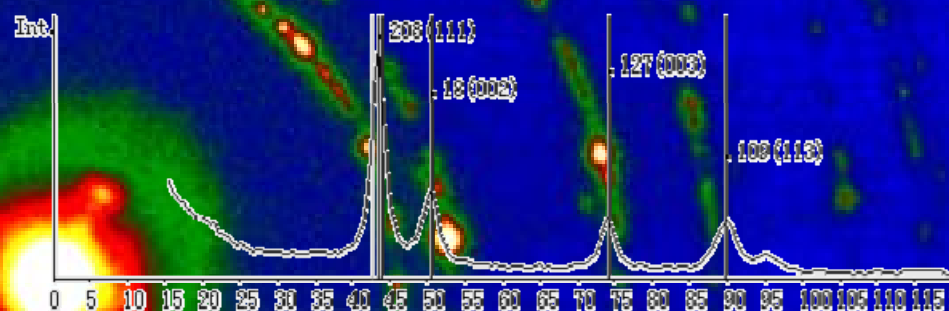


EDP2XRD

Version 1.0.0



Dr Hongwei Liu
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2015.07.12

Instructions

- Specific description
- About the author
- Main functions
- Basic operation
- Acknowledgement

Specific description

Computer language:	Visual Basic 6.0
Core algorithm:	Robot vision
Knowledge background:	Crystal diffraction
Key technology:	Image processing
Script Line number:	5050
Running environment:	Windows9X/2000/xp/7 Operation system; 64 MB; inner memory; 50MBhard disk space

About the Author

- Name: Hongwei Liu
- Research field: Advanced materials preparing and characterization
- Affiliation: ACMM, The University of Sydney
- Email: microscopy.liu@gmail.com

Main functions

- Convert electron diffraction pattern into X-ray diffraction pattern both in auto mode and manual mode
- Work for single or multiple crystalline crystal electron diffraction pattern
- Work for non-complete electron diffraction pattern



