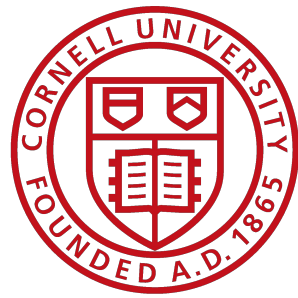




PARADIM
AN NSF MATERIALS INNOVATION PLATFORM

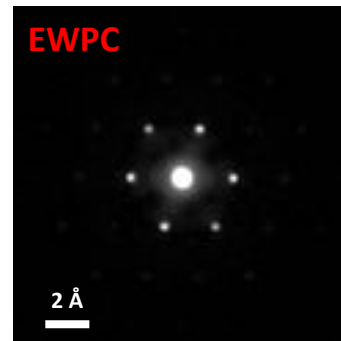
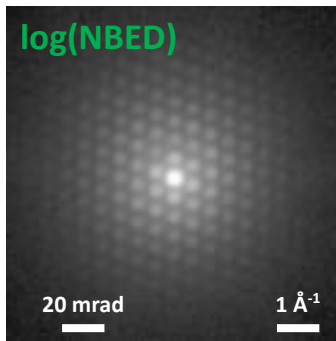
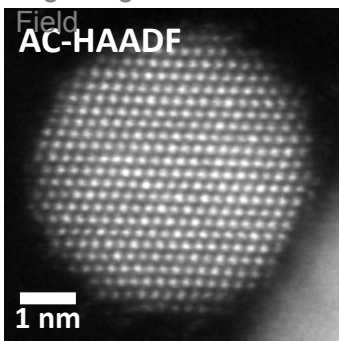


T5 - 4D STEM data analysis

The **Exit Wave Power Cepstrum** (EWPC):

$$| \text{FT}(\ln(I(k))) |$$

Aberration Corrected
High Angle Annular Dark
Field



- Points correspond to local projected interatomic spacings
- Robust to
 - sample mistilts
 - thickness
 - randomly-oriented nanoparticles

The “classic” power cepstrum (PC),*

$$PC(f(t)) = \left| \mathcal{F} \left(\ln \left(|\mathcal{F}(f(t))|^2 \right) \right) \right|^2$$

separates convolved signals :

$$PC(\alpha(t) * \beta(t)) \approx PC(\alpha(t)) + PC(\beta(t))$$

Since the diffraction pattern is : $I(\mathbf{q}) = |\mathcal{F}(\phi(\mathbf{x}))|^2$

An “exit wave power cepstrum” (EWPC) can be calculated as:

$$EWPC_{\phi}(\mathbf{x}) = PC(\phi(\mathbf{x})) = \left| \mathcal{F} \left(\ln(I(\mathbf{q})) \right) \right|^2$$

Or simply

$$EWPC = \left| \mathcal{F} \left(\ln(I(\mathbf{q})) \right) \right|$$

[*] Bogert, B. P. (1963). The quefrency analysis of time series for echoes; Cepstrum, pseudo-autocovariance, cross-cepstrum and saphe cracking. *Time series analysis*, 209-243.

Strong phase approximation for diffraction:

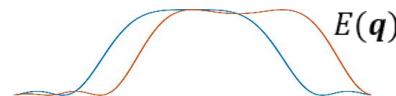
$$I(\mathbf{q}) = |\Phi_p(\mathbf{q}) \otimes (E(\mathbf{q}) \cdot V(\mathbf{q}))|^2 \approx |E(\mathbf{q})|^2 \cdot |\Phi_p(\mathbf{q}) \otimes V(\mathbf{q})|^2$$

where $\Phi_p(\mathbf{q})$ - probe function,

$V(\mathbf{q})$ - projected atomic potential,

$E(\mathbf{q})$ - slowly varying envelope damping function
(carries tilt and thickness information)

Envelope damping diffraction pattern

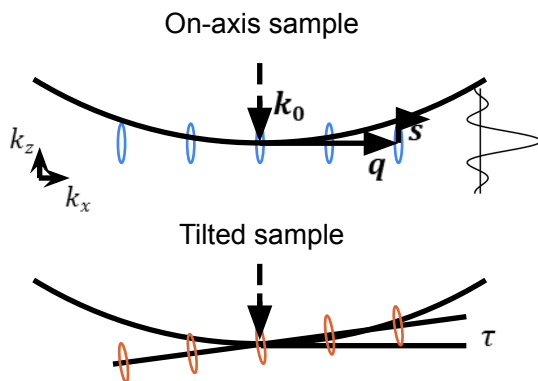


$$\text{EWPC}_\phi(\mathbf{x}) = \left| \mathcal{F} \left(\ln(I(\mathbf{q})) \right) \right| \approx \text{PC}(\epsilon(\mathbf{x})) + |\phi_P(\mathbf{x})|^2 \cdot \text{PC}(v_0(\mathbf{x}))$$

