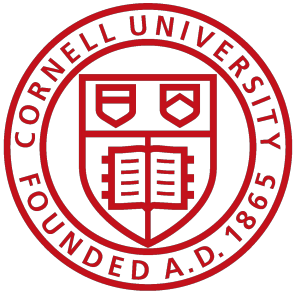
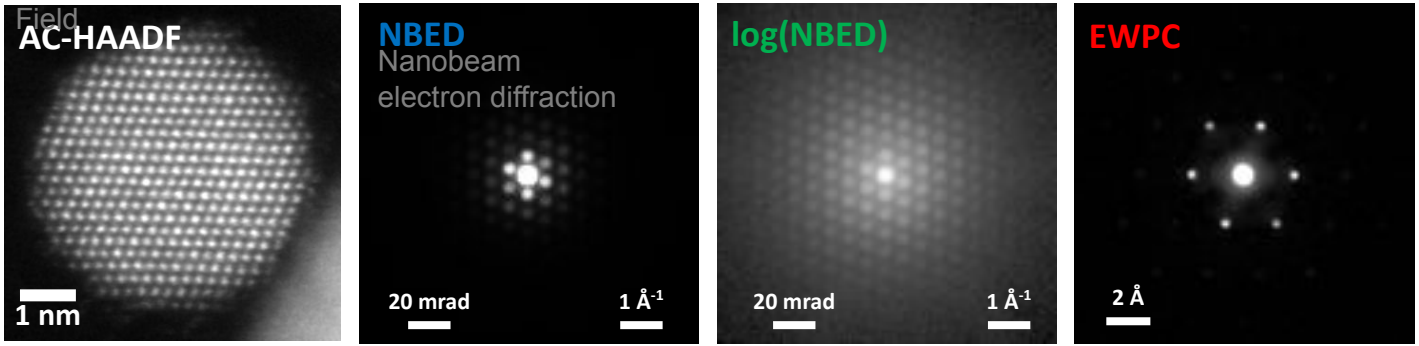


T5 - 4D STEM data analysis

Exit Wave Power Cepstrum

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

$$\left| \mathrm{FT}\left(\ln\left(I(\boldsymbol{k}) \right) \right) \right|$$



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

Padgett et al. *Ultramicroscopy*, **2020**, Vol 214,112994

Cepstrum (spectrum) transform

The "classic" power cepstrum (PC),*

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

separates convolved signals :

$$\mathrm{PC}\big(\alpha(t) * \beta(t)\big) \approx \mathrm{PC}\big(\alpha(t)\big) + \mathrm{PC}\big(\beta(t)\big)$$

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

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

$$\mathrm{EWPC}_{\phi}(\boldsymbol{x}) = \mathrm{PC}\big(\phi(\boldsymbol{x})\big) = \left|\mathcal{F}\left(\ln\big(I(\boldsymbol{q})\big)\right)\right|^2$$

Or simply

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

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

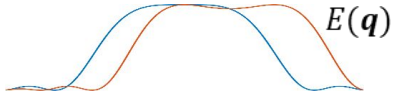
Exit-Wave Power Cepstrum (EWPC)

Strong phase approximation for diffraction:

$$I(\boldsymbol{q}) = \left|\Phi_{\mathrm{p}}(\boldsymbol{q}) \otimes \left(E(\boldsymbol{q}) \cdot V(\boldsymbol{q})\right)\right|^2 \approx |E(\boldsymbol{q})|^2 \cdot \left|\Phi_{\mathrm{p}}(\boldsymbol{q}) \otimes V(\boldsymbol{q})\right|^2$$

where $\Phi_{\mathrm{p}}(\boldsymbol{q})$ - probe function,
$V(\boldsymbol{q})$ - projected atomic potential,
$E(\boldsymbol{q})$ - slowly varying envelope damping function
(carries tilt and thickness information)