- Image processing for electron diffraction pattern

Histogram

Contrast inversion

Gradation conversion

Smoothing

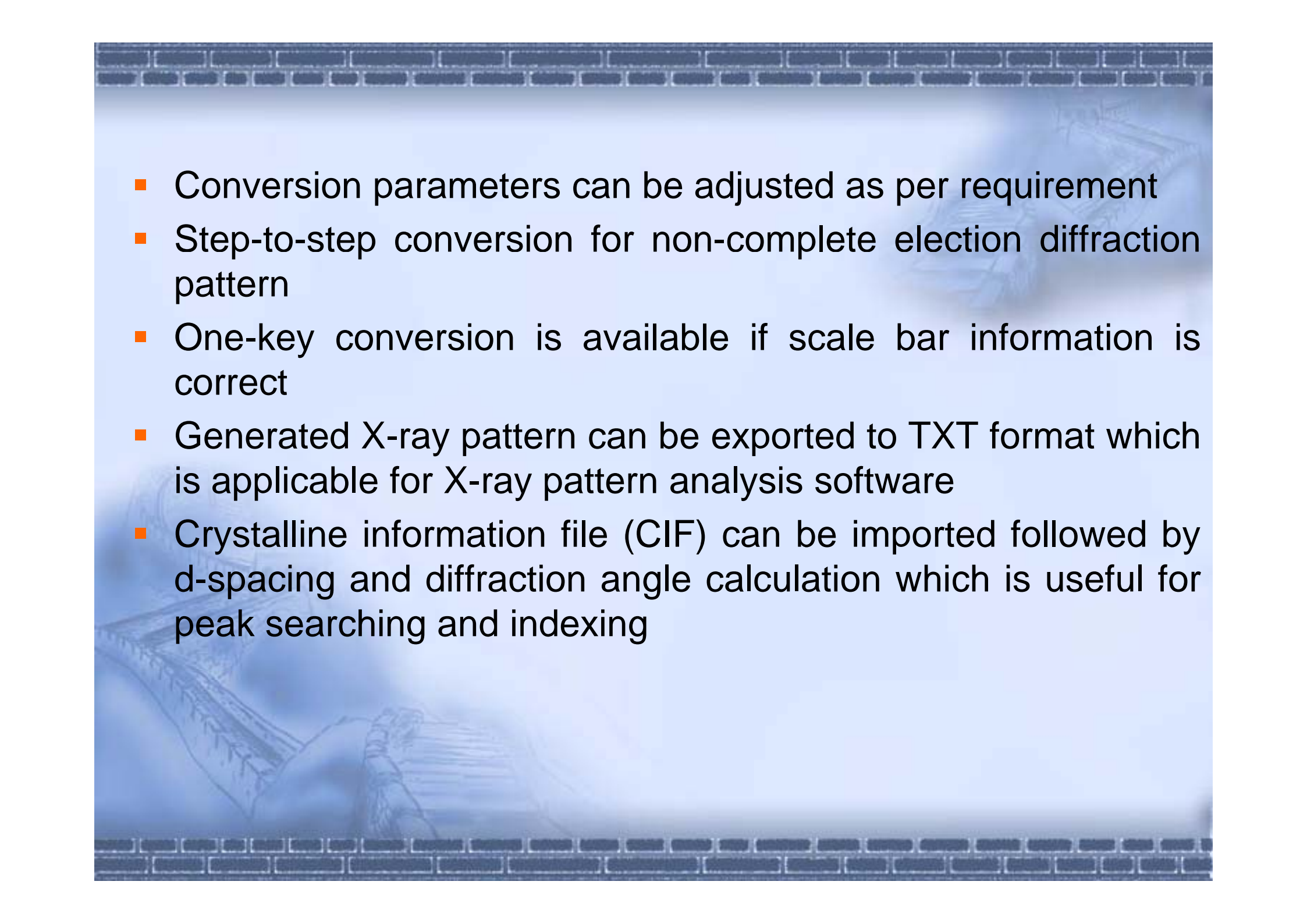
Sharpening

Edge searching

Binarization

Scale bar searching

Circle centre searching

- 
- Conversion parameters can be adjusted as per requirement
 - Step-to-step conversion for non-complete electron diffraction pattern
 - One-key conversion is available if scale bar information is correct
 - Generated X-ray pattern can be exported to TXT format which is applicable for X-ray pattern analysis software
 - Crystalline information file (CIF) can be imported followed by d-spacing and diffraction angle calculation which is useful for peak searching and indexing

Operation

1. Set conversion parameters:

- Input reciprocal scale bar (defaulted as 5), unit is 1/nm;
- Input X-ray wavelength (defaulted as 0.154), unit is nm;
- Input normal resolution (defaulted as 0.1), unit is deg;
- Input radius resolution (defaulted as 0.1), unit is deg;
- Input start angle (defaulted as 15), unit is deg.

Remark: one-key conversion is available if all the above parameter have been set correctly.

EDP convert

Step I - Set calibration

Scale Length (Pixel)

Reciprocal Distance (1/nm)

Calibration (1/nm)

Step II - Set the centre

Beam centre (Pixel) X

Y

Distance Range (1/nm)

Real space Distance (nm)

X-ray angle (°)

Step III - Conversion into X-ray diffraction pattern

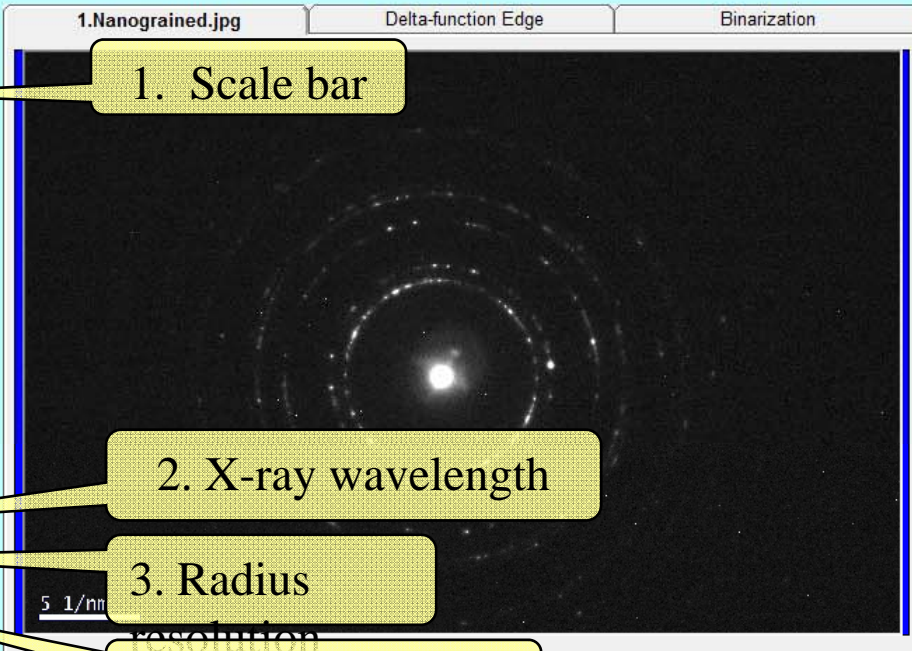
Electron wavelength (nm)