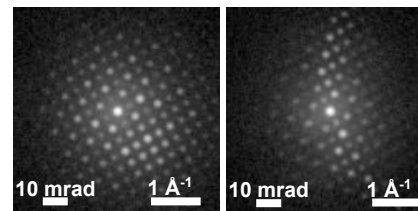
Ewald sphere
envelope
Probe function
Projected
lattice potential

Tilt and thickness artifacts are decomposed from the atomic distance information

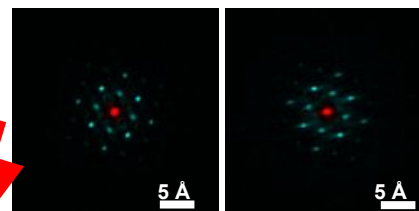
$$\text{EWPC}_{\phi}(\mathbf{x}) = \text{PC}(\epsilon(\mathbf{x})) + |\phi_P(\mathbf{x})|^2 \cdot \text{PC}(v_0(\mathbf{x}))$$



log(NBED)



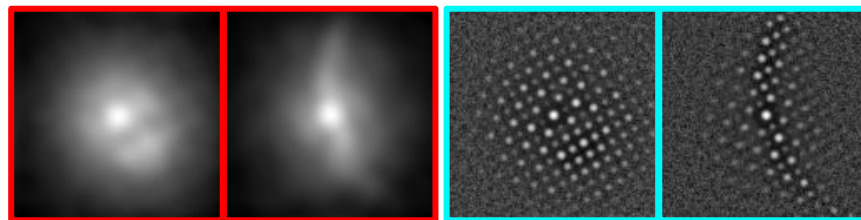
log(EWPC)

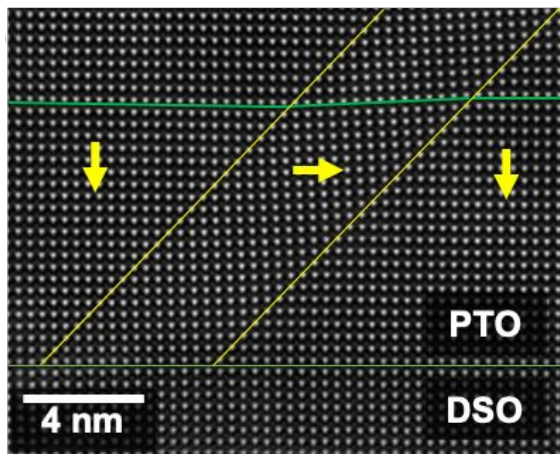


Low frequency

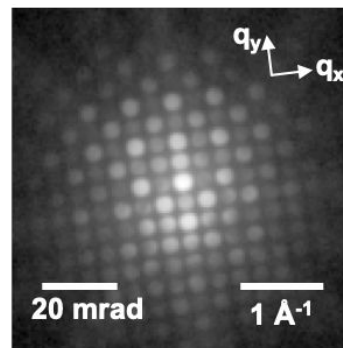
Filtered log(NBED)

