

# ***CLS STXM and Ptychography Data Analysis***

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# Outline

## ❖ aXis2000

- Installation and Introduction
- Images
- Spectra
- Linescans
- Stacks: alignment, spectra, mapping, fitting, etc.
- Cryo-STXM

## ❖ PyPIE: STXM-Ptychography

## ❖ PCA\_GUI and Mantis

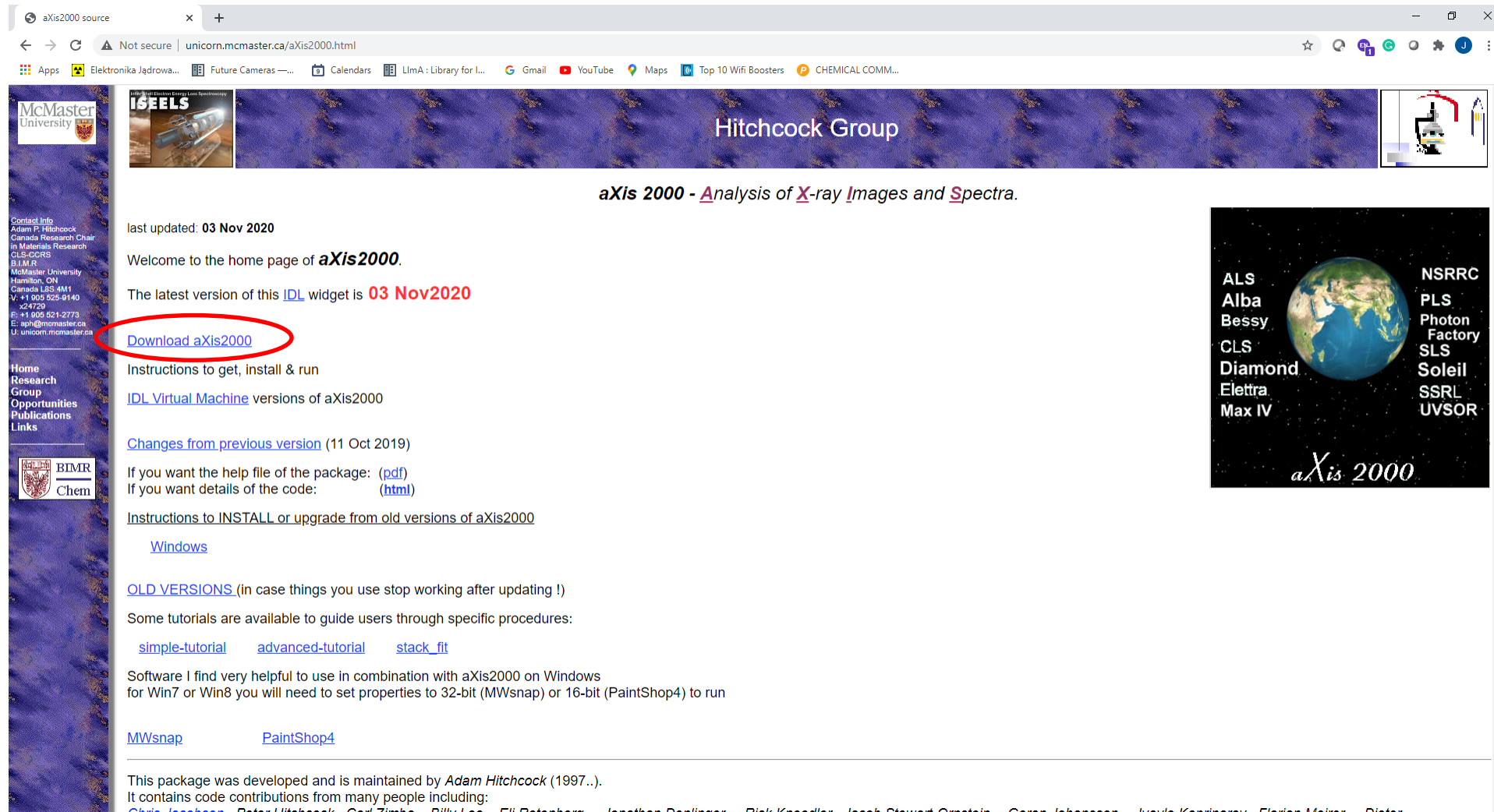
## ❖ ImageJ Plugins - ScatterJ



# STXM and Ptychography Data Analysis Software

- aXis2000, Interactive Data Language (IDL) Virtual Machine, <http://unicorn.mcmaster.ca/aXis2000.html>.
- Other IDL based: stack\_analyze.sav, pca\_gui.sav
- Python based: Mantis 2.3.02
- Ptychography: PyPIE, Sharpcamera, PtychoLib, etc.
- Other imaging processing: ImageJ and plugins, MATLAB, etc.
- Other spectroscopy processing: Athena, Fityk 0.9.8

# aXis2000 – Analysis of X-ray Images and Spectra



The screenshot shows the aXis2000 website in a web browser. The browser's address bar shows the URL `unicorn.mcmaster.ca/aXis2000.html`. The website has a blue header with the McMaster University logo on the left and the Hitchcock Group logo on the right. Below the header, the text *aXis 2000 - Analysis of X-ray Images and Spectra.* is displayed. The main content area includes a 'last updated: 03 Nov 2020' notice, a welcome message, and a link to download the latest version (03 Nov 2020). A red circle highlights the 'Download aXis2000' link. Other links include 'Instructions to get, install & run', 'IDL Virtual Machine versions of aXis2000', 'Changes from previous version' (dated 11 Oct 2019), and 'Instructions to INSTALL or upgrade from old versions of aXis2000'. A sidebar on the left contains contact information for Adam P. Hitchcock and a list of links. A right sidebar features a globe image and lists various synchrotron facilities: ALS, Alba, Bessy, CLS, Diamond, Elettra, Max IV, NSRRC, PLS, Photon Factory, SLS, Soleil, SSRL, and UVSOR. The footer of the website mentions that the package was developed and maintained by Adam Hitchcock (1997..) and lists several contributors.

McMaster University

Hitchcock Group

*aXis 2000 - Analysis of X-ray Images and Spectra.*

last updated: 03 Nov 2020

Welcome to the home page of **aXis2000**.

The latest version of this [IDL](#) widget is **03 Nov2020**

[Download aXis2000](#)

Instructions to get, install & run

[IDL Virtual Machine](#) versions of aXis2000

[Changes from previous version](#) (11 Oct 2019)

If you want the help file of the package: ([pdf](#))  
If you want details of the code: ([html](#))

[Instructions to INSTALL or upgrade from old versions of aXis2000](#)

[Windows](#)

[OLD VERSIONS](#) (in case things you use stop working after updating !)

Some tutorials are available to guide users through specific procedures:

[simple-tutorial](#) [advanced-tutorial](#) [stack\\_fit](#)

Software I find very helpful to use in combination with aXis2000 on Windows  
for Win7 or Win8 you will need to set properties to 32-bit (MWsnap) or 16-bit (PaintShop4) to run

[MWsnap](#) [PaintShop4](#)

This package was developed and is maintained by Adam Hitchcock (1997..).  
It contains code contributions from many people including:  
[Chris Jacobsen](#) [Peter Hitchcock](#) [Carl Zimba](#) [Billy Lee](#) [Eli Rotenberg](#) [Jonathan Denlinger](#) [Rick Kneadler](#) [Jacob Stewart-Ornstein](#) [Goran Johansson](#) [Ivaylo Konradinov](#) [Florian Meier](#) [Dieter](#)

ALS  
Alba  
Bessy  
CLS  
Diamond  
Elettra  
Max IV

NSRRC  
PLS  
Photon  
Factory  
SLS  
Soleil  
SSRL  
UVSOR

*aXis 2000*



# aXis2000 – Analysis of X-ray Images and Spectra

aXis2000 download (Windows, M x +

Not secure | unicorn.mcmaster.ca/axis/aXis2000-download.html

Apps Elektronika Jądrowa... Future Cameras... Calendars UIMA : Library for L... Gmail YouTube Maps Top 10 Wifi Boosters CHEMICAL COMM...

McMaster University

Hitchcock Group  
aXis2000

*aXis 2000 - Analysis of X-ray Images and Spectra.*

last updated: 03 Nov 2020

**aXis2000**

The latest version is 03 Nov 2020

Note this code works on Windows, Unix or Mac\_OSX operating systems. There are known issues with the Mac version that I am in the process of correcting. Please send me an email with test data that demonstrates bugs so I can fix them.

[Download aXis2000](#)

**For windows:** please make a folder c:\aXis2000 and expand all files in the downloaded aXis2000.zip file into c:\aXis2000 using folder names (there will be four sub-folders).

**For Mac\_OS:** please place all files & folders in the zip file in Users\laXis2000

If you are using IDL Virtual Machine here are some instructions to get & install [IDL Virtual Machine](#) version (same code)

[Changes from previous version](#) (11 Oct 2019)

If you want the help file of the package: [\(pdf\)](#)  
If you want details of the code: [\(html\)](#)

**Do NOT use folder names with blanks for the source code or your data !!!**

[Instructions to INSTALL or upgrade from old versions of aXis2000](#)

[Windows](#) Please make a folder c:\aXis2000 and expand all files in the downloaded aXis2000-pre-IDL8.3 zip file into c:\aXis2000 using folder names (there will be four sub-folders).

[OLD VERSIONS](#) (in case things you use stop working after updating I)

Some tutorials are available to guide users through specific procedures  
[simple tutorial](#) [advanced tutorial](#) [stack\\_fit](#)

I find the following 2 programs very helpful to use in combination with aXis2000 on Windows.