X-ray wavelength (nm)

ED Radius Resolution (°)

ED ring Resolution (°)

Start Angle (°)



Crystal		Refined spots		Hough Trans	
Crystal:					
a	0.368 nm	Alpha	90 °	N max	
b	0.368 nm	Beta	90 °		3
c	0.368 nm	Gamma	90 °		List
No	2 theta	d (nm)	H	K	L
54	103.054	.098	3	1	
55	131.581	.084	3	1	
56	97.95	.102	3	2	
57	103.054	.098	3	2	
58	119.245	.089	3	2	
59	157.874	.078	3	2	
60	125.178	.087	3	3	
61	131.581	.084	3	3	
62	157.874	.078	3	3	

No	Angle (2-th)	Intensity	Normalized	D-spacing

1. Scale bar

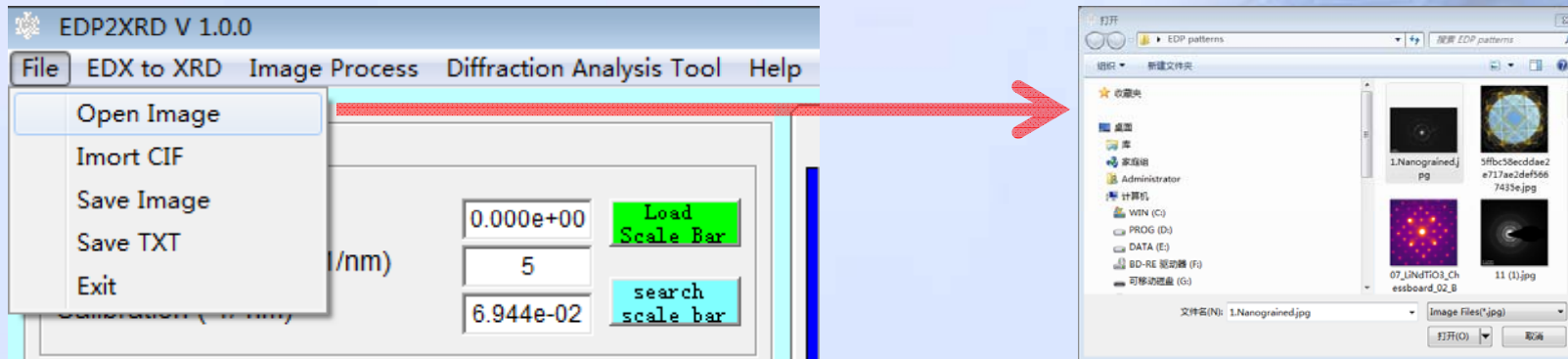
2. X-ray wavelength

3. Radius

4. Angle resolution

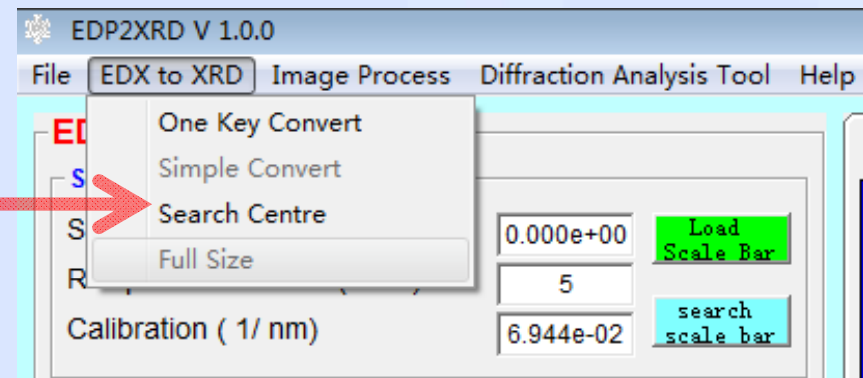
5. Start angle

2. Open or drag JPG format image of electron diffraction pattern into Image frame area



3. Auto Mode1: One-key conversion

- From Main menu → EDX to XRD → One Key Convert
- Wait until conversion finished.



One-key conversion utilizes image processing for the pattern which contains lots of noise, low quality and non-apparent diffraction ring feature.

Output X-ray pattern as TXT format file

EDP2XRD V 1.0.0

File EDX to XRD Image Process Diffraction Analysis Tool Help

Open Image
 Import CIF
 Save Image
 Save TXT
 Exit

72
 5
 6.944e-02

Calibration
 Search Scale Bar

Step II - Set the centre

Beam centre (Pixel) X 296
 Y 232
 Distance Range (1/nm) 3.25e+01
 Real space Distance (nm) 4.434e-01
 X-ray angle (°) 170

Load Centre
 Search Centre

Step III - Conversion into X-ray diffraction pattern

Electron wavelength (nm) 0.00251
 X-ray wavelength (nm) 0.154