Envelope damping diffraction pattern



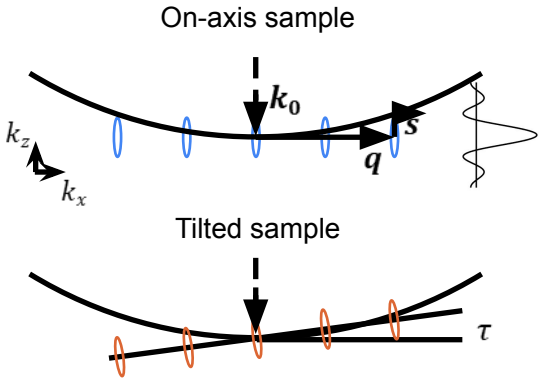
$$\mathrm{EWPC}_{\phi}(\mathbf{x}) = \left|\mathcal{F}\left(\ln\left(I(\boldsymbol{q})\right)\right)\right| \approx \mathrm{PC}\left(\epsilon(\boldsymbol{x})\right) + |\phi_P(\boldsymbol{x})|^2 \cdot \mathrm{PC}\left(v_0(\boldsymbol{x})\right)$$

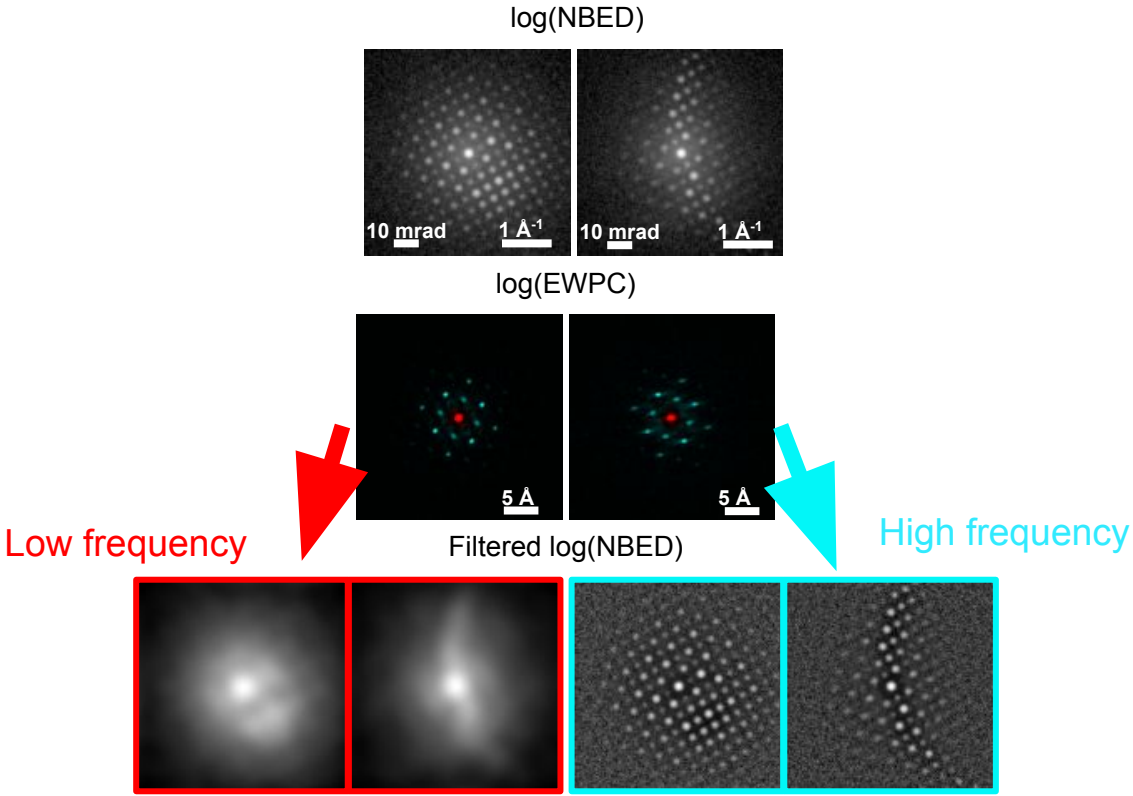
Ewald sphere envelope — Probe function — Projected lattice potential