**Windows installation location: c:\aXis2000**

**Mac installation location: Users\laXis2000**

**aXis2000.sav is the IDL executable file.**

**Old versions and online tutorials**

ALS  
Alba  
Bessy  
CLS  
Diamond  
Electra  
NSRRC  
PLS  
Photon  
Factory  
SLS  
Soleil  
SSRL  
UVSOR

*aXis 2000*

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# aXis 2000

## Analysis of X-ray microscopy Images and Spectra (30 June 2014)

aXis2000 - Analysis of X-ray microscopy Images and Spectra - is an [IDL widget](http://www.exelisvis.com/) for viewing, comparing and processing X-ray microscopy images and spectra. IDL stands for [Interactive Data Language](http://www.exelisvis.com/), a scientific computing platform developed by Research Systems Inc (RSI), currently part of Exelis Visual Information Solutions (<http://www.exelisvis.com/>). aXis2000 contains scripts developed by Chris Jacobsen, Carl Zimba, Adam Hitchcock and others. The widget platform was written by Adam & Peter Hitchcock. It is maintained and occasionally updated by Adam Hitchcock. It can be obtained from [unicorn.mcmaster.ca/aXis2000](http://unicorn.mcmaster.ca/aXis2000). It operates on Windows (WIN), Unix (X) and Macintosh (MAC) versions of IDL, although there are problems at present with operating it on a Mac, if you use IDL 7.0 and later versions.

Since May-04 a compiled version (aXis2000.sav) for use with [IDL Virtual Machine](http://www.exelisvis.com/) has been available. This allows access to the power of aXis2000 without needing to purchase an IDL license. Please note that there are often features of aXis2000 that work with the licensed version, but not with the VM version, and that the specific details of these problems depend on the version of both IDL and aXis2000.

I would appreciate it if you would notify me by email ([aph@mcmaster.ca](mailto:aph@mcmaster.ca)) about problems with the code or if you wish to make suggestions for improvements. If you make extensions or corrections, I would appreciate receiving a copy of your code revisions with sample data, so I can evaluate and incorporate in future versions.

I thank all the people who have written scripts that went into this. Carl Zimba (Photons Unlimited) who supplied ZSTACK and extensively improved the overall package in 2000; my son, Peter who helped set up the basic widget structure; Eli Rotenberg, Jonathan Denlinger, Stefano Cerasari, Tolek Tyliczszak, Andy Smith, Andreas Scholl, Göran Johansson, Jacob Stewart Ornstein, and many others. SPECIAL thanks to Chris Jacobsen (Stony Brook, nsls) for sharing his STACK\_ANALYZE and PCA\_GUI codes, Rick Kneidler, for providing the basis for the stack-fit routine, and Billy Loo (UCSF) for providing SF, the Henke mass absorption routine and the Conjugate Gradient Optimization routine (ax\_cgo).

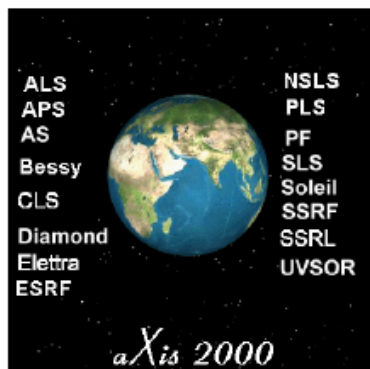
**TO START aXis2000:** after [installing aXis2000](#) (see end of this file)  
Windows and Mac OS:

Start IDL ;

If you have set the [Preferences](#) (in IDL) so that axis2000\_batch.pro is the start file, aXis2000 will launch automatically.

Otherwise, type axis2000 on the IDL command line.

If you quit aXis2000 and stay in IDL, you can restart by typing axis2000



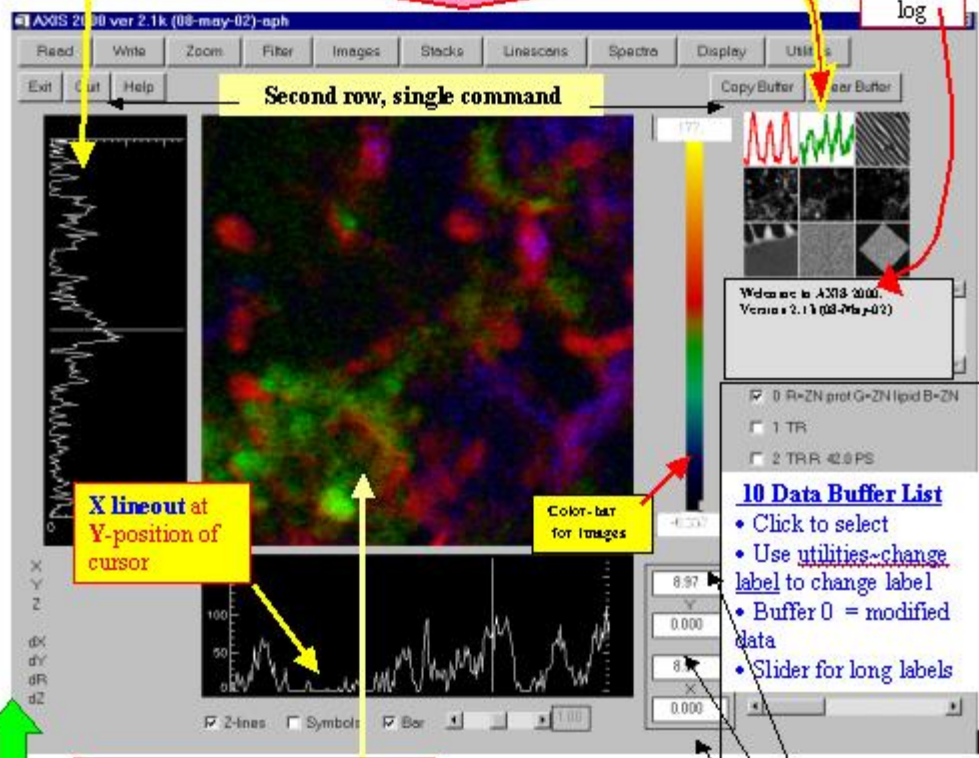
## Features of the aXis2000 widget

Y lineout at X-position of cursor

First-row pull-down menus

Thumbnails  
• Click to select a buffer

Axis Messages, Hints and log



Lineouts, symbols & scale bar options

Gamma for Images

X, Y, (Z) limits for Images & spectra (display & control)

### Cursors

(X,Y,Z) - at cursor  
(dX,dY,dZ) - change over line (images) or between cursors (spectra)  
dR - distance along line (images only)

### Main Image

- Displays currently selected image or selected spectrum (or group of spectra, if Spectra-Overplot used)
  - Size of aXis2000 display can be adjusted (0.5 to 2.0) of a nominal size (360x360 pixels in Main Image) by size parameter in axis.ini
- Mouse** (if Z-lines is selected)
- First click - cursor and lineout; arms the line generator
  - Second click - draws and documents line (image) ;  
- reports difference in cursors (spectra)
  - Third click - clears line and cursor information



# aXis2000 GUI Structure

- Think of as a **TOOLBOX** rather than a **Workflow** (Mantis is workflow oriented)
- User can follow pre-set sequence(s)

Tutorials on web site <http://unicorn.mcmaster.ca/aXis2000.html> (rather dated!!)

**aXis2000 Manual** (Help) describes function of each button, not workflow

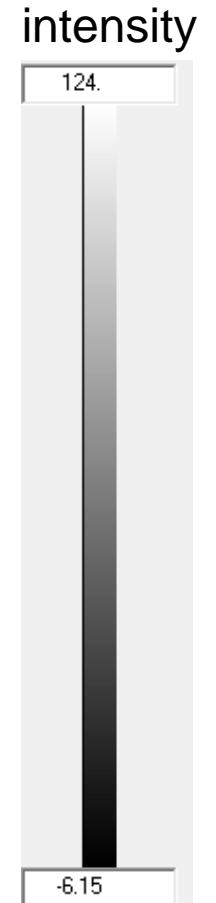
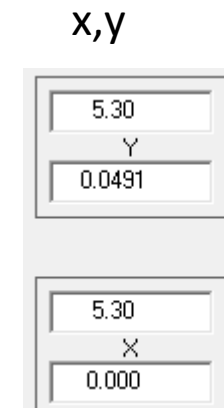
Top level menus organized by **process** (read/write/zoom/filter/utilities)  
and by **type of data**: images / stacks/linescans/spectra



## Main panel features



|     |           |    |
|-----|-----------|----|
| X   | 0.052719  | 1  |
| Y   | 1.2904    | 25 |
| Z   | 2.3799    |    |
| d-X | 0.46469   |    |
| d-Y | -0.012539 |    |
| d-R | 0.46485   |    |
| d-Z | 41.570    |    |



