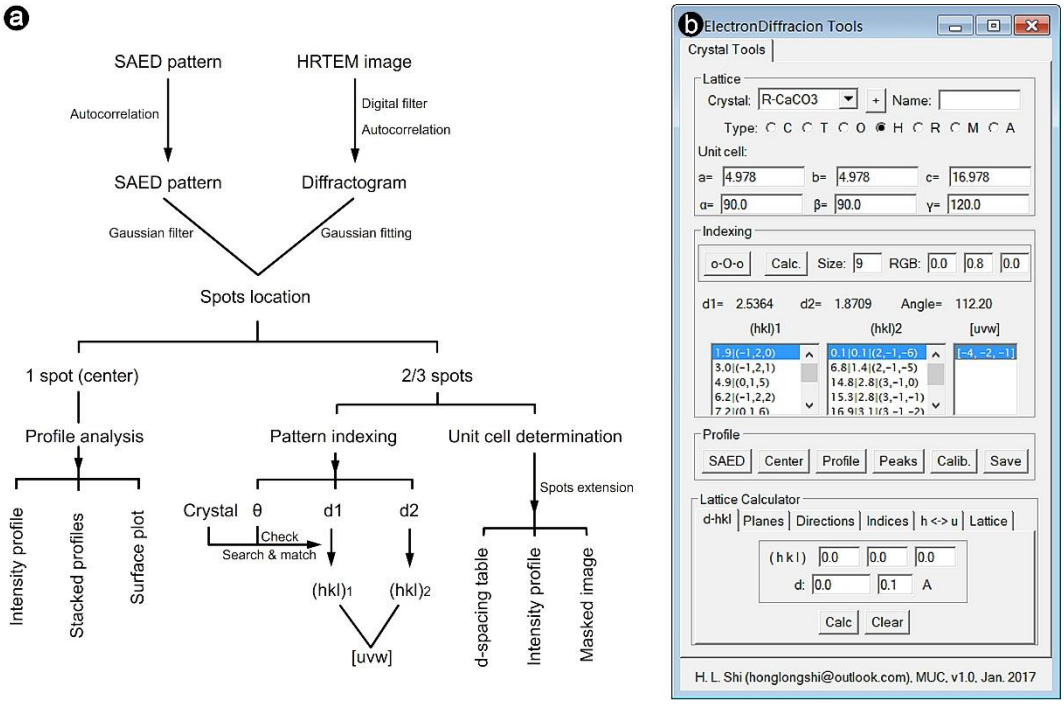

Figure 1 (a) Flowchart of ElectronDiffraction Tools, (b) GUI of ElectronDiffraction Tools.

2.1 Pattern calibration

If your loaded pattern is un-calibrated, e.g., the greyscale images, they should be correctly calibrated before other analysis.

2.1.1 Profile calibration

- Drag an ROI spanning a known peak (see Fig 2),
- Click Calib. Button,
- Set the value of the d-spacing of this peak in prompted dialogue, e.g., 2.5692 Å for (-1 2 0) peak of the calcite crystal.

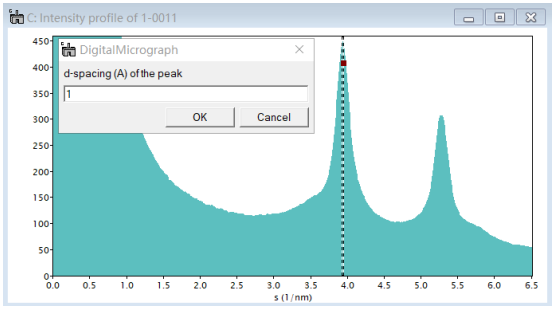

Figure 2 Profile calibration by a known peak.

2.1.2 SAED calibration by a known d-spacing

- Select a SAED pattern,
- CTRL + Calib. Button, set '1' in prompted dialogue to calibrate it using the d-spacing between two spots (See Fig 3),
- Move the cursor to the first spot and hit the spacebar, and then move the cursor to the second spot and hit the spacebar.
- If you use high-order spots to calibrate, you should set a divisor in the prompted dialogue,

e.g., 2 in this example.