Tilt and thickness artifacts are decomposed from the atomic distance information

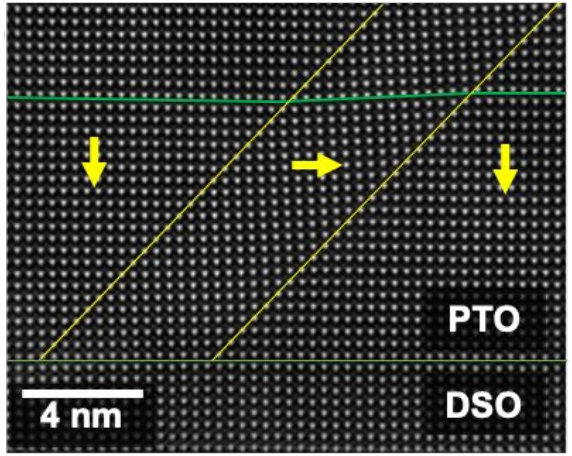
EWPC: Tilt and thickness decomposition

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

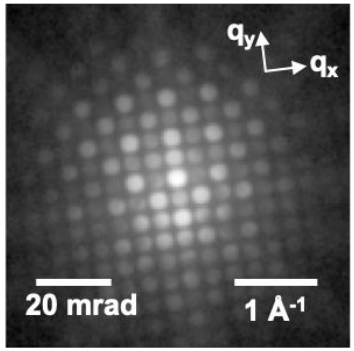




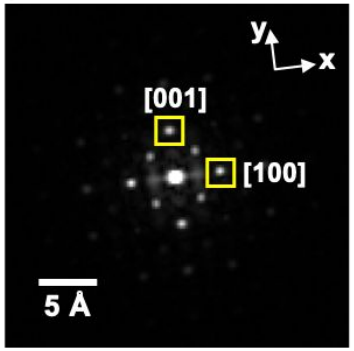
EWPC application: $PbTiO_3$ domains in strained film



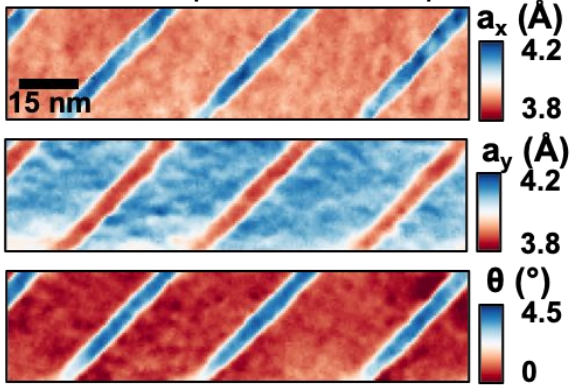
log (NBED)

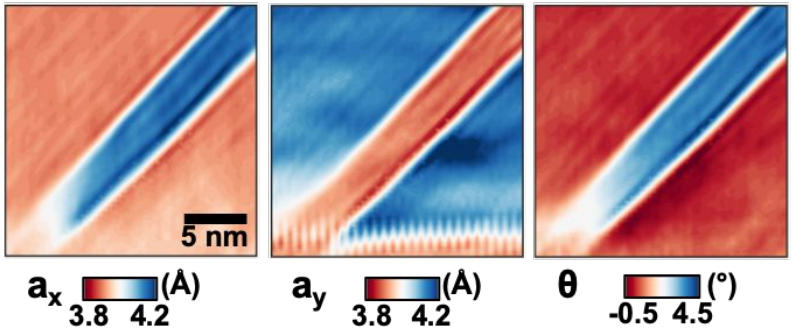


log (EWPC)



Lattice parameter map





Padgett, Elliot, et al. *Ultramicroscopy* (2020): 112994.