# Images

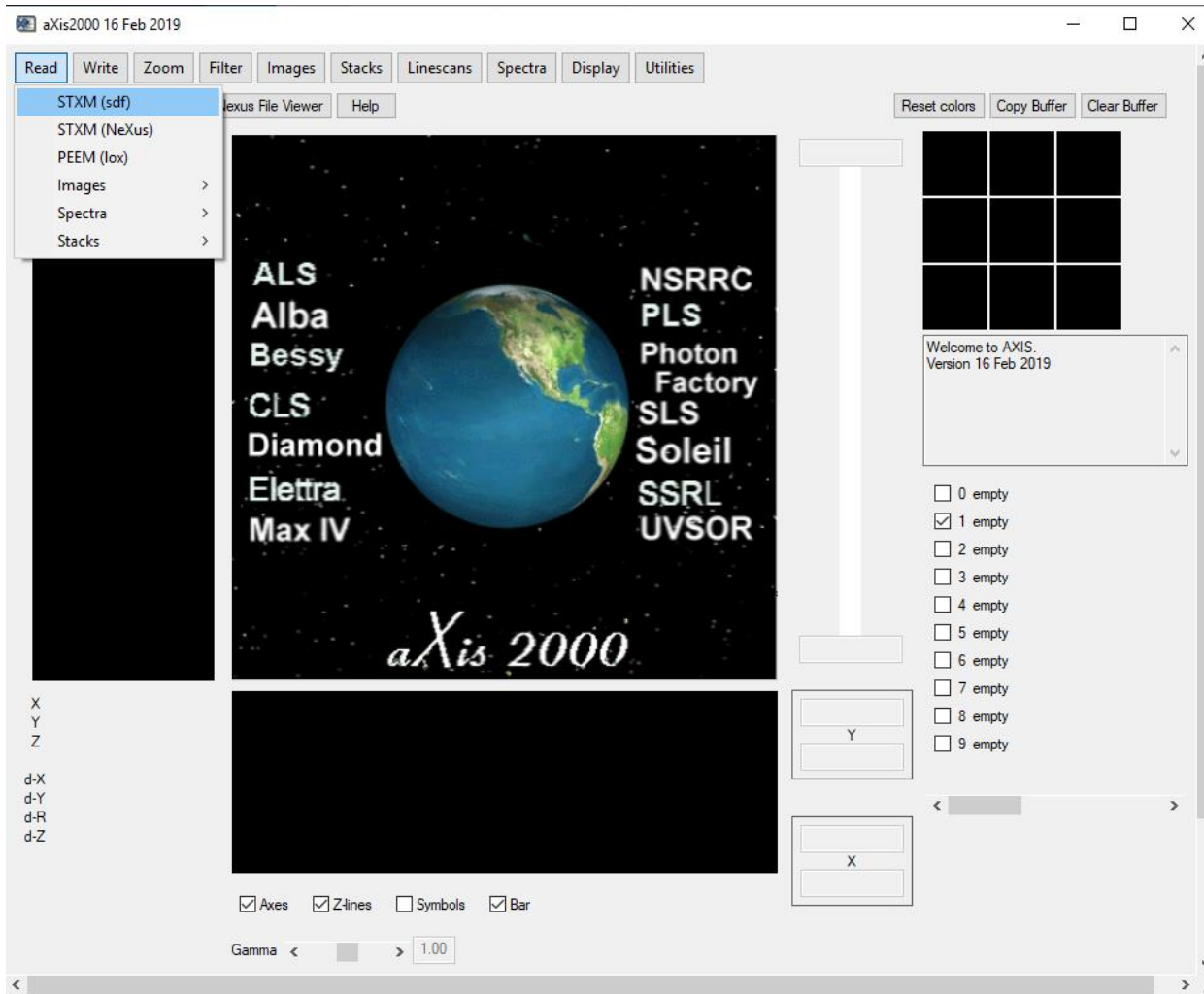


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synchrotron

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# aXis2000 – Read Data



- **Read → STXM (sdf)**, for standard CLS Ambient-STXM data files
- **Read → STXM (NeXus)**, for CLS Cryo-STXM data files
- **Read → PEEM (lox)**, for CLS PEEM data files
- **Read → Images**, for many other synchrotron instruments data files, graphics files, etc.
- **Read → Spectra**, for many other synchrotron instruments data files, text files, etc.
- **Read → Stacks**, for many other synchrotron instruments data files



# Ambient-STXM Data Format

**Header File:** e.g. **A091111005.hdr**,  
Scans, STXM, and Beamline settings

```
A091111005.hdr - Notepad
File Edit Format View Help
ScanDefinition = { Label = "A091111005.hdr"; Type = "Image Scan"; Flags = "Image"; Dwell = 1.095;
  Regions = (1,
    {
      PAxis = { Name = "Sample X"; Unit = "um"; Min = -196.629; Max = -186.629; Dir = 1;
        Points = (250, -196.629, -196.589, -196.549, -196.509, -196.469, -196.429, -196.389,
629, -192.589, -192.549, -192.509, -192.469, -192.429, -192.389, -192.349, -192.309, -192.269, -192.229, -192.189, -
-188.509, -188.469, -188.429, -188.389, -188.349, -188.309, -188.269, -188.229, -188.189, -188.149, -188.109, -188.0
);
      QAxis = { Name = "Sample Y"; Unit = "um"; Min = 4796.553; Max = 4806.553; Dir = 1;
        Points = (250, 4796.553, 4796.593, 4796.633, 4796.673, 4796.713, 4796.753, 4796.793,
553, 4800.593, 4800.633, 4800.673, 4800.713, 4800.753, 4800.793, 4800.833, 4800.873, 4800.913, 4800.953, 4800.993, 4
4804.673, 4804.713, 4804.753, 4804.793, 4804.833, 4804.873, 4804.913, 4804.953, 4804.993, 4805.033, 4805.073, 4805.1
);
    });
    StackAxis = { Name = "Energy"; Unit = "eV"; Min = 300.003; Max = 300.003; Dir = -1;
      Points = (1, 300.003);
    };
  };
  Channels = (1,
    { Name = "counter0"; Unit = "counts"; });
  };
  Time = "2009 November 11 22:50:37"; BeamFeedback = false; ShutterAutomatic = true;
  Channels = (1,
    { ID = 1; Type = 0; Name = "counter0"; Controller = 0; DeviceNumber = 0; UnitName = "counts"; LinearCoefficient = 1;
  });
  Monochromator = { Name = "Energy"; LastPosition = 300.002; Status = 1; Type = 1; ControllerID = 63; Vel = 0; };
  EntranceSlit = { Name = "M3STXMPitch"; LastPosition = 3.064; Status = 0; Type = 1; ControllerID = 67; Vel = 1; };
  ExitVSlit = { Name = "SlitX"; LastPosition = 30.1; Status = 1; Type = 1; ControllerID = 62; Vel = 200; };
  ExitHSlit = { Name = "SlitY"; LastPosition = 30.2; Status = 1; Type = 1; ControllerID = 61; Vel = 200; };
  SampleFineX = { Name = "SampleX"; LastPosition = -184.33349; Status = 0; Type = 0; ControllerID = 41; Vel = 1; };
  SampleFineY = { Name = "SampleY"; LastPosition = 4796.5631; Status = 0; Type = 0; ControllerID = 42; Vel = 1; };
  SampleFineZ = { Name = "SampleFineZ"; LastPosition = -25.004884; Status = 0; Type = 0; ControllerID = 40; Vel = 1; };
  SampleCoarseX = { Name = "CoarseX"; LastPosition = -166; Status = 0; Type = 1; ControllerID = 82; Vel = 1.9; };
  SampleCoarseY = { Name = "CoarseY"; LastPosition = 4832.2; Status = 0; Type = 1; ControllerID = 83; Vel = 0.5; };
  SampleCoarseZ = { Name = "CoarseZ"; LastPosition = 819; Status = 0; Type = 1; ControllerID = 11; Vel = 1; };
  ZonePlateZ = { Name = "ZonePlateZ"; LastPosition = -1162.7178; Status = 1; Type = 1; ControllerID = 88; Vel = 600; };
};
```

**Image Data File:**  
e.g. **A091111005\_a.xim**

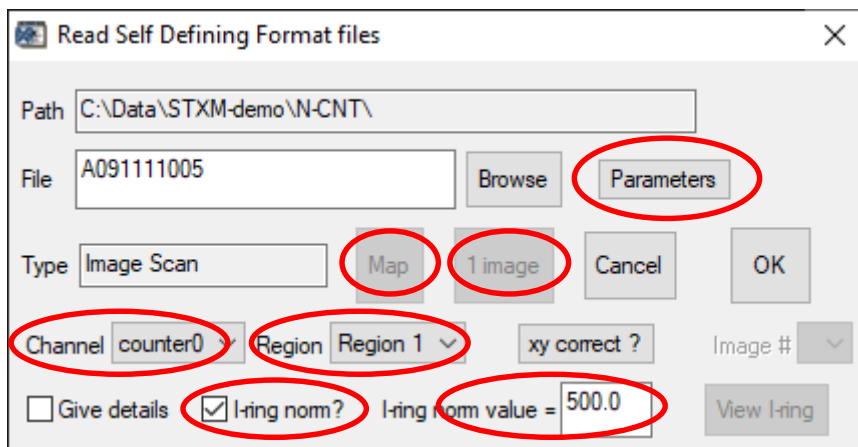
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 541 | 539 | 551 | 548 | 551 | 543 | 550 | 562 | 539 | 566 | 566 | 574 | 558 | 566 | 570 |
| 566 | 550 | 558 | 562 | 554 | 561 | 554 | 561 | 559 | 551 | 569 | 569 | 553 | 541 | 546 |
| 548 | 556 | 548 | 546 | 542 | 557 | 562 | 544 | 542 | 556 | 546 | 562 | 552 | 539 | 537 |
| 566 | 569 | 551 | 527 | 570 | 556 | 563 | 557 | 559 | 535 | 554 | 556 | 554 | 560 | 564 |
| 561 | 545 | 552 | 563 | 554 | 554 | 546 | 553 | 578 | 575 | 553 | 561 | 550 | 544 | 550 |
| 552 | 547 | 560 | 567 | 535 | 558 | 559 | 563 | 554 | 567 | 555 | 564 | 554 | 547 | 559 |
| 565 | 545 | 562 | 572 | 554 | 554 | 570 | 565 | 545 | 542 | 549 | 551 | 558 | 547 | 560 |
| 563 | 554 | 555 | 557 | 561 | 552 | 557 | 538 | 545 | 534 | 541 | 536 | 565 | 541 | 556 |
| 538 | 555 | 567 | 542 | 562 | 551 | 552 | 565 | 555 | 563 | 568 | 561 | 557 | 545 | 557 |
| 545 | 544 | 567 | 567 | 559 | 561 | 564 | 558 | 553 | 556 | 563 | 557 | 564 | 552 | 562 |
| 544 | 545 | 557 | 539 | 560 | 570 | 549 | 544 | 568 | 549 | 541 | 547 | 565 | 545 | 547 |
| 550 | 565 | 552 | 536 | 536 | 565 | 553 | 563 | 563 | 557 | 558 | 549 | 566 | 554 | 539 |
| 548 | 581 | 562 | 559 | 568 | 571 | 570 | 564 | 549 | 554 | 551 | 566 | 565 | 557 | 547 |
| 543 | 542 | 543 | 562 | 557 | 548 | 545 | 536 | 537 | 548 | 565 | 537 | 553 | 550 | 561 |
| 552 | 553 | 544 | 552 | 559 | 550 | 567 | 560 | 557 | 545 | 547 | 549 | 550 | 552 | 553 |
| 554 | 569 | 563 | 552 | 545 | 546 | 545 | 553 | 553 | 546 | 551 | 552 | 550 | 556 | 553 |
| 544 | 550 | 556 | 544 | 556 | 563 | 571 | 557 | 557 | 558 | 558 | 563 | 561 | 552 | 546 |