- Set the value of d-spacing in prompted dialogue, e.g., 2.5692.
- And then set the unit of this d-spacing.

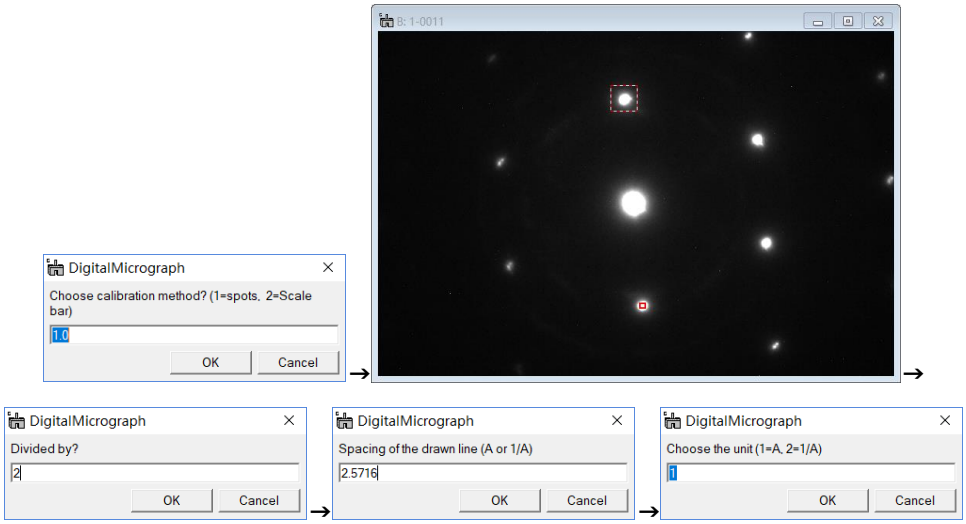

Figure 3 SAED calibration by a known d-spacing between two spots.

2.1.3 SAED calibration by a scale bar

- Select a SAED pattern,
- CTRL + Calib. Button, set '2' in prompted dialogue to calibrate it using a scale bar (See Fig 4),
- Move the cursor to the left side of the scale bar and hit the spacebar, and then move the cursor to the right side of the scale bar and hit spacebar
- Set the spacing of the scale bar in prompted dialogue, e.g., 5.

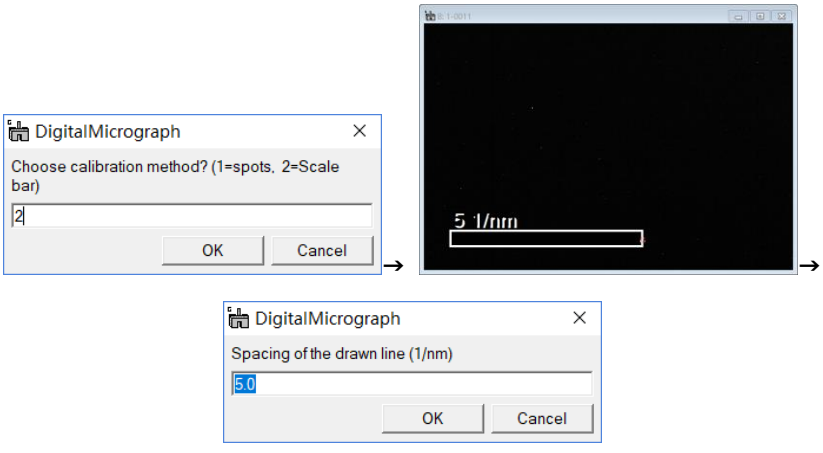

Figure 4 SAED calibration by a scale bar.

2.2 Pattern indexing for a known phase

2.2.1 Define a crystal

- Set lattice type, C(cubic), T(tetragonal), O(orthorhombic), H(hexagonal),

R(rhombohedral), M(monoclinic), A(triclinic), e.g., 'H' for calcite crystal (See Fig 5).

- Set unit cell: a, b, c, α, β, γ, e.g., a=b=4.978 Å, α=β=90°, γ=120° for calcite crystal.
- Click '+' to add this crystal.