High frequency

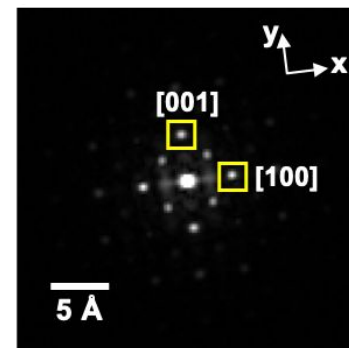


PARADIM EWPC application: PbTiO_3 domains in strained film

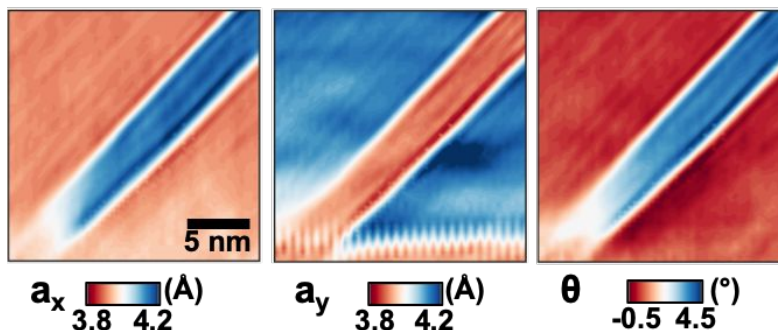
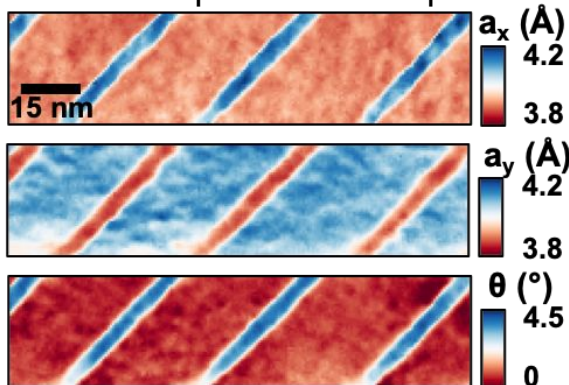
log (NBED)



log (EWPC)



Lattice parameter map



(Optional)

Browsing 4D STEM data on NION Swift

Windows

Copy the folders into

“C:\Users\#userName\AppData\Roaming\Nion\Nion Swift\Plugins”



```
Anaconda Prompt - nionswift

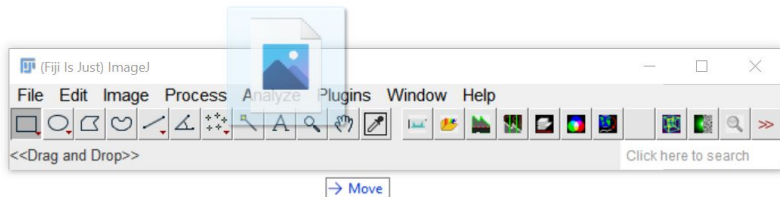
(base) C:\Users\UserName>conda activate nionswift

(nionswift) C:\Users\UserName>nionswift
```

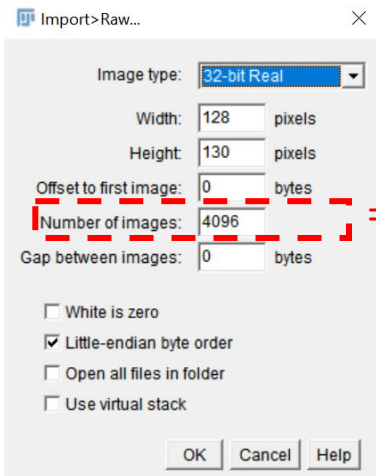
Mac

Users/#userName/Library/Application Support/Nion/Nion Swift/Plugins

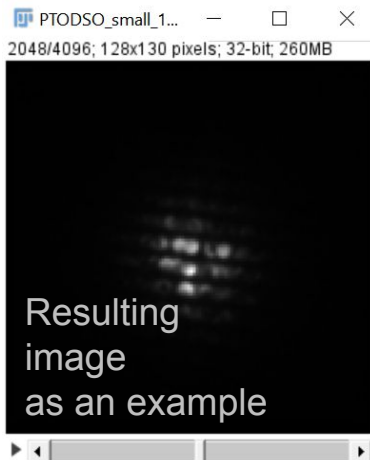
1. Nion Swift 4D Tools only accepts `tif` format 4D data. Use ImageJ to make your file into a tif. Drag & drop the file.



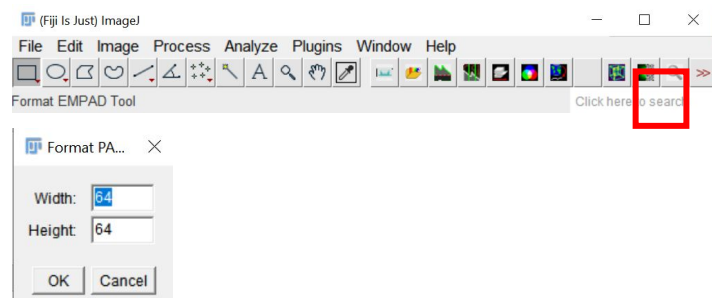
2. Once the 4D data is loaded, the following popup window will show up. Change number of images accordingly.