**Spectrum Data File:**  
e.g. **A100219012\_0.xsp**

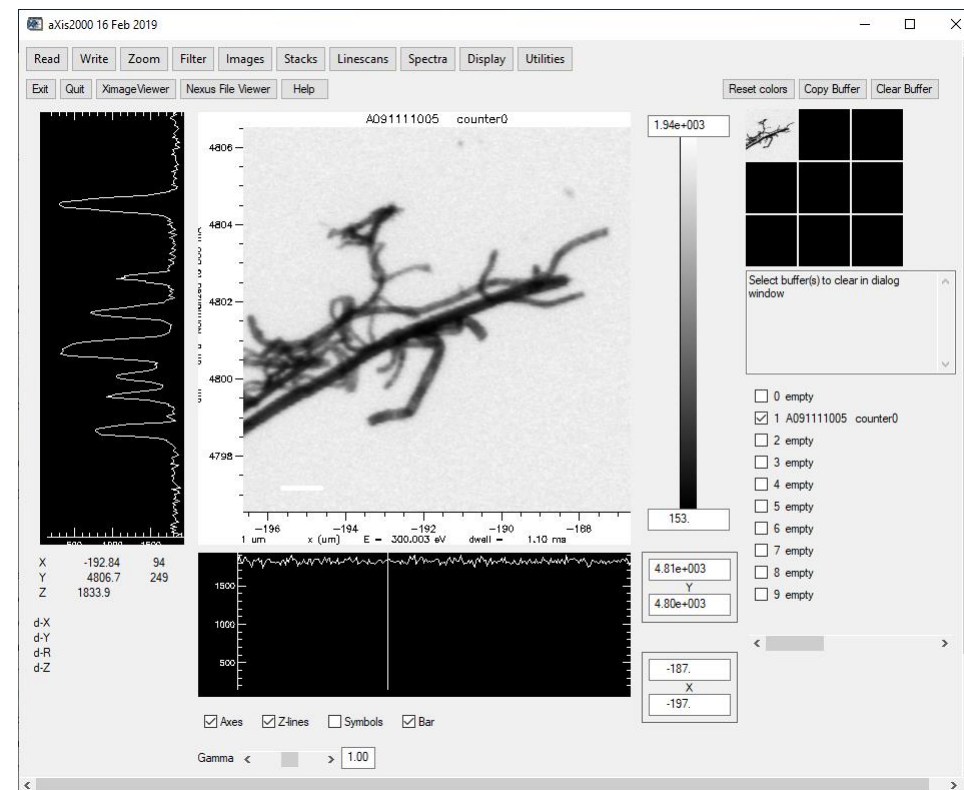
```
A100219012_0.xsp - Notepad
File Edit Format View Help
395 472473
395.196 474819
395.392 472304
395.588 473986
395.784 472452
395.98 472916
396.176 469059
396.372 469666
396.568 468513
396.764 467277
396.96 468773
397.156 467601
397.352 468312
397.548 467831
397.744 466367
397.94 464330
398.136 460334
398.332 450769
398.528 441331
```



# aXis2000 – Read Ambient-STXM Images

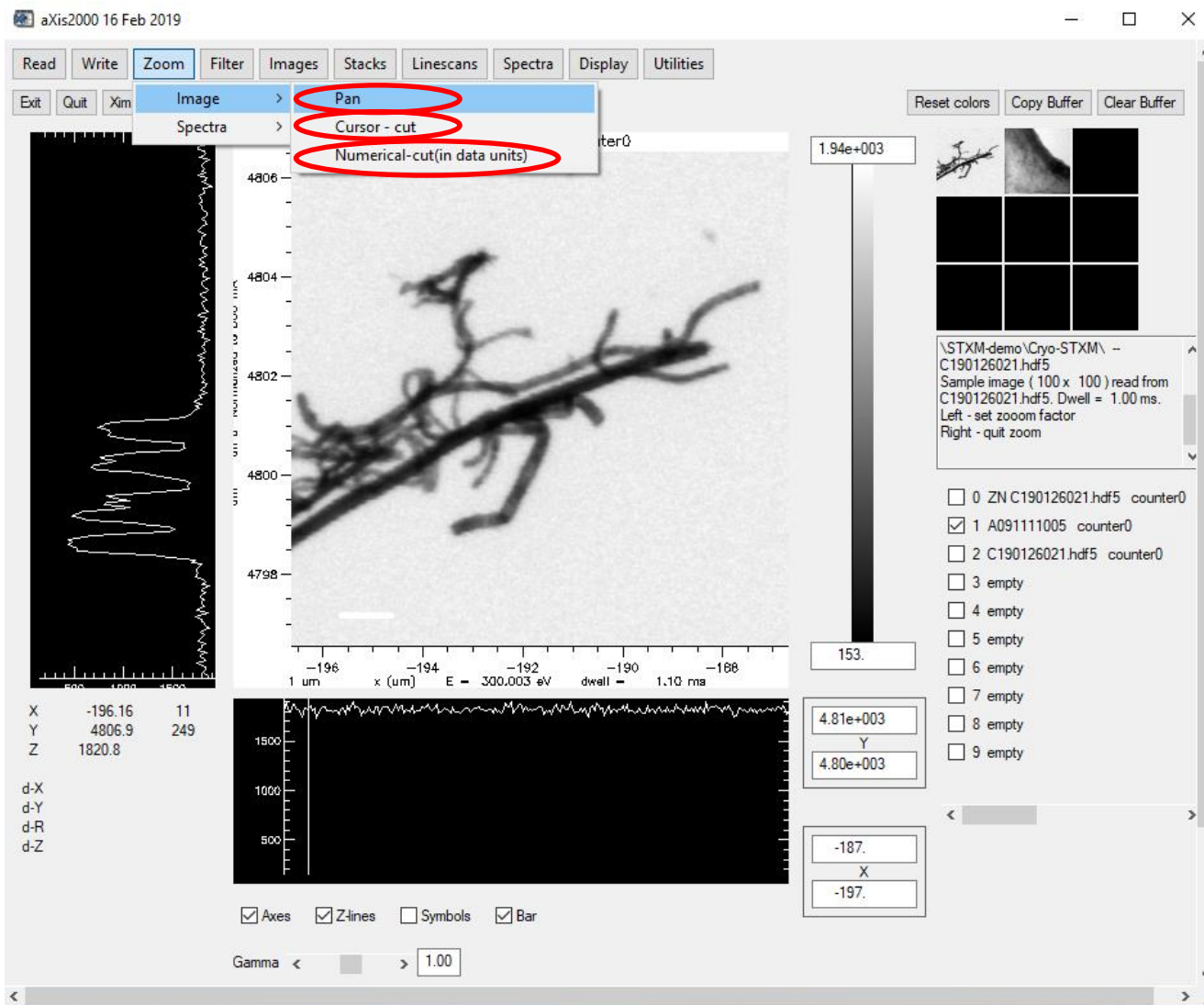


- **Parameters:** access all information in the header file
- **Map:** obtain a two-image subtraction map directly without alignment
- **1 image:** read an image from a selected photon energy for a stack
- **Channel:** select data channel if more than one detector is used
- **Region:** select sample region if more than one image region is defined
- **I-ring norm?:** normalization to I-ring
- **I-ring norm value:** CLS 220 mA



- **First click on image:** select the starting point
- **Second click on image:** select the ending point, then calculate the d-X, d-Y, d-R, and d-Z of the two points
- **Third click on image:** clear the selected points