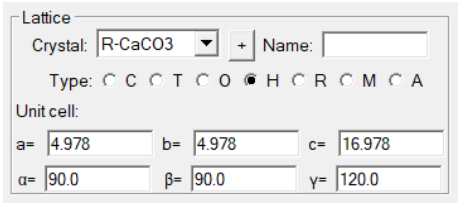

Figure 5 Define a crystal.

2.2.2 Spot measurements

- Select a SAED pattern,
- Click o-O-o button,
- Move the cursor to the first spot and hit the spacebar, and then move the cursor to the second spot (direct beam) and hit the spacebar, move the third spot and hit the spacebar. (↑↓←→use to change the size of the ROI) (See Fig 6).
- Click 'Calc.' button.
- Select (always) the first one in (hkl)1 list, a calculated spot will be overlaid on the SAED pattern.
- Select (always) the first one in (hkl)2 list, a calculated zone axis pattern will be overlaid on the SAED pattern.
- The zone axis direction will be displayed in [uvw] list.

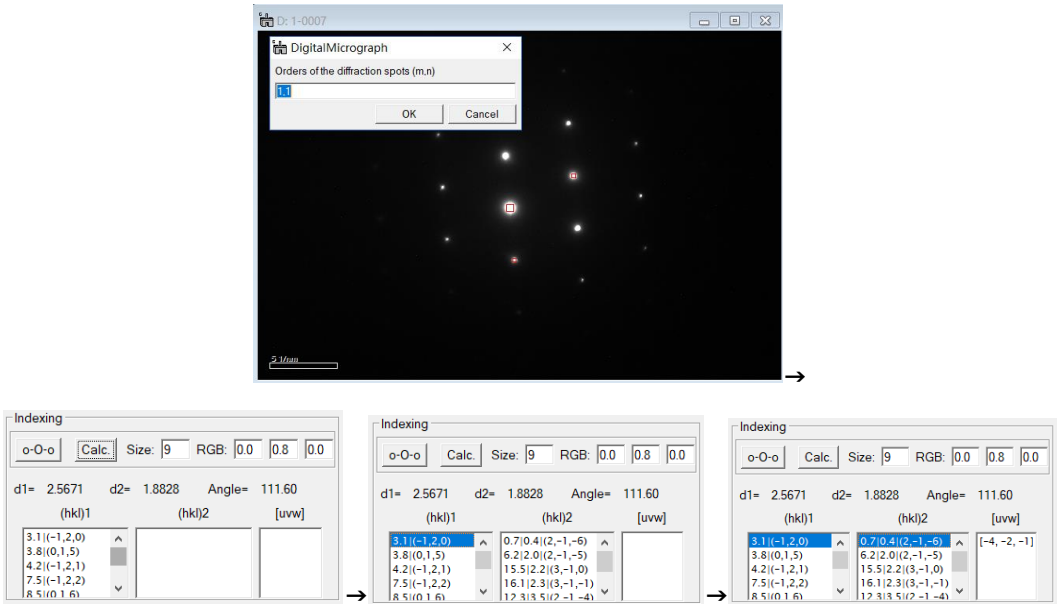

Figure 6 Pattern indexing for a known phase.

2.3 Extraction of a d-spacing table

- Select a SAED pattern,
- Click o-O-o button,
- Move the cursor to the first spot and hit the spacebar, and then move the cursor to the

second spot (direct beam) and hit the spacebar, move the third spot and hit the spacebar. (↑↓←→use to change the size of the ROI) (See Fig 7).

- Click CTRL+'Calc.' button.
- Set orders of (m, n) in prompted dialogue, e.g., 2,2
- Set d1, d2 and theta in prompted dialogue successively (it is necessary to geometrically correct when the measured values are not ideal),
- And then an intensity profile and a masked image are displayed, and a dialogue is prompted to save the derived d-spacing table as '*.dsp' file, which can be directly imported in Mdi Jade.