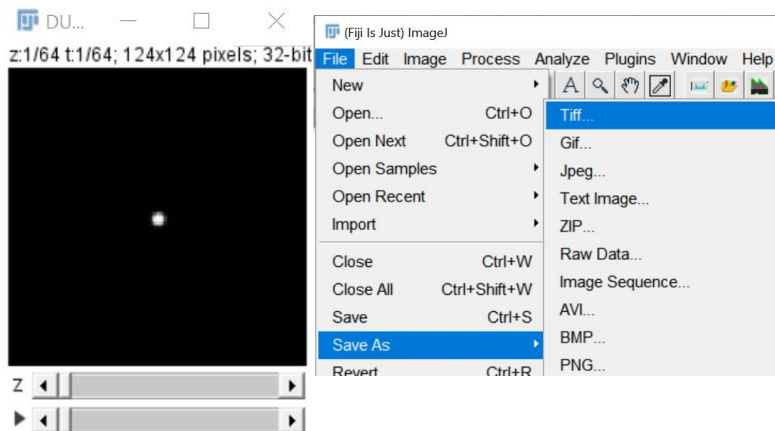
#pixels in x1 axis
of real space
X
#pixels in x2 axis
of real space



3. Click on "Format EMPAD Tool" icon. Type real space coordinates.



4. Once you see a window like the following, save as a tif format.



1. Drag & drop .tif format 4D-STEM data

Note: Steps to follow

Optional explanations

Nion Swift - Nion Swift Project 20210507: Workspace

File Edit Display Graphics Processing Workspace 4D Tools EELS Multi-Dimensional Processing Window Help

Toolbar

Data Panel

afterHyperstack_PTODSO_small_128x130x64.tif
C(64 x 64) x D(124 x 124), Real (32-bit)
Thu May 13 01:06:34 2021

Filter: No Filter

Metadata

Task Panel

Import Data Items
Done Thu May 13 01:06:34 2021
Number File
1 afterHyperstack_PTODSO_small_128x130x64.tif

Copy to Clipboard

afterHyperstack_PTODSO_small_128x130x64.tif_x64

Histogram

max 2.45866e+06
mean 4225.85
min 165.397

rms 780.18
std 77903.5
sum 6.49766e+07

Inspector

Image Data

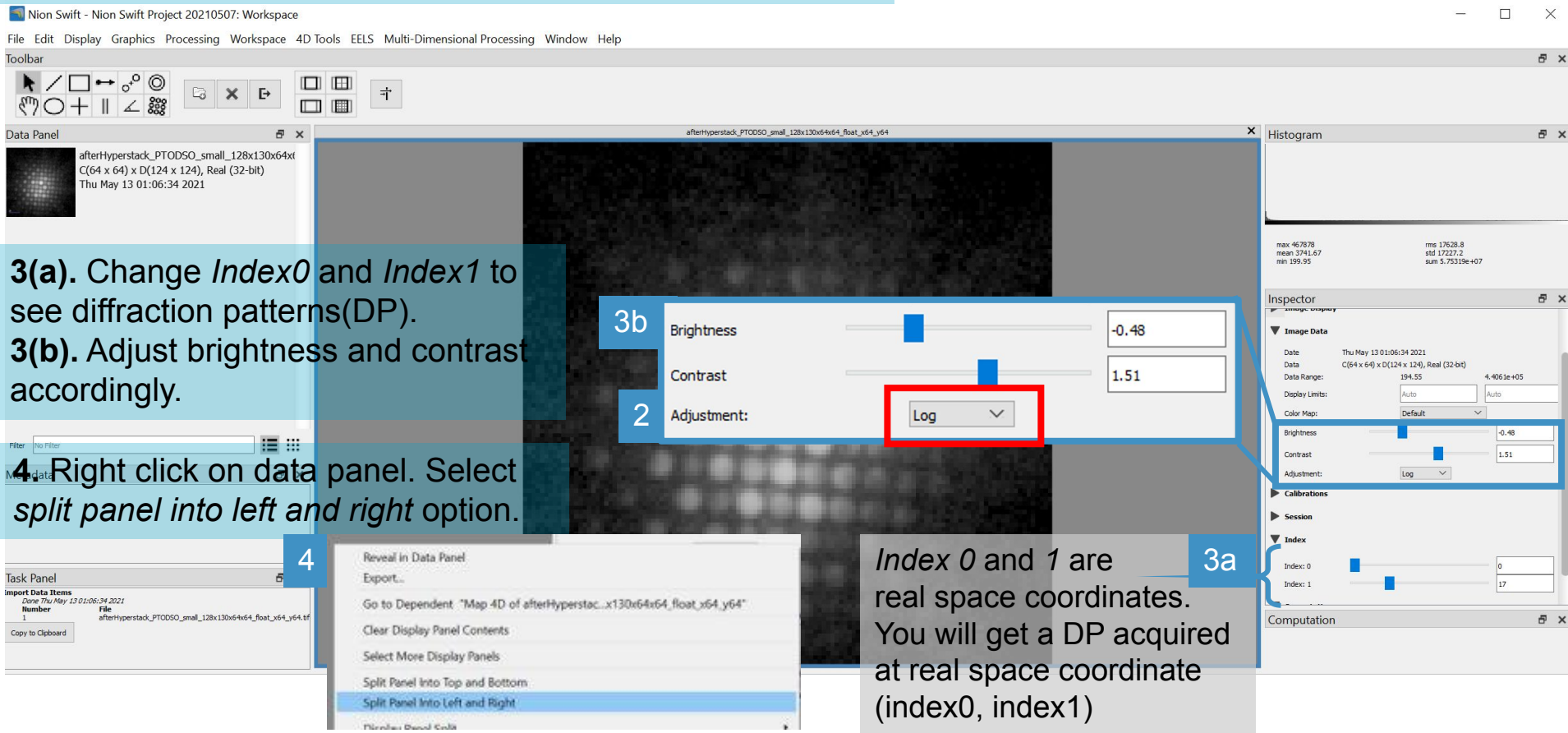
Date Thu May 13 01:06:34 2021
Data C(64 x 64) x D(124 x 124), Real (32-bit)
Data Range: 165.40 2.4587e+06
Display Limits: Auto Auto
Color Map: Default
Brightness 0.00
Contrast 1.00
Adjustment: None