# aXis2000 – Image Zoom



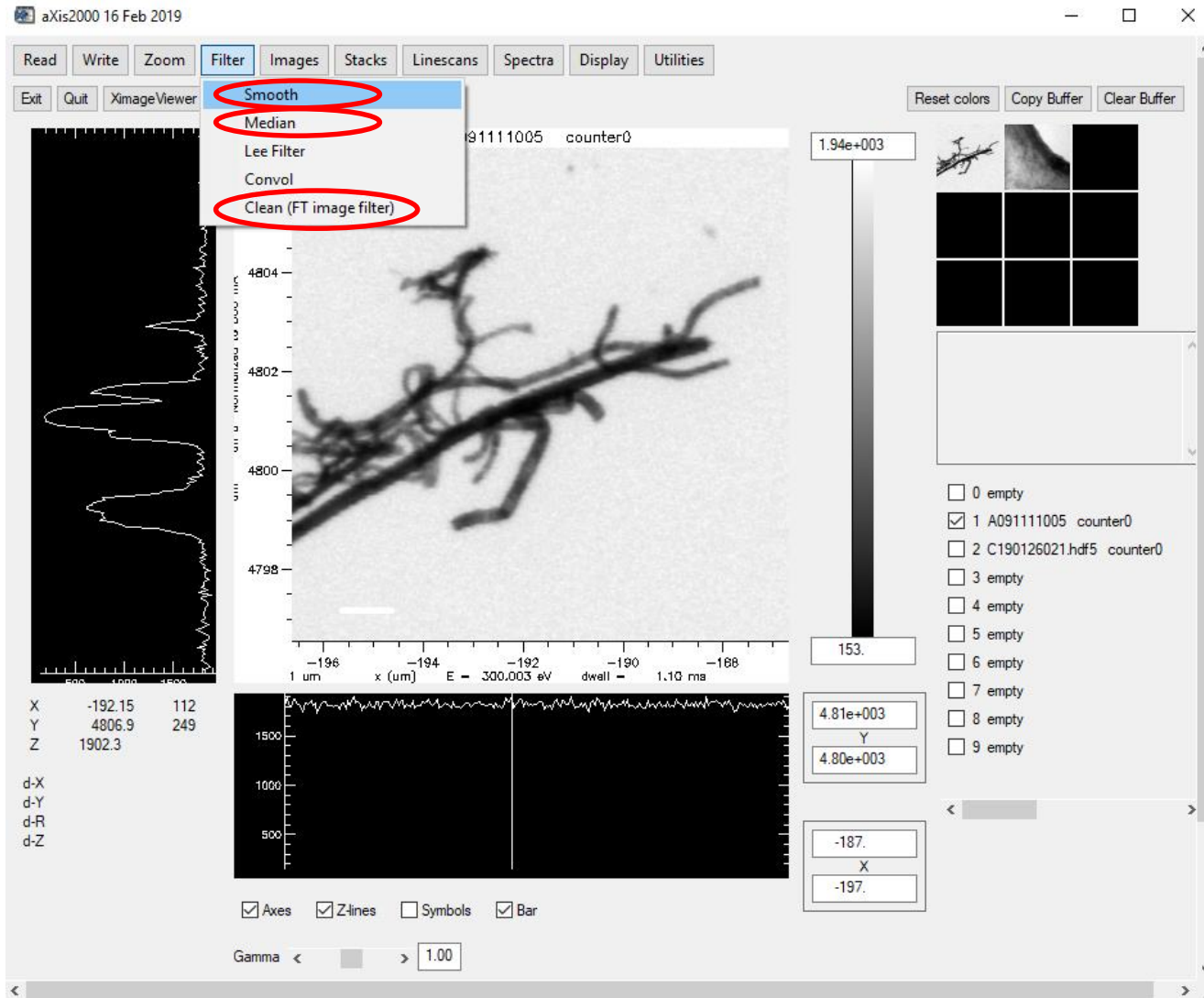
## Functions

- **Pan:** pops-up a zoom window with a ~3x expansion of the region around the cursor
- **Cursor - cut:** use cursor to define a stretchable box on the image to cut
- **Numerical - cut:** numerical input of the coordinates X-min, X-max, Y-min, and Y-max for image cut





# aXis2000 – Image Filter



## Some Useful Functions

- **Smooth:** Boxcar average over n-points
- **Median:** n-point Savitsky-Golay averaging
- **Clean (FT image filter):** 2d-FT filter. The FT is displayed on a 1:1 pixel format.



# aXis2000 – Image Processing



## Some Useful Functions

- **Add:** add/append image or constant
- **Average pixels:** average image or region pixels
- **Clip signal:** two clicks to select image intensity range
- **Convert\_to\_OD:** normalize to the maximum intensity value of the image
- **Delete region:** select an image region and replace the intensity value by arbitrary number
- **Gain:** multiply or divide the image intensity by a number
- **Generate mask:** threshold the image intensity as 0 and 1
- **Multiply buffers:** multiple two images
- **Power:** power the image intensity
- **Ratio to:** divided by another image
- **Replace line:** remove bad/black lines



# aXis2000 – Image Display



## Some Useful Functions

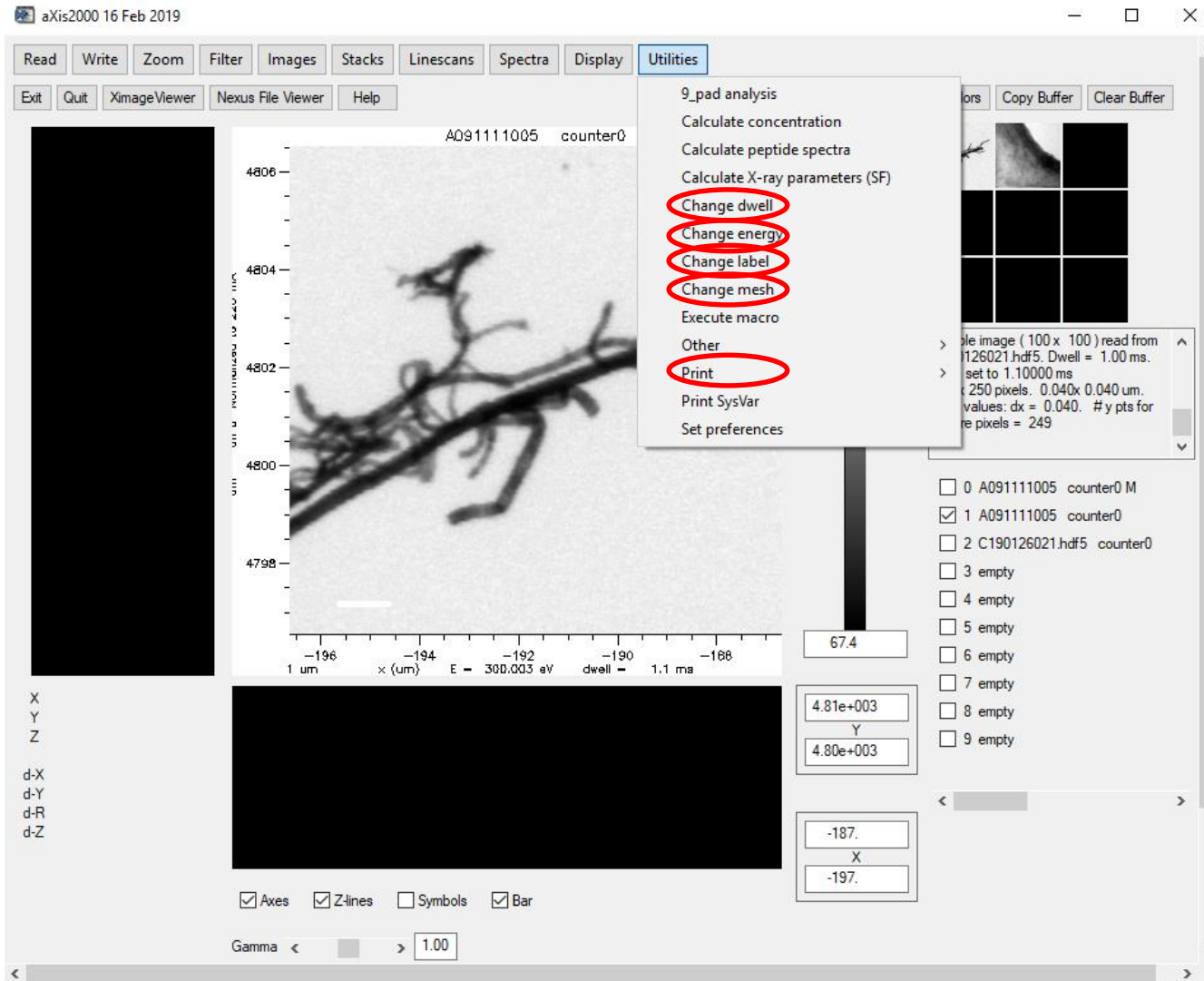
- **3d plot:** X, Y and Intensity 3d image plot
- **Modify image colors:** change image colors



- **Scale bar position:** click on image to manually place the scale bar
- **Thumbnails:** display multiple images together