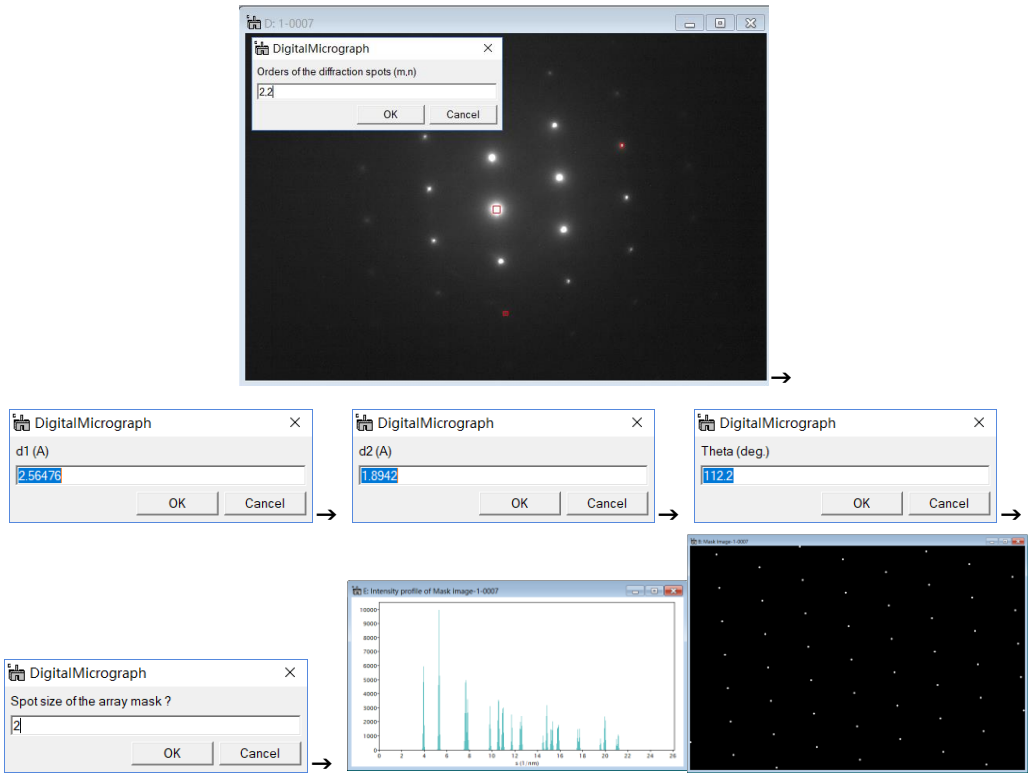

Figure 7 Extraction of a d-spacing table from a spot-like pattern.

2.4 Pattern correction

2.4.1 Get an FT pattern (direct diffractogram) of an HRTEM

- Select an HRTEM image (e.g. ex3.dm3, See Fig 8),
- Drag a squared ROI. (Shift key for square ROI or ALT key for 2^n ROI)
- Click SAED button, you will get a magnitude pattern of the FT diffractogram,
- Click Yes in the prompted dialogue if you want to get an autocorrelation pattern.

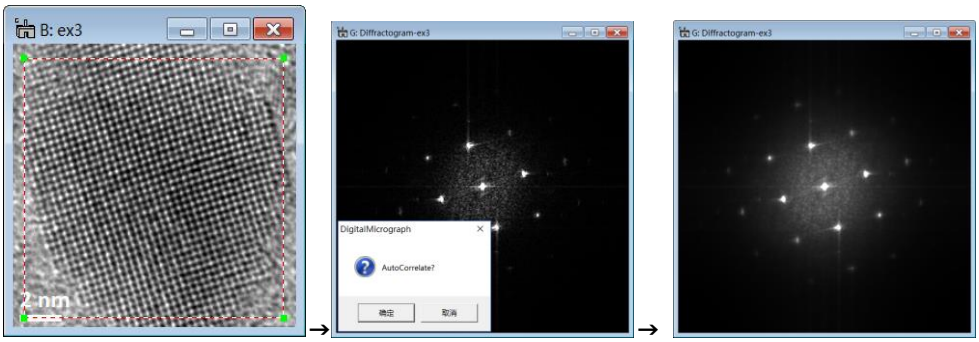

Figure 8 How to obtain a diffractogram from an HRTEM image.