PARADIM
AN NSF MATERIALS INNOVATION PLATFORM

(Optional)
Browsing 4D STEM data on NION Swift

Install Nion Swift Plugins

Windows

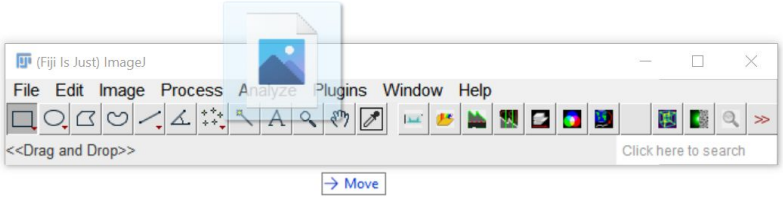
Copy the folders into "C:\Users\#userName\AppData\Roaming\Nion\Nion Swift\PlugIns"

Mac

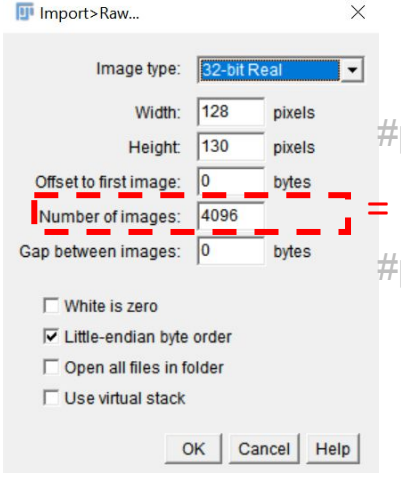
Users/#userName/Library/Application Support/Nion/Nion Swift/PlugIns

Optional: Prepare your own data

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

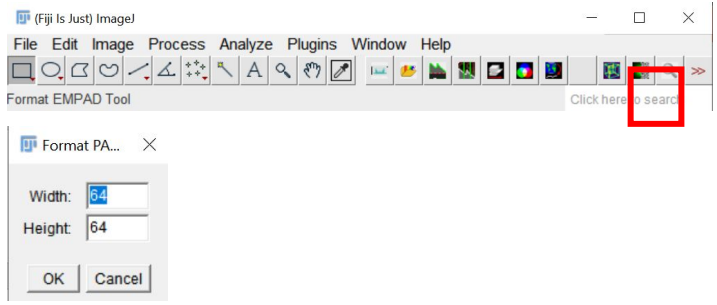


2. Once the 4D data is loaded, the following popup window will show up. Change number of images accordingly.

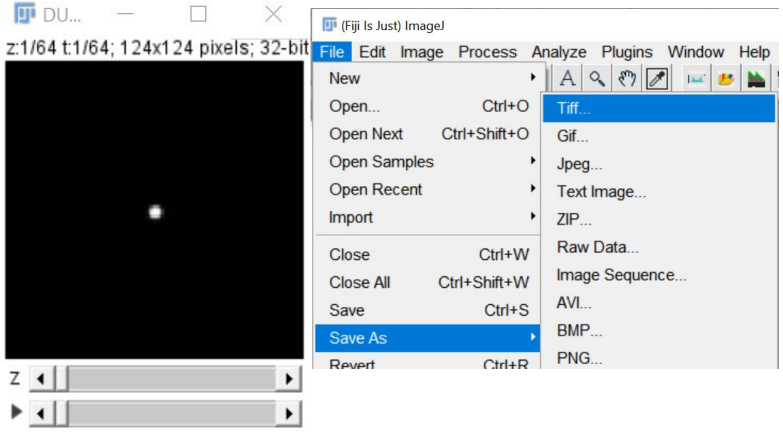


= #pixels in x1 axis of real space X #pixels in x2 axis of real space

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.