# aXis2000 – Image Utilities



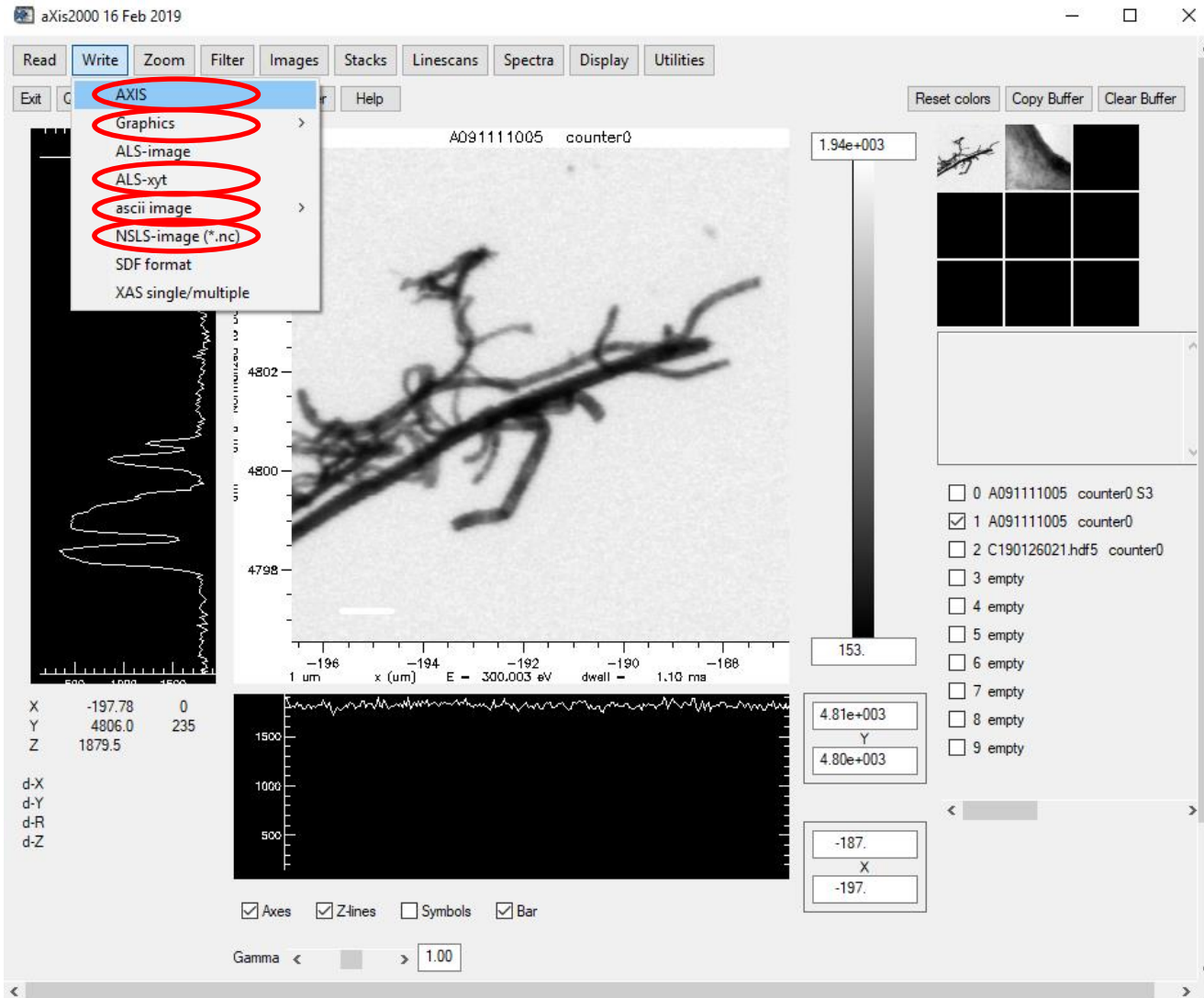
## Some Useful Functions

- **Change dwell:** change image dwell time
- **Change energy:** change image photon energy
- **Change label:** change label for image or other files like spectra
- **Change mesh:** change image X and Y pixel number
- **Print:** print image or other files like spectra with or without IDL annotation





# aXis2000 – Write Images



## Some Useful Functions

- **AXIS**: images written into \*.axb binary format
- **Graphics**: images written into graphics formats, such as GIF, JPG, PNG and TIF, with and without axes or labels
- **ALS-xyt**: images written into X, Y, intensity, X-pixel, and Y-pixel
- **ascii image**: images written into coordinates, and 2d array of image intensity
- **NSLS-image (\*.nc)**: images written into NSLS netCDF image format (\*.nc)



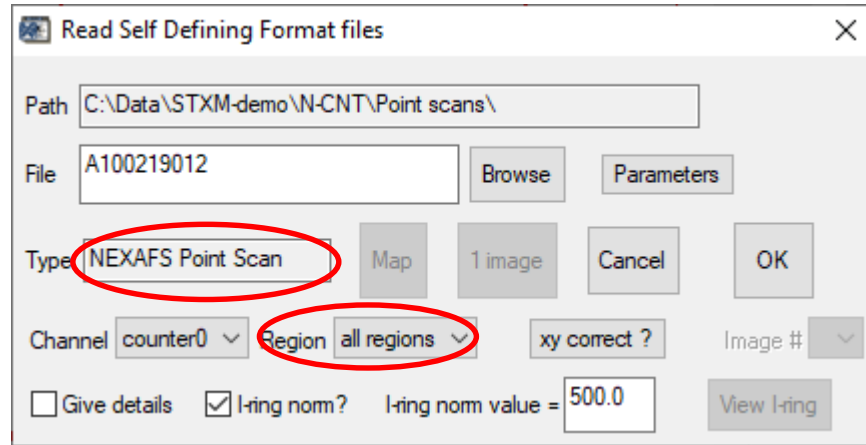
# Spectra



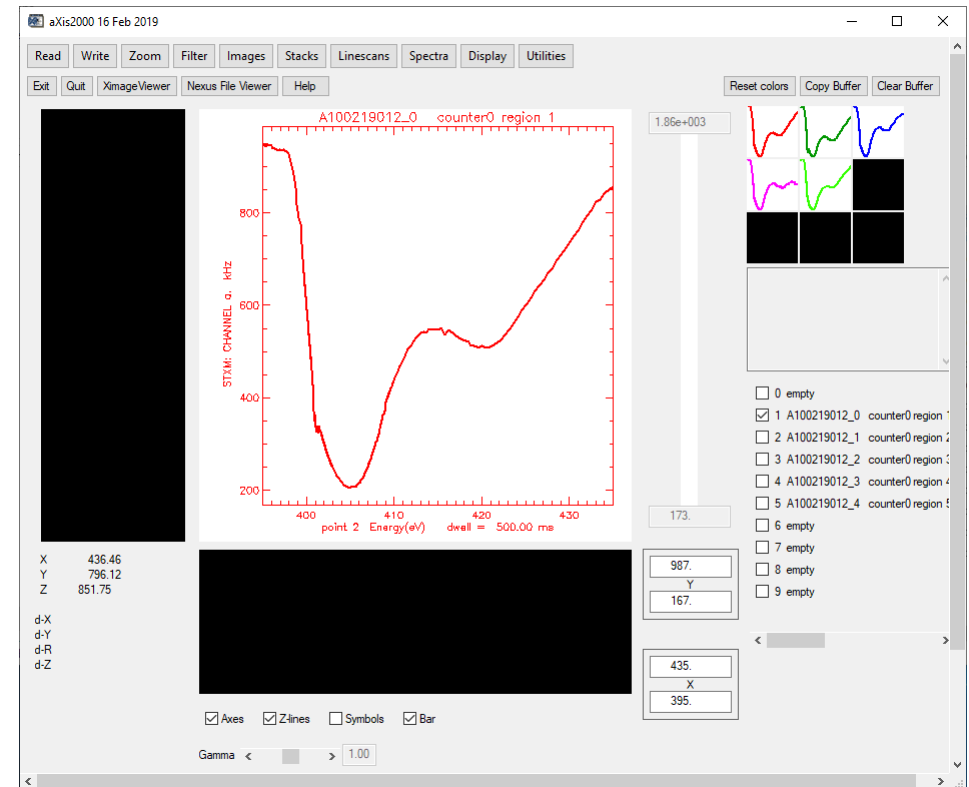
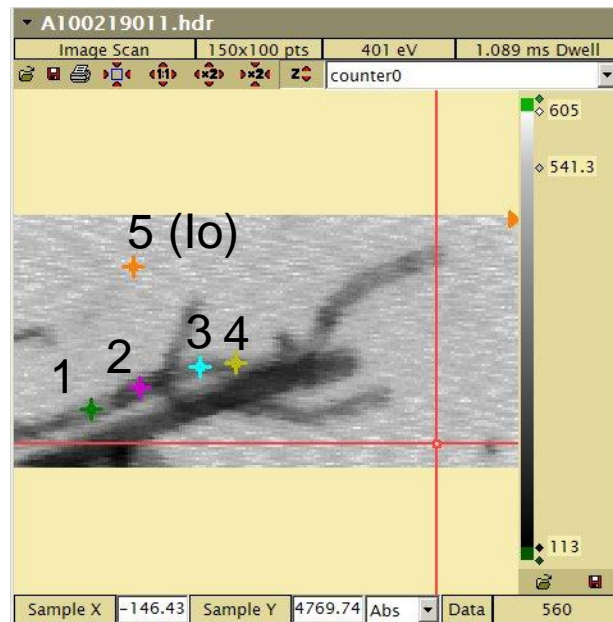
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de rayonnement  
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# aXis2000 – Read Ambient-STXM Point Spectra