2.4.2 Get a filtered diffractogram of an HRTEM

- Select an HRTEM image (e.g. ex3.dm3, See Fig 9),
- Drag a squared ROI. (Shift key for square ROI or ALT key for 2^n ROI)
- Click SAED button with ALT key, you will get a magnitude pattern of the filtered-FT pattern,
- Click Yes in the prompted dialogue if you want to get an autocorrelation pattern.

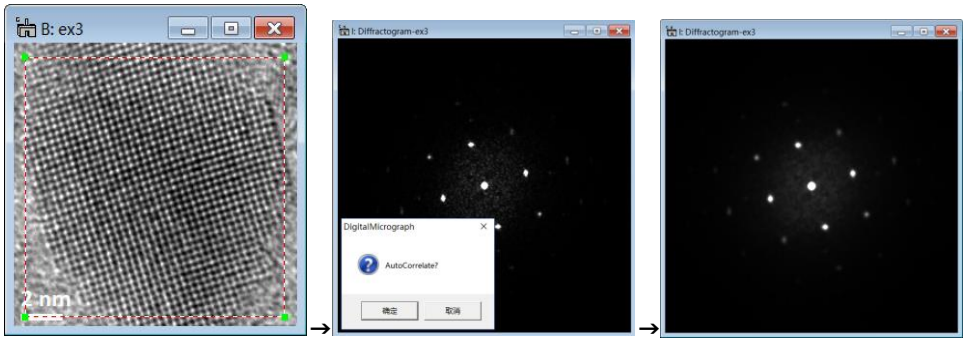

Figure 9 How to obtain a filtered diffractogram from an HRTEM image.

2.4.3 Correction of a SAED pattern

- Select a SAED pattern (e.g. ex1.dm3, See Fig 10),
- Click SAED button with CTRL key, you will get an autocorrelation pattern of the specified pattern.

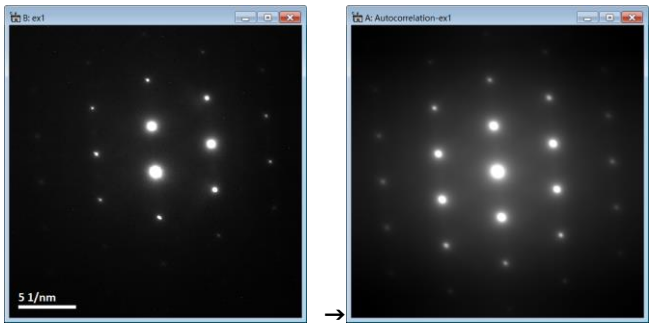

Figure 10 How to correct a SAED pattern.

2.5 Profile analysis

2.5.1 Get an intensity profile and the linear image from a SAED pattern

- Select a SAED pattern (e.g., ex1.dm3, see Figure 11),
- Click Center button, and then move the cursor to the direct beam and hit the spacebar.
- Click Profile button to get an intensity profile and the linear image.

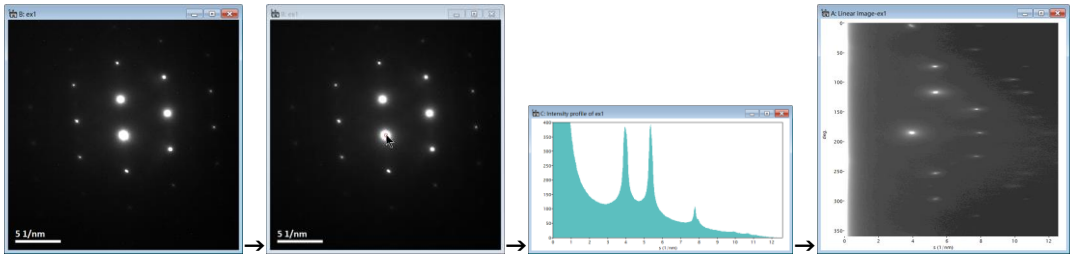

Figure 11 How to get an intensity profile and the linear image.