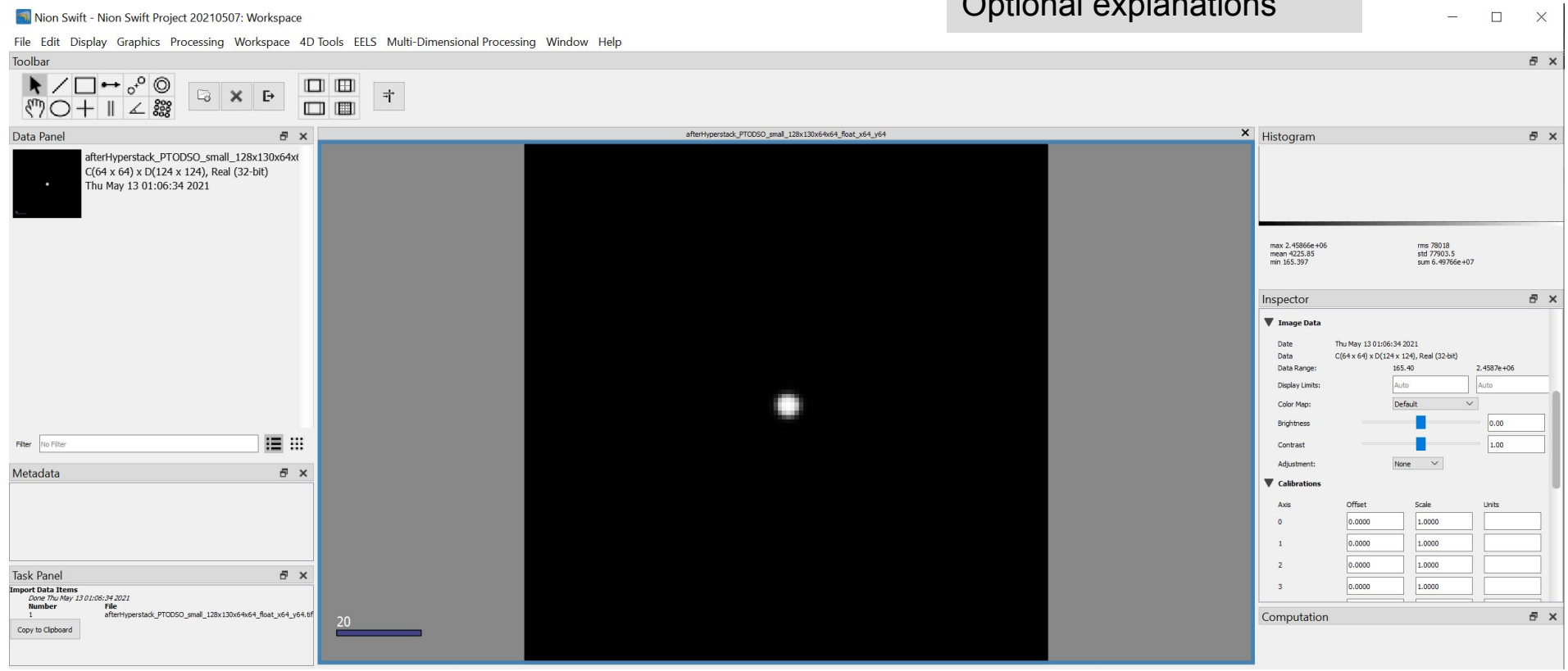


Load Data

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

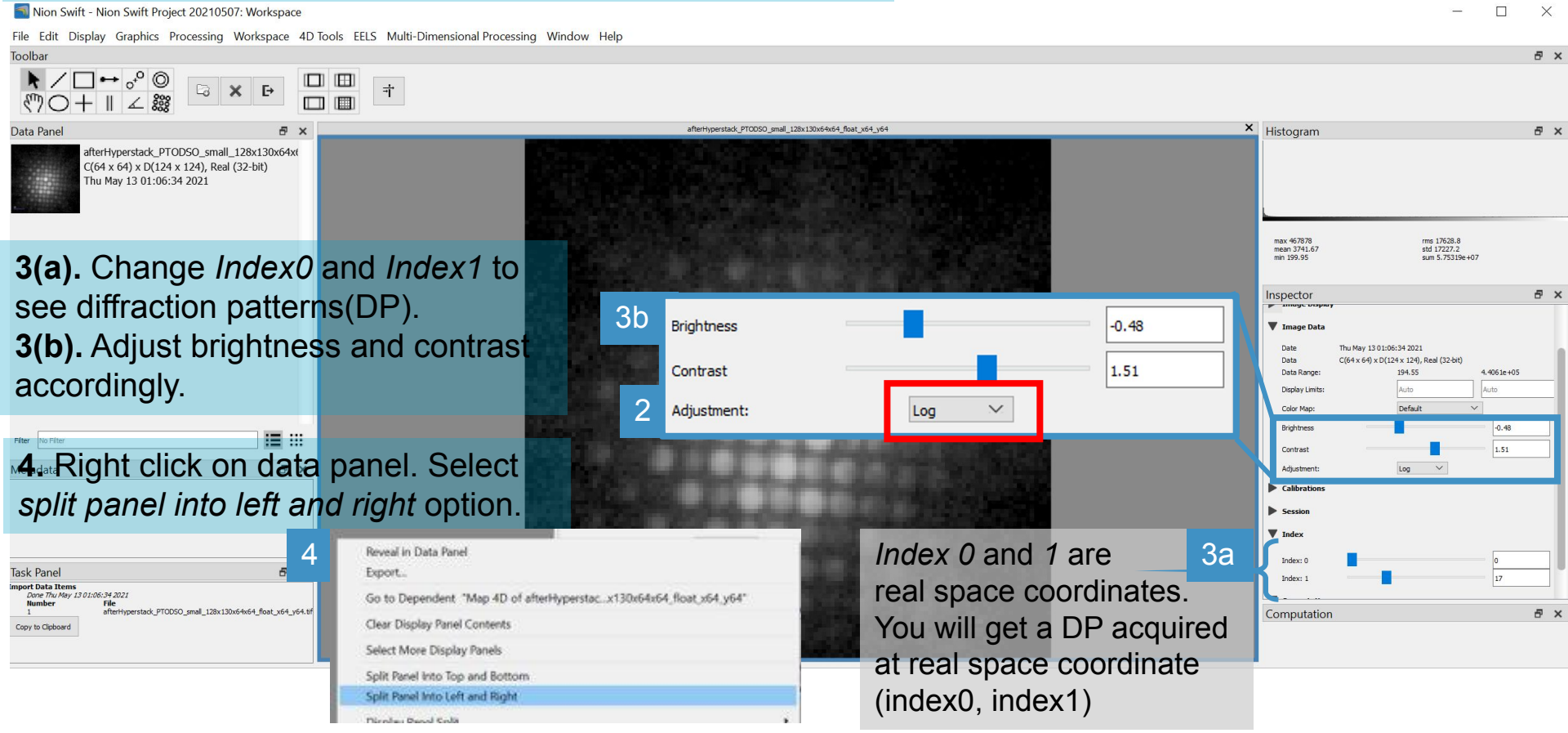
Note: Steps to follow

Optional explanations



Set Variables

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



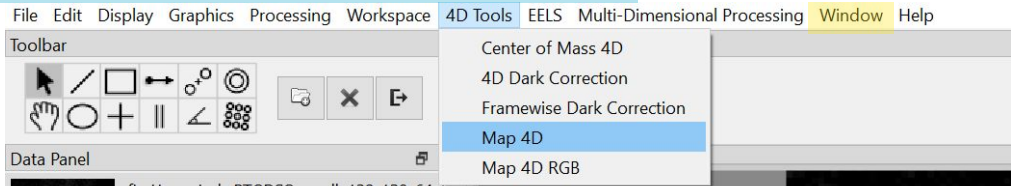
3(a). Change *Index0* and *Index1* to see diffraction patterns(DP).
3(b). Adjust brightness and contrast accordingly.

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

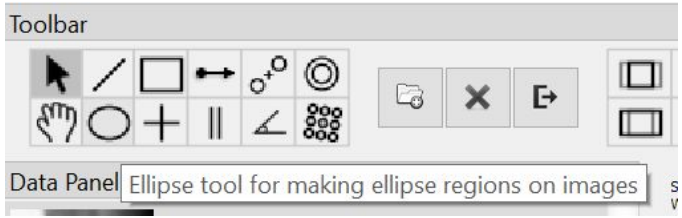
Index 0 and *1* are real space coordinates. You will get a DP acquired at real space coordinate (index0, index1)

Map 4D

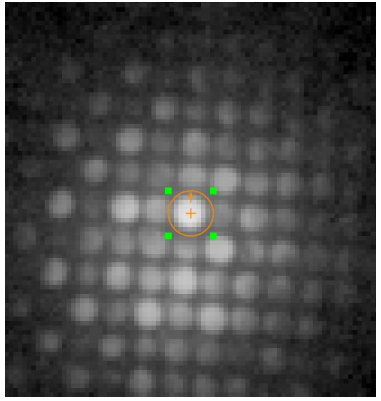
5. *4D Tools > Map 4D*



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.