 ED Radius Resolution (°) 0.5
 ED ring Resolution (°) 1
 Start Angle (°) 15

Convert

No	2 theta	Intensity	Normalized	d (nm)	H	K	L
131	89.56	24237	404	.1192	1	1	3
53	4.42	37990	633	.2173	1	1	1
105	7.13	19189	320	.1386	0	2	2
65	6.93	24028	400	.1912	0	0	2
130	88.49	22270	371	.1198			
129	87.8	20380	339	.1204			
1	15.5	33585	559	.571			
128	87.11	18682	311	.1211			

2-theta = 32.3°, d-spacing = .277 nm

1.Nanograined.jpg Delta-function Edge Binarization

5 1/nm

Crystal

Crystal	Refined spots	Hough Trans
a 0.368 nm	Alpha 90°	N max 3
b 0.368 nm	Beta 90°	
c 0.368 nm	Gamma 90°	List

No	2 theta	d (nm)	H	K	L
54	103.054	.098	3	1	
55	131.581	.084	3	1	
58	97.95	.102	3	2	
57	103.054	.098	3	2	
58	119.245	.089	3	2	
59	157.874	.078	3	2	
60	125.178	.087	3	3	
61	131.581	.084	3	3	
62	157.874	.078	3	3	

Int I

208 (111)
 127 (003)
 18 (002)

2-theta (°)

NUM 1:39 PM 9/08/2015

Indexing result

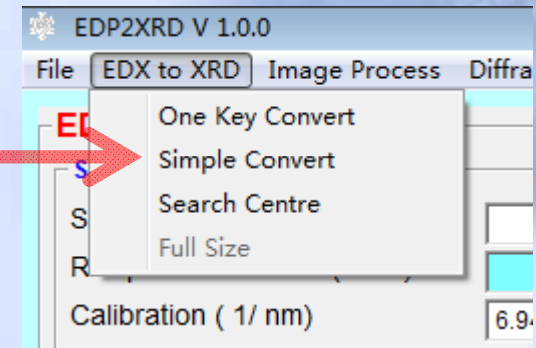
Mouse detecting diffraction angle of RXD and corresponding ring of EDP

Mouse left click for indexing diffracted peaks according to CIF file if structural factor is known

Input or drag CIF file to calculate planar d-spacing and diffraction angle 2-theta.

4. Auto Mode 2: Simple conversion

- From Main menu → EDX to XRD → Simple Convert
- Wait until conversion finishes.



Remark: Simple conversion omits all image processing to fast convert EDP which is high quality and low noise. The final conversion pattern is the same as that obtained by one-key conversion with the only difference of conversion time.