2.5.2 Get a surface plot of the linear image

- Select a linear image (see Figure 12),
- Click Profile button with CTRL key to get surface plot of the linear image.

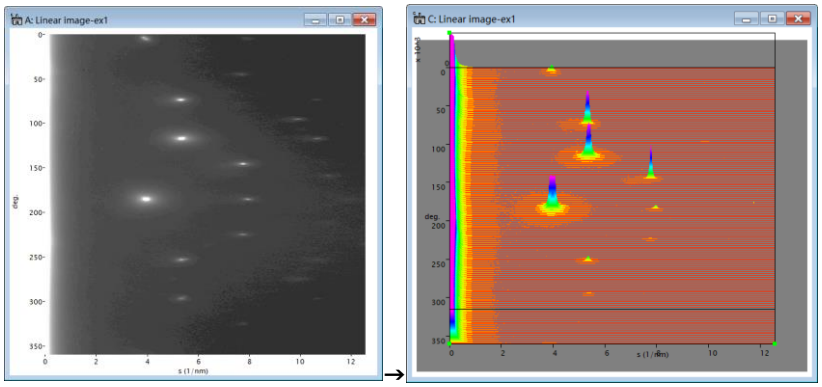

Figure 12 How to get a surface plot of the linear image.

2.5.3 Get stacked profiles of the SAED pattern

- Select a SAED pattern (see Figure 13), and center it.
- Click Profile button with ALT key, input the number of profiles, e.g., 10

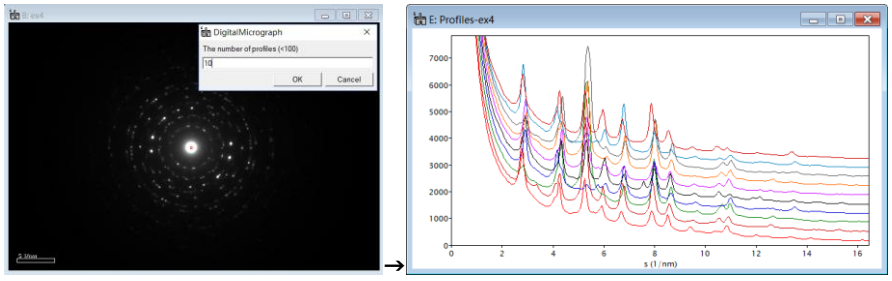

Figure 13 How to get stacked profiles from a SAED pattern.

2.5.4 Location of peaks

(a) locate only one peak

- Select an intensity profile (see Figure 14),
- Drag an ROI spanning the interest peak,
- Click Peaks button to locate it.

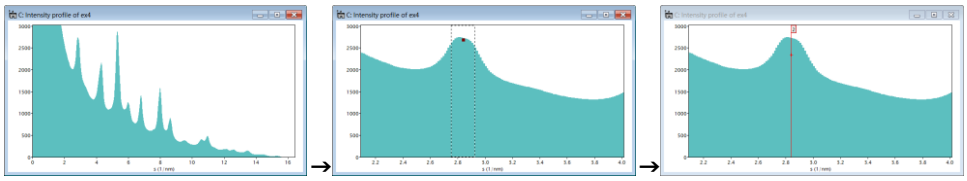

Figure 14 How to locate one peak in the intensity profile.

(b) locate multi-peaks automatically

- Select an intensity profile (see Figure 15),
- Drag an ROI spanning the interest peak (define FWHM of the peak),
- Click Peaks button with CTRL key to locate peaks.

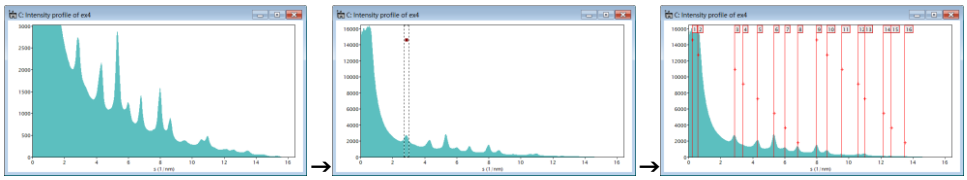

Figure 15 How to locate multi-peak in the intensity profile.