Calibrations

Axis	Offset	Scale	Units
0	0.0000	1.0000	
1	0.0000	1.0000	
2	0.0000	1.0000	
3	0.0000	1.0000	

Computation

2. Set *Adjustment* under *Inspector* window to *Log*



The screenshot shows the Nion Swift software interface. The main window displays a diffraction pattern (DP) acquired at real space coordinate (index0, index1). The Inspector window is open, showing the Adjustment dropdown menu set to Log. The Brightness and Contrast sliders are also visible. The Data Panel shows the file name and acquisition date. The Task Panel shows the file name and acquisition date. The Histogram window shows the statistics of the DP.

3(a). Change *Index0* and *Index1* to see diffraction patterns(DP).

3(b). Adjust brightness and contrast accordingly.

4. Right click on data panel. Select *split panel into left and right* option.

2 Brightness: -0.48
Contrast: 1.51
Adjustment: Log

3a Index 0 and 1 are real space coordinates. You will get a DP acquired at real space coordinate (index0, index1)

4 Right click on data panel. Select *split panel into left and right* option.

Task Panel
Import Data Items
Done Thu May 13 01:06:34 2021
File
1 afterHyperstack_PTODSO_small_128x130x64x64_float_x64_y64.tif
Copy to Clipboard

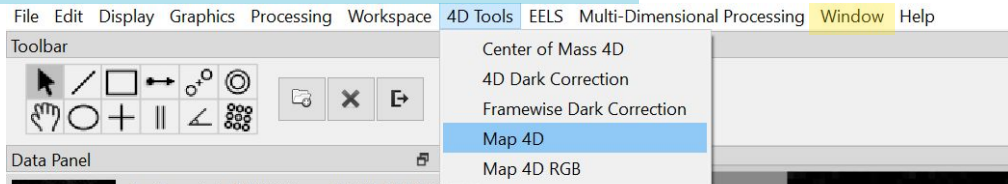
Data Panel
afterHyperstack_PTODSO_small_128x130x64x64_float_x64_y64.tif
C(64 x 64) x D(124 x 124), Real (32-bit)
Thu May 13 01:06:34 2021

Histogram
max: 467878
mean: 3741.67
min: 199.95
rms: 17628.8
std: 17227.2
sum: 5.75319e+07