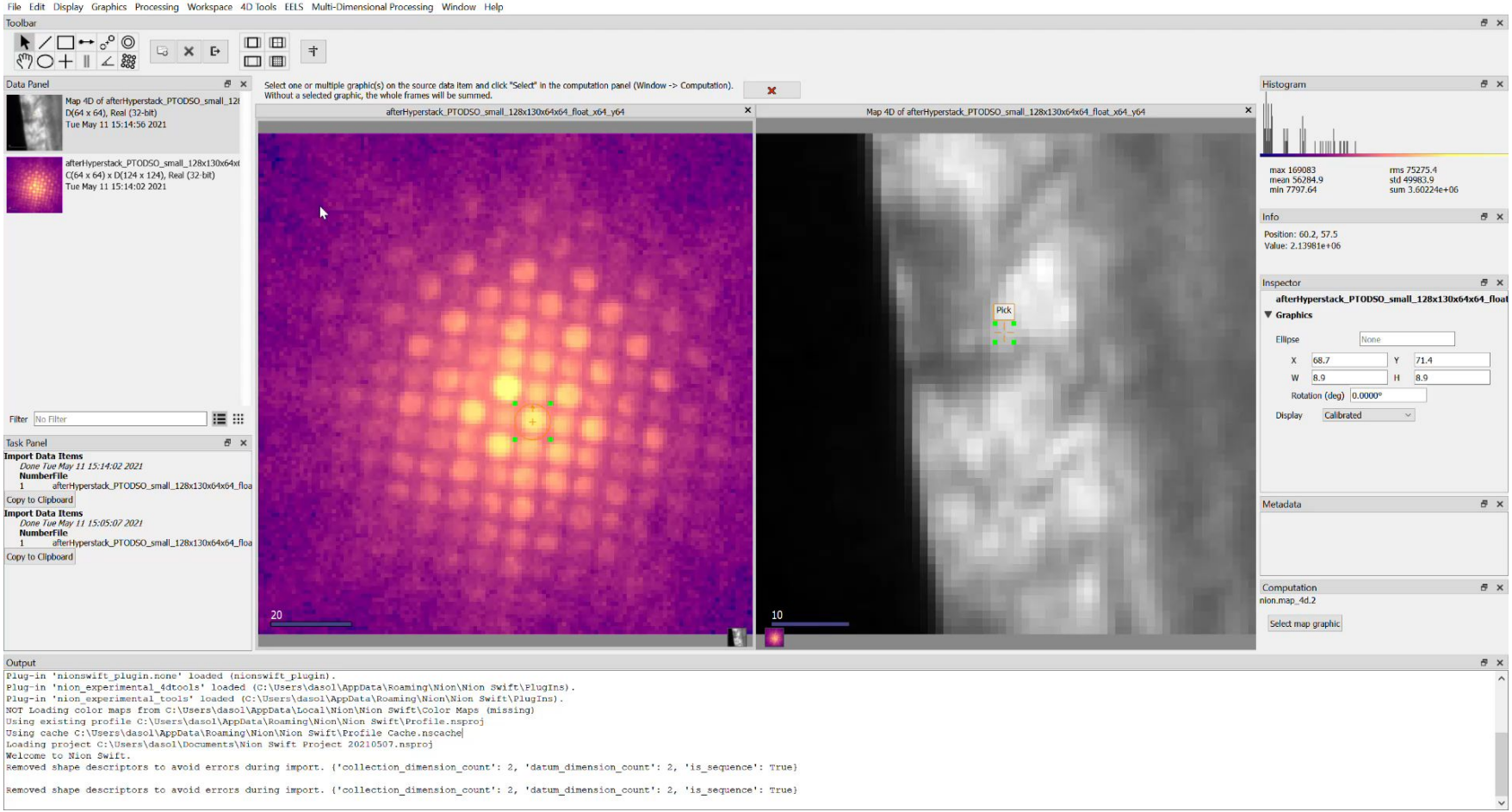
7. Click *Select map graphic* from the *Computation* window. (You can open this window from *Window*> *Computation*).