(c) Save peaks

- Select an intensity profile (see Figure 16),
- Locate all peaks and delete your unwanted peaks,
- Click Peaks button with ALT key to save peaks.
- Input 1 or 2 to choose the file type of the peak list: *.dsp (d-spacing table for Mdi Jade) and *.pks (peak list file for Crystallographica Search-Match).

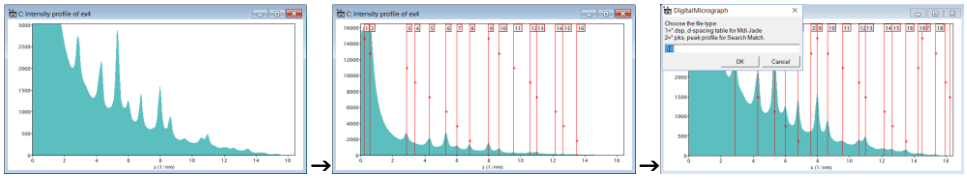

Figure 16 How to locate multi-peaks in the intensity profile.

2.6 Save data

Note: *.dif contains multi-profiles and it can be dragged into Mdi Jade directly;
*.txt is a XYY file, you can make a 3D plot in Origin or Surfer.

2.6.1 Save profiles

- Select an intensity profile (see Figure 17),
- Click Save button, and set the file type to save all slices.

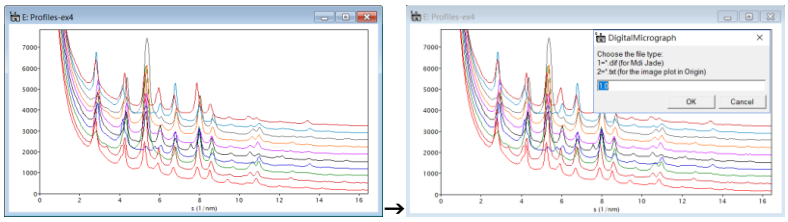

Figure 17 Save profiles to *.dif or *.txt file.

2.6.2 Save the linear image or its surface plot

- Select a linear image (see Figure 18),
- Click Save button with CTRL key, and set the file type (1=*.dif and 2=*.txt)
- Set the number of profiles, and the linear image will be saved.

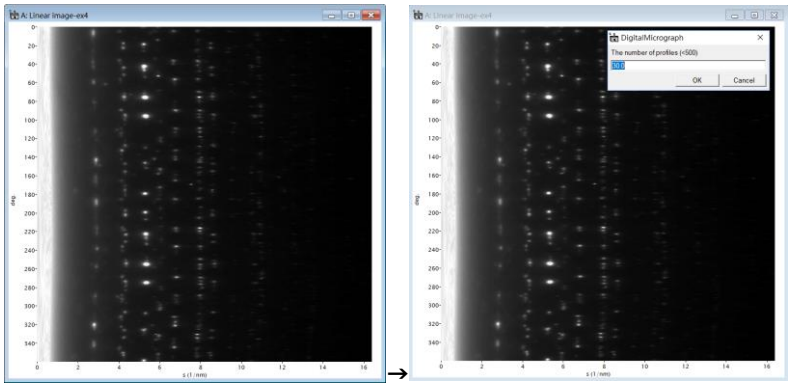

Figure 18 Save a linear image or surface plot as *.dif or *.txt file.

2.6.3 Save a SAED pattern

- Select a SAED pattern (see Figure 19),
- Click Save button with ALT key, and set the file type (1=*.dif and 2=*.txt)
- Set the number of profiles, and the SAED will be saved.