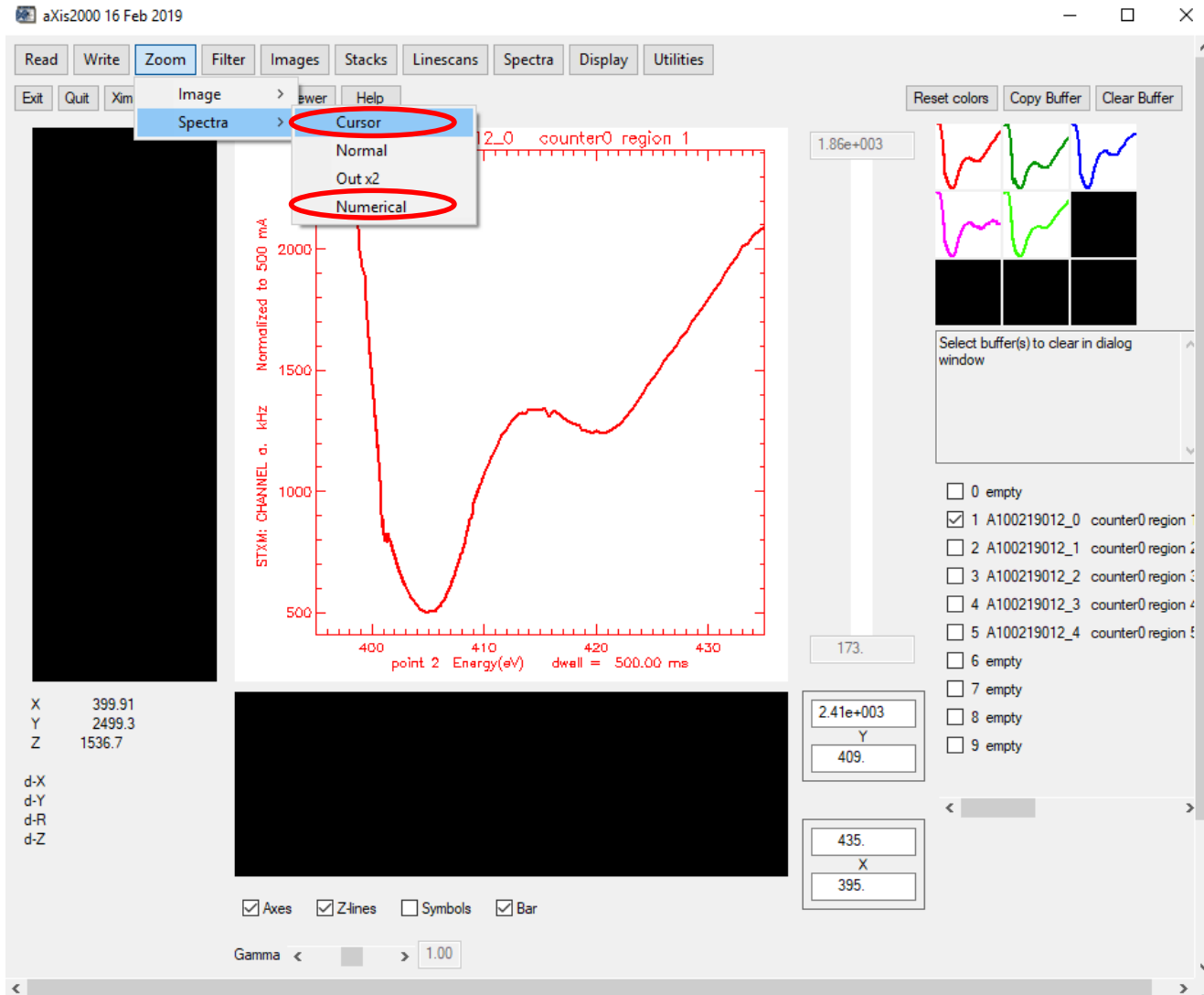
A100219012–point scan–500 ms



- **First click on spectrum:** select the starting point
- **Second click on spectrum:** select the ending point, then calculate the d-X, d-Y, and d-Z of the two points
- **Third click on spectrum:** clear the selected points



# aXis2000 – Spectrum Zoom



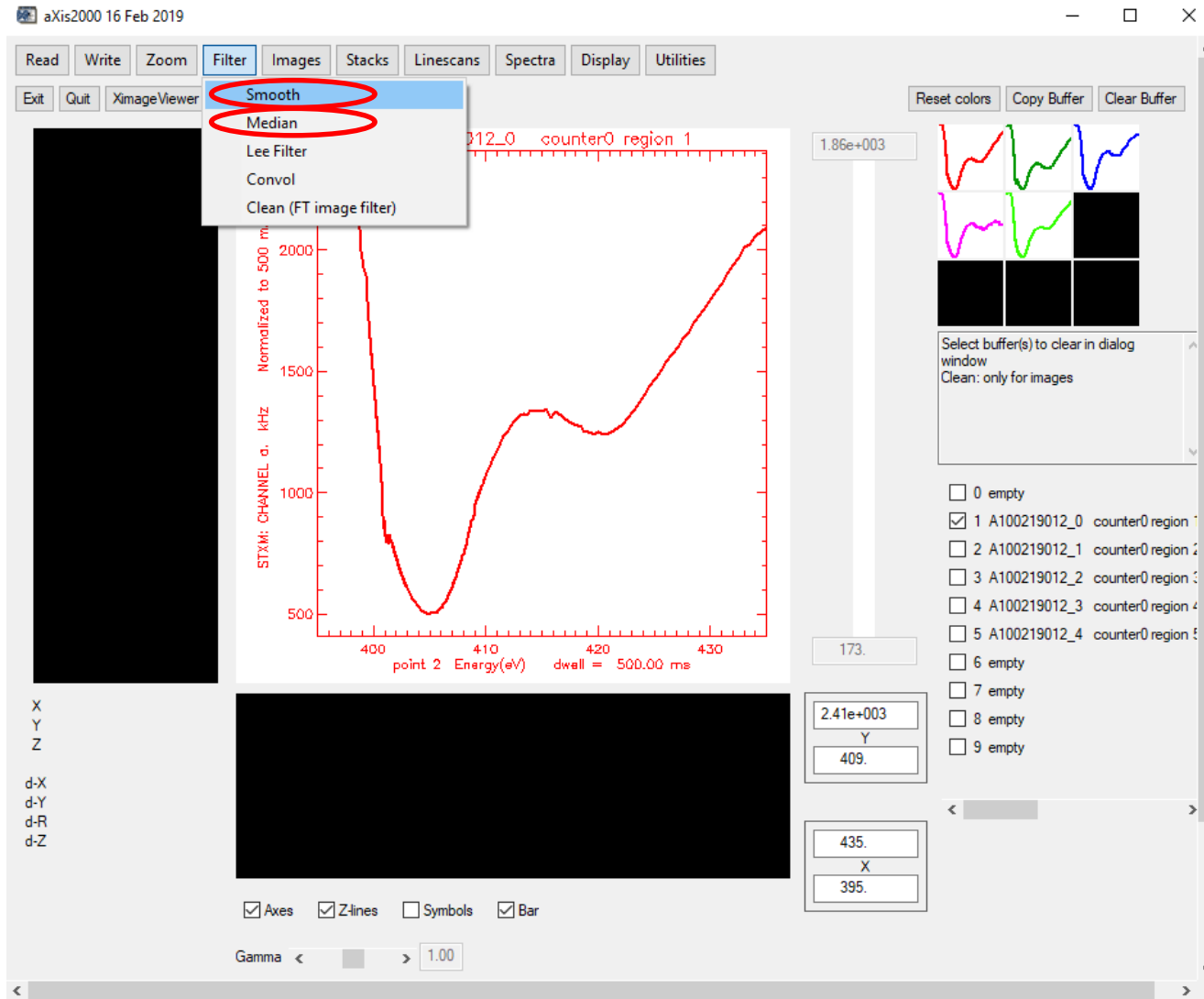
## Some Useful Functions

- **Cursor:** use cursor to define a stretchable box on the spectrum to cut
- **Numerical:** numerical input of the limits of X-min, X-max, Y-min, and Y-max for spectrum cut





# aXis2000 – Spectrum Filter

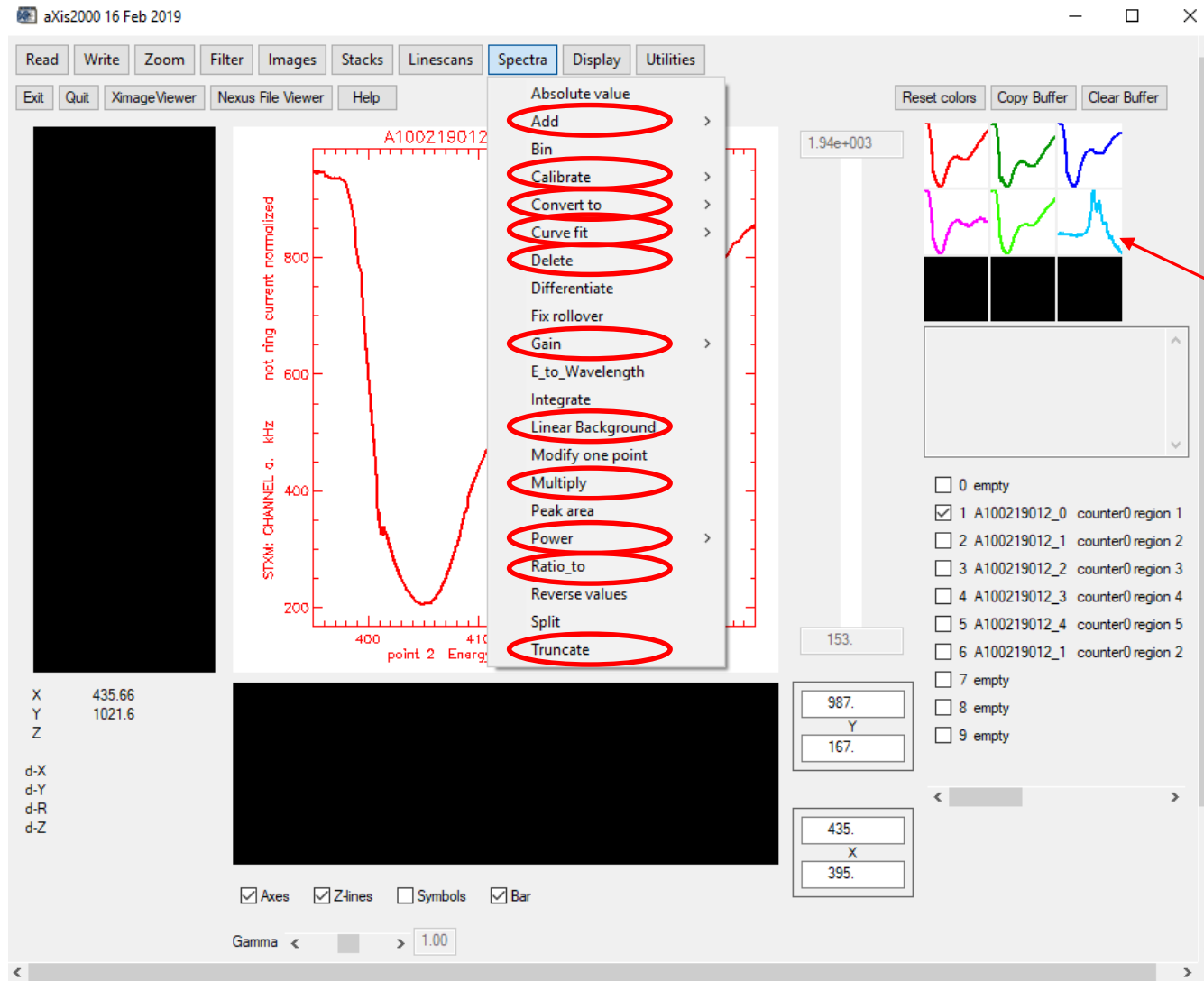


## Some Useful Functions

- **Smooth:** Boxcar average over n-points
- **Median:** n-point Savitsky-Golay averaging