5. Manual Mode1:Simple conversion

The screenshot displays the EDP2XRD V 1.0.0 software interface. The main window shows a diffraction pattern titled "1.Nanogained.jpg" with a central spot and concentric rings. Three red arrows point to the left sidebar, indicating the steps: "Step 1: Calibration", "Step 2: search centre", and "Step 3: convert".

Step I - Set calibration

Scale Length (Pixel)	0	Calibration
Reciprocal Distance (1/nm)	5	Search Scale Bar
Calibration (1/ nm)	1	

Step II - Set the centre

Beam centre (Pixel)	X	0	Load Centre
	Y	0	
Distance Range (1/nm)		0	
Real space Distance (nm)		0	Search Centre
X-ray angle (°)		170	

Step III - Conversion into X-ray diffraction pattern

Electron wavelength (nm)	0.00251	Convert
X-ray wavelength (nm)	0.154	
ED Radius Resolution (°)	0.5	
ED ring Resolution (°)	1	
Start Angle (°)	15	

Crystallographic Data

No	2 theta	d (nm)	H	K	L
54	103.054	.098	3	1	
55	131.581	.084	3	1	
56	97.95	.102	3	2	
57	103.054	.098	3	2	
58	119.245	.089	3	2	
59	157.874	.078	3	2	
60	125.178	.087	3	3	
61	131.581	.084	3	3	
62	157.874	.078	3	3	

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Manual mode simple conversion is similar as auto mode simple conversion but with the freedom of controlling each step of conversion.

6. Manual Mode 2: Manual conversion

Step 1: Click “Load centre”, enter scale bar definition mode.

The screenshot shows the EDP2XRD V 1.0.0 software interface. The main window displays a diffraction pattern titled "1.Nanograined.jpg" with a scale bar of "5 1/nm". A red arrow points to the "Load Centre" button in the "Step II - Set the centre" section. The "Step I - Set calibration" section includes buttons for "Calibration", "Search Scale Bar", and "Convert". The "Step III - Conversion into X-ray diffraction pattern" section includes a "Convert" button. The right panel shows a histogram and a table of refined spots.

No	2 theta	d (nm)	H	K	L
54	103.054	.098	3	1	
55	131.581	.084	3	1	
56	97.95	.102	3	2	
57	103.054	.098	3	2	
58	119.245	.089	3	2	
59	157.874	.078	3	2	
60	125.178	.087	3	3	
61	131.581	.084	3	3	
62	157.874	.078	3	3	

Crystal: a 0.368 nm Alpha 90 ° N max 3
b 0.368 nm Beta 90 °
c 0.368 nm Gamma 90 ° List

No	Angle (2-th)	Intensity	Normalized	D-spacing			

Ready NUM 1:36 PM 9/08/2015

Manual conversion is for a pattern with poor information of scale bar.

6. Manual Mode 2: Manual conversion

Step 2: Define scale bar length

Mouse left key click P1 the start point of scale bar, Keep left key down and move to P2 the end point of scale bar, the release left key. Input the calibration value in the Dialogue box. The length of scale bar will be input into Scale length (Pixel) .

The screenshot displays the EDP2XRD V 1.0.0 software interface. The main window shows a diffraction pattern with a scale bar labeled '1/nm'. Two points, P1 and P2, are marked on the scale bar. A dialog box titled 'Option of Calibrate EDP' is open, showing the 'Calibration' section with the following options:

- Measure Scale Bar Length [5] 1/nm
- Measure d-spacing [0.2] nm

The 'OK' button is highlighted in green. The interface also includes a sidebar with various settings and a table of refined spots.