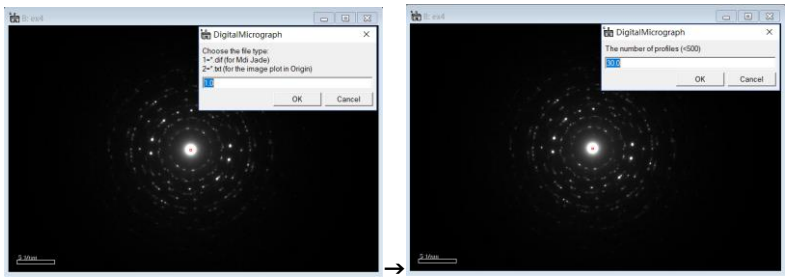

Figure 19 Save a SAED pattern as *.dif or *.txt file.

2.7 Preferences

Preferences are used to save the default parameters of ElectronDiffraction Tools, you can edit them to meet your needs.

- Choose the menu ‘File/ Global Info…’ or hit the hotkey ‘CTRL+I’, a window will be prompted (see Figure 20),
- Click ‘General/ Tags’, and preferences of ElectronDiffraction Tools will be displayed in the right panel.
- You can edit each item by double-click it.

Error Angle and Error d: the default errors of the d-spacing and angle for the pattern indexing.
Wavelength: the default wavelength used to convert electron diffraction pattern into two theta (note: the default radiation should be defined for phase analysis in Crystallographica Search-Match)
Window position X and Y: the default position of ElectronDiffraction Tools. If it is out of your PC screen, you need to change them to small values, e.g., (20,20). If you move the window to your preferred position, close this window with 'ALT key' and the position will be saved as default.

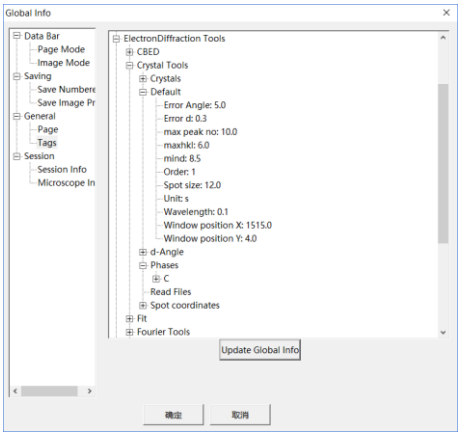

Figure 20 Preferences of ElectronDiffraction Tools.

3. Buttons and hotkeys in ElectronDiffraction Tools

Buttons	Keys	Description
+		Add a new crystal.
	ALT	Delete the selected crystal.
o-O-o		Automatically locate 3 spots, spacebar to locate them.
	ALT	Manually locate 3 spots, spacebar to locate them.
	CTRL	Automatically locate 2 spots, spacebar to locate them.
Calc.		Calculate a d-spacing table for a specified crystal.
	CTRL	Extract a d-spacing table (*.dsp), a masked image and the intensity profile.
SAED		Get an FT pattern (diffractogram) of an HRTEM image.
	ALT	Get an autocorrelation-masked diffractogram of an HRTEM image.
	CTRL	Get an autocorrelation SAED from a selected SAED pattern.
Center		Automatically locate the center of a SAED pattern (Spacebar to locate it).
	ALT	Define the center of a SAED pattern by an oval component or the origin.
Profile		Get an intensity profile and the linear image from the selected SAED pattern.
	ALT	Get a stacked profiles from the selected SAED pattern.
	CTRL	Get a surface plot from the selected linear image.
	Space	Align a linear image or stacked profiles.
Peaks		Mark a peak by the specified ROI on the intensity profile.
	ALT	Save peaks as *.dsp (peak list file for Mdi Jade) or *.pks file (peak list file for Crystallographica Search-Match)

	CTRL	Locate peaks automatically on an intensity profile.
Calib.		Calibrate the intensity profile by a known peak.
	ALT	Get scale parameters.
	CTRL	Calibrate a SAED pattern by a known spacing between two spots or a scale bar.
Save		Save profiles as *.dif (for Mdi Jade) or *.txt (for image plot in Origin)
	ALT	Save SAED pattern as *.dif (for Mdi Jade) or *.txt (for image plot in Origin)
	CTRL	Save Linear image or Surface plot as *.dif (for Mdi Jade) or *.txt (for image plot in Origin)