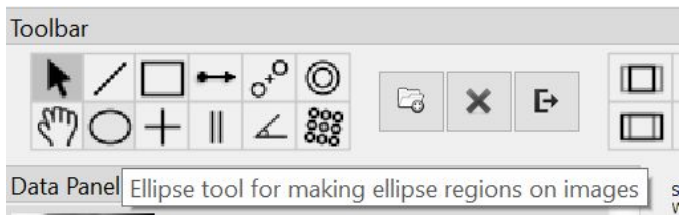
Inspector
Image Data
Date: Thu May 13 01:06:34 2021
Data: C(64 x 64) x D(124 x 124), Real (32-bit)
Data Range: 194.55
Display Limits: Auto
Color Map: Default
Brightness: -0.48
Contrast: 1.51
Adjustment: Log
Calibrations
Session
Index
Index 0: 0
Index 1: 17
Computation

Right-click context menu:
Reveal in Data Panel
Export...
Go to Dependent: "Map 4D of afterHyperstack...x130x64x64_float_x64_y64"
Clear Display Panel Contents
Select More Display Panels
Split Panel into Top and Bottom
Split Panel into Left and Right
Pin/Unpin Board Editor

5. 4D Tools > Map 4D



6. Select *Ellipse tool* from *Toolbar*. Draw a circle on the DP.



Tip: shift+drag allows you to draw a circle rather than an ellipse.

Only the region within this circle will be used to get real space image. Select a diffraction spot you're interested in looking at. You can move/adjust size of this circle later.