EDP convert

Step I - Set calibration

Scale Length (Pixel) [0] Calibration
Reciprocal Distance (1/nm) [5] Search Scale Bar
Calibration (1/ nm) [1] Search Scale Bar

Step II - Set the centre

Beam centre (Pixel) X [0] Load Centre
Y [0] Load Centre
Distance Range (1/nm) [0] Search Centre
Real space Distance (nm) [0] Search Centre
X-ray angle (°) [170] Search Centre

Step III - Conversion into X-ray diffraction pattern

Electron wavelength (nm) [0.00251] Convert
X-ray wavelength (nm) [0.154] Convert
ED Radius Resolution (°) [0.5] Convert
ED ring Resolution (°) [1] Convert
Start Angle (°) [15] Convert

Crystal | Refined spots | Hough Trans

Crystal:

a [0.368] nm Alpha [90] ° N max
b [0.368] nm Beta [90] ° 3
c [0.368] nm Gamma [90] ° List

No	2 theta	d (nm)	H	K	L
54	103.054	.098	3	1	
55	131.581	.084	3	1	
56	97.95	.102	3	2	
57	103.054	.098	3	2	
58	119.245	.089	3	2	
59	157.874	.078	3	2	
60	125.178	.087	3	3	
61	131.581	.084	3	3	
62	157.874	.078	3	3	

No | Angle (2-th) | Intensity | Normalized | D-spacing

Clear

6. Manual Mode 2: Manual conversion

Step 3: Set diffraction ring centre

Mouse left key clicks "Load Centre". Move the mouse icon into diffraction pattern area. A red hollow circle will appear using mouse icon as the centre. Carefully move the mouse so that red color circle has the same centre as that of diffracted rings. Then click and release mouse left key. The centre position of diffracted pattern will be input into Beam centre (Pixel) X Y.

The screenshot shows the EDP2XRD V 1.0.0 software interface. The main window displays a diffraction pattern with a central crosshair. A red arrow points to the 'Load Centre' button in the 'Set the centre' section. Another red arrow points to the 'Convert' button in the 'Conversion into X-ray diffraction pattern' section. The diffraction pattern has a scale bar of 5 1/nm. The right panel shows a histogram and a table of refined spots.

No	2 theta	d (nm)	H	K	L
54	103.054	.098	3	1	
55	131.581	.084	3	1	
56	97.95	.102	3	2	
57	103.054	.098	3	2	
58	119.245	.089	3	2	
59	157.874	.078	3	2	
60	125.178	.087	3	3	
61	131.581	.084	3	3	
62	157.874	.078	3	3	

Step 4: Click "Convert" and conversion starts.

Image processing

Histogram

Gradation conversion

Contrast inversion

Smoothing

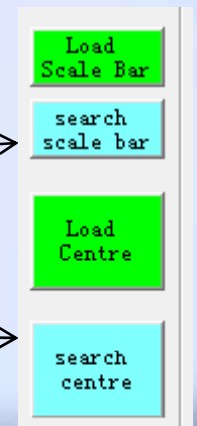
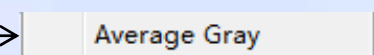
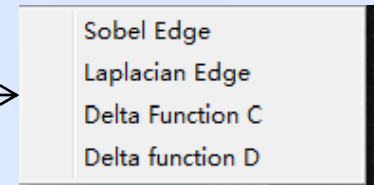
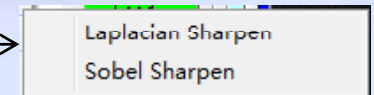
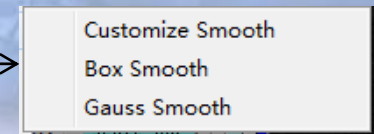
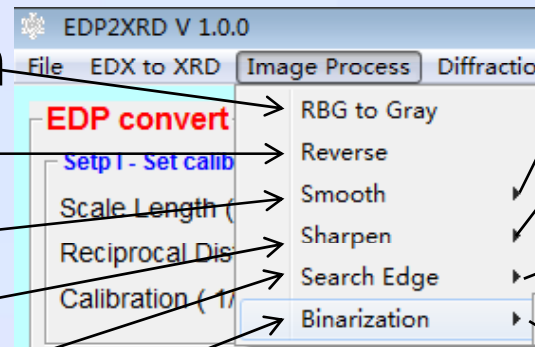
Sharpening