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

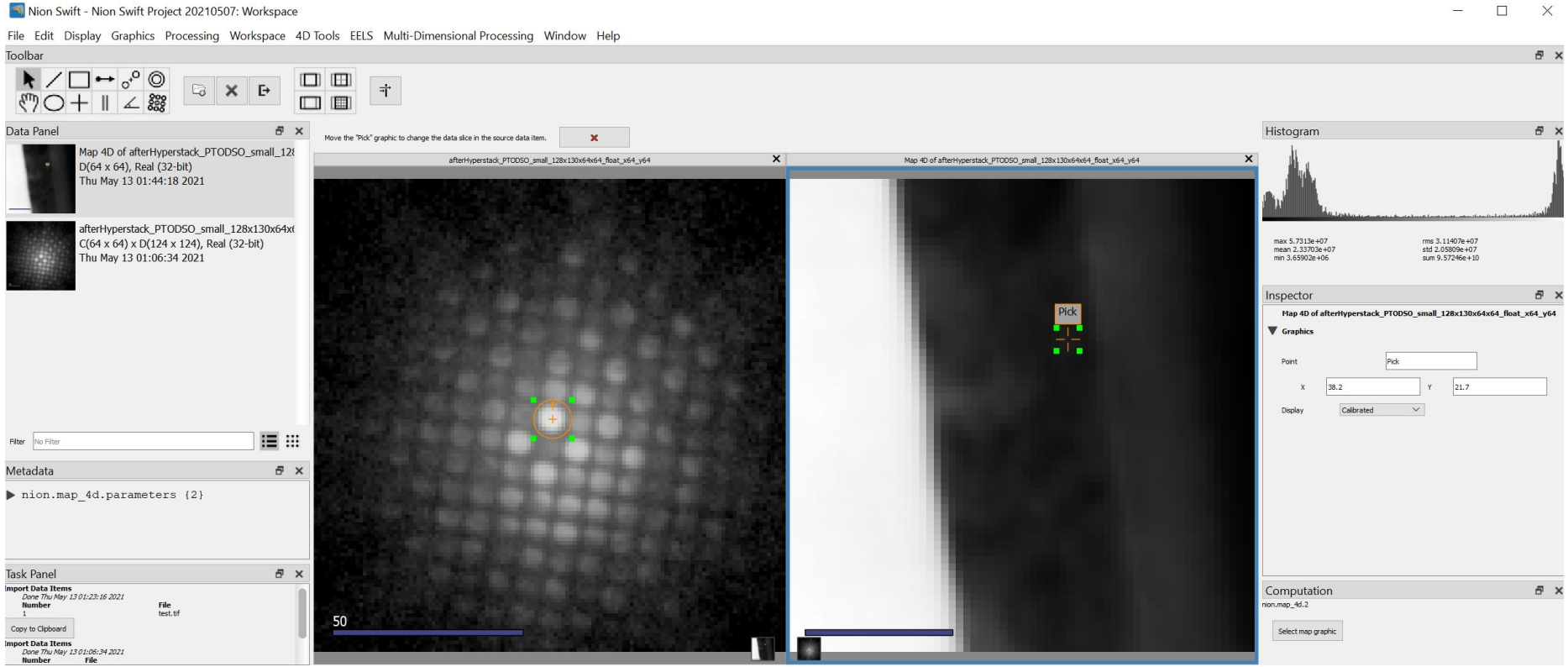
Q: What happens when you move the circular mask around?

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

Example Windows



Example Windows



Example Windows