7. Click *Select map graphic* from the *Computation* window. (You can open this window from *Window>* *Computation*).

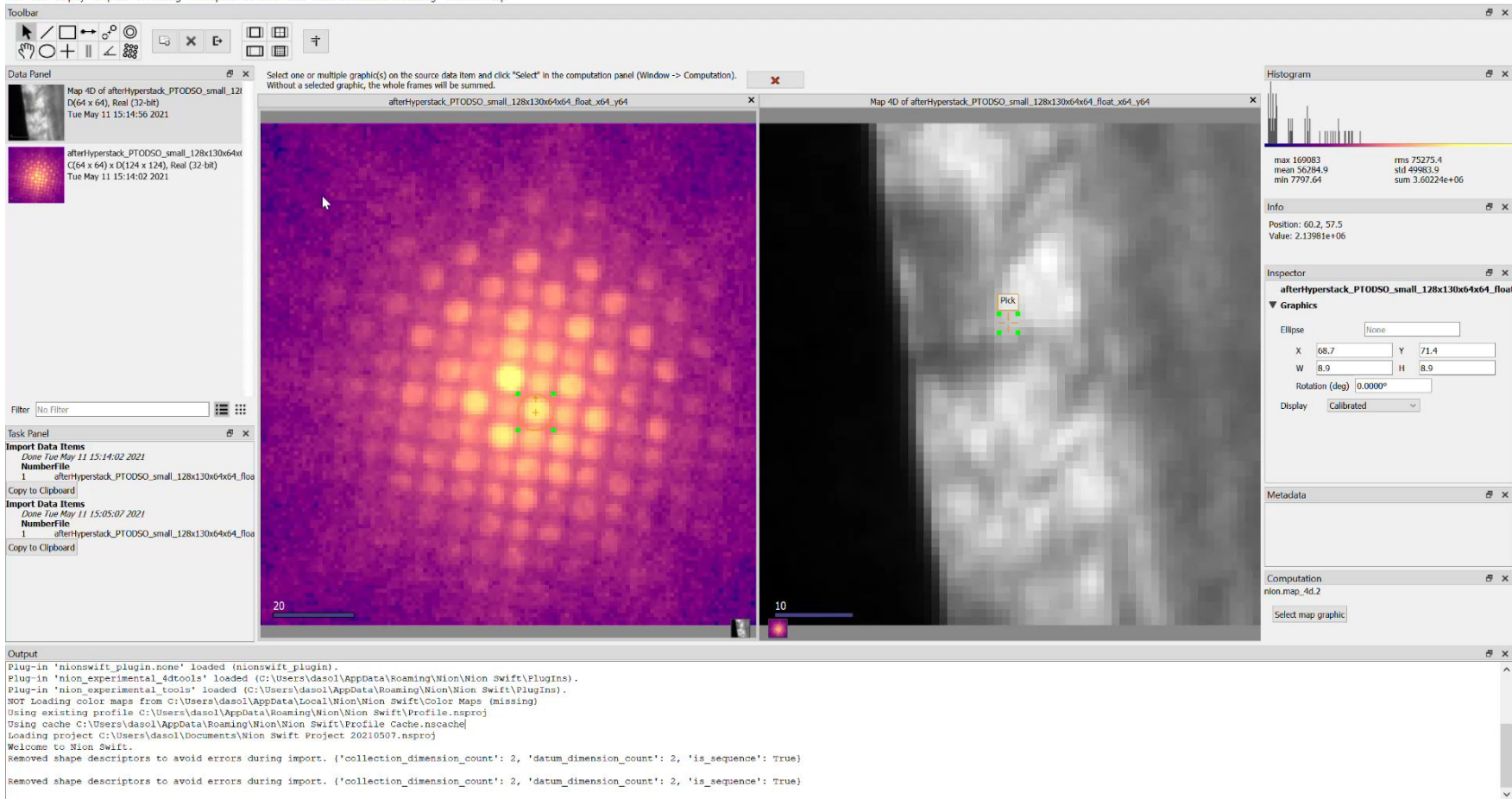


8. You can now view the 4D STEM data!

Q: What happens when you move the circular mask around?

Q: What is the role of this mask? What is the equivalent part in the microscope?

File Edit Display Graphics Processing Workspace 4D tools EELS Multi-Dimensional Processing Window Help



Nion Swift - Nion Swift Project 20210507: Workspace

File Edit Display Graphics Processing Workspace 4D Tools EELS Multi-Dimensional Processing Window Help

Toolbar

Data Panel

Map 4D of afterHyperstack_PTODSO_small_128x130x64x64_float_x64_y64
D(64 x 64), Real (32-bit)
Thu May 13 01:44:18 2021

afterHyperstack_PTODSO_small_128x130x64x64_float_x64_y64
C(64 x 64) x D(124 x 124), Real (32-bit)
Thu May 13 01:06:34 2021

Filter: No Filter

Metadata

nion.map_4d.parameters {2}

Task Panel

Import Data Items
Done Thu May 13 01:23:16 2021
Number 1
File test.tif
Copy to Clipboard

Import Data Items
Done Thu May 13 01:06:34 2021
Number File

Move the "Pick" graphic to change the data slice in the source data item.

afterHyperstack_PTODSO_small_128x130x64x64_float_x64_y64

Map 4D of afterHyperstack_PTODSO_small_128x130x64x64_float_x64_y64

Pick

Histogram

max 5.7313e+07 rms 3.11407e+07
mean 2.33703e+07 std 2.05809e+07
min 3.65902e+06 sum 9.57246e+10

Inspector

Map 4D of afterHyperstack_PTODSO_small_128x130x64x64_float_x64_y64

▼ Graphics

Point Pick

X 38.2 Y 21.7

Display Calibrated

Computation

nion.map_4d.2

Select map graphic

Nion Swift - Nion Swift Project 20210507: Workspace

File Edit Display Graphics Processing Workspace 4D Tools EELS Multi-Dimensional Processing Window Help

Toolbar

Data Panel

Map 4D of afterHyperstack_PTODSO_small_128x130x64x64_y64
D(64 x 64), Real (32-bit)
Thu May 13 01:44:51 2021

afterHyperstack_PTODSO_small_128x130x64x64_y64
C(64 x 64) x D(124 x 124), Real (32-bit)
Thu May 13 01:06:34 2021

Filter: No Filter

Metadata

Task Panel

Import Data Items
Done Thu May 13 01:23:16 2021
Number
1
File
test.tif
Copy to Clipboard

Import Data Items
Done Thu May 13 01:06:34 2021
Number
File

Select one or multiple graphic(s) on the source data item and click "Select" in the computation panel (Window -> Computation).
Without a selected graphic, the whole frames will be summed.

afterHyperstack_PTODSO_small_128x130x64x64_float_x64_y64

Map 4D of afterHyperstack_PTODSO_small_128x130x64x64_float_x64_y64

Pick

Histogram

max 123531
mean 31685.6
min 4016.03

rms 47746.6
std 35717.9
sum 3.16856e+05

Inspector

afterHyperstack_PTODSO_small_128x130x64x64_float_x64_y64

▼ Graphics

Ellipse

X 54.2 Y 69.1
W 10.1 H 10.1
Rotation (deg) 0.0000°

Display Calibrated

Computation

nion.map_4d.2

Select map graphic