Edge searching

Binarization

Scale bar searching

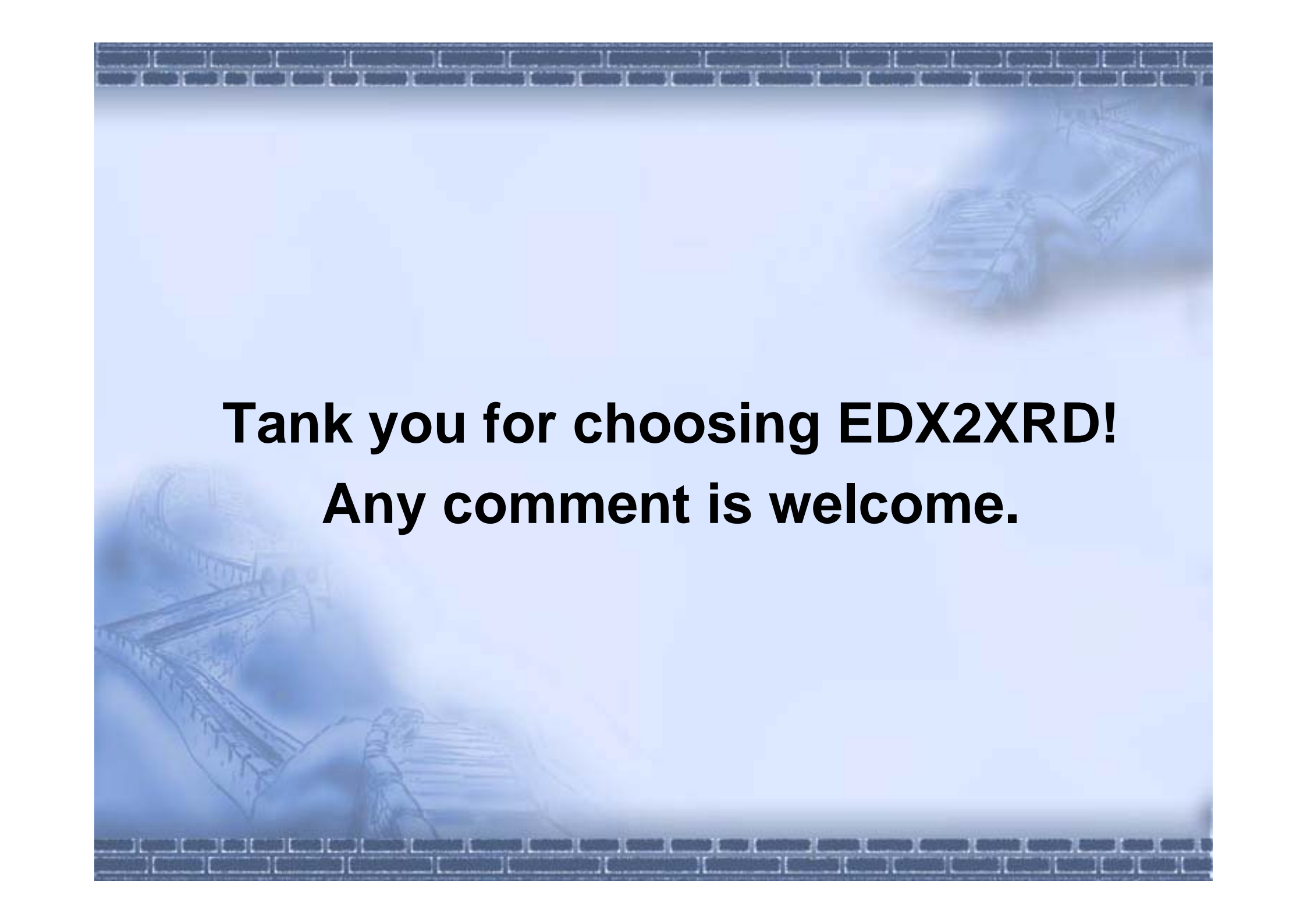
Circle centre searching



Acknowledgements

Enlightening discussion with Dr Matthew Foley, Dr Anna Ceguerra at ACMM, The University of Sydney and Dr Qingyun Lin at AMME, The University of Sydney is greatly appreciated.

Dr Hongwei Liu
Sydney
20150725

The background features a light blue gradient with faint, semi-transparent architectural drawings of classical structures, including columns and arches. A dark blue brick border runs horizontally across the top and bottom of the image. Centered in the middle is the text:

Tank you for choosing EDX2XRD!
Any comment is welcome.