# aXis2000 – Spectrum Processing

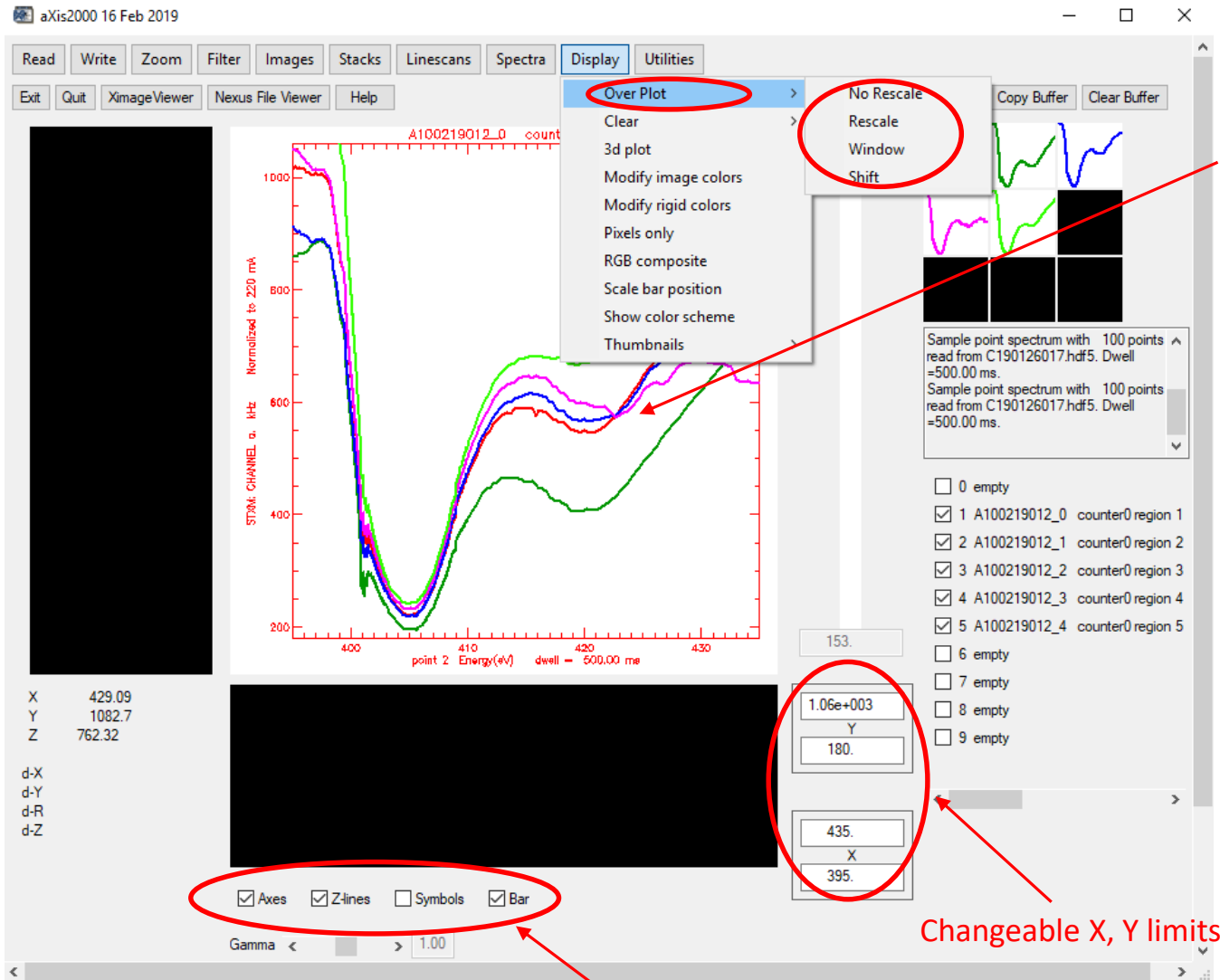


## Some Useful Functions

- **Add**: add/append spectrum or constant
- **Calibrate**: calibrate X or Y scale
- **Clip signal**: two clicks to select image intensity range
- **Convert to**: normalize to an I<sub>0</sub> spectrum to get OD spectrum
- **Curve fit**: linear combination curve fit and other
- **Delete**: delete the region between two selected points
- **Gain**: multiply or divide the Y scale (intensity) by a number
- **Linear Background**: select two points on spectrum for background baseline
- **Multiply**: multiple two spectra
- **Power**: power the spectrum intensity
- **Ratio to**: divided by another spectrum
- **Truncate**: truncate the spectral regions beyond the two selected points



# aXis2000 – Spectrum Display



## Some Useful Functions

- **Over plot:** display multiple spectra on the same plot based on **No Rescale, Rescale, Window, and Shift**

Changeable settings

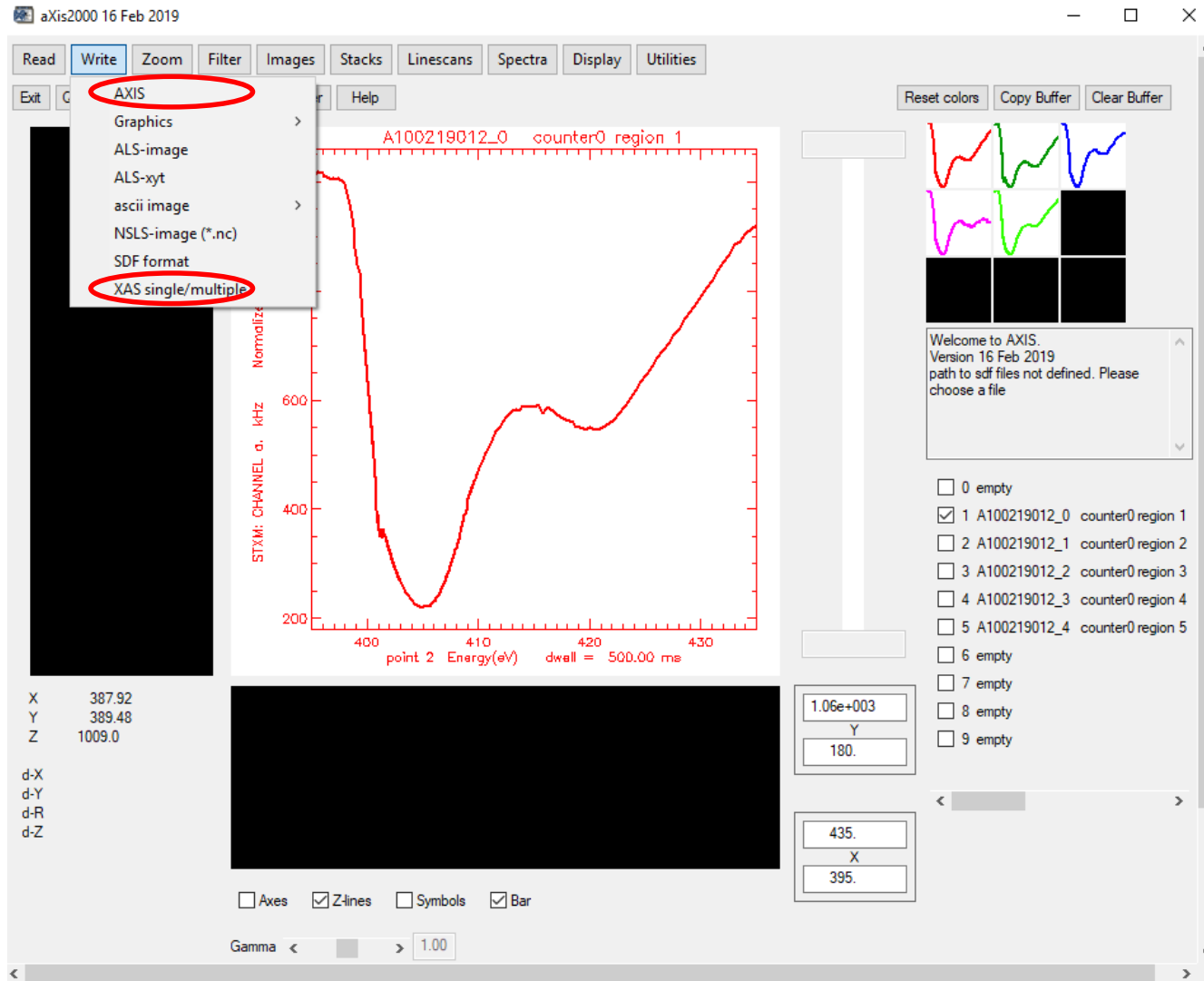
Changeable X, Y limits



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# aXis2000 – Write Spectra



## Some Useful Functions

- **AXIS**: spectra written into \*.txt ASCII format
- **XAS single/multiple**: images written into NSLS XAS format (\*.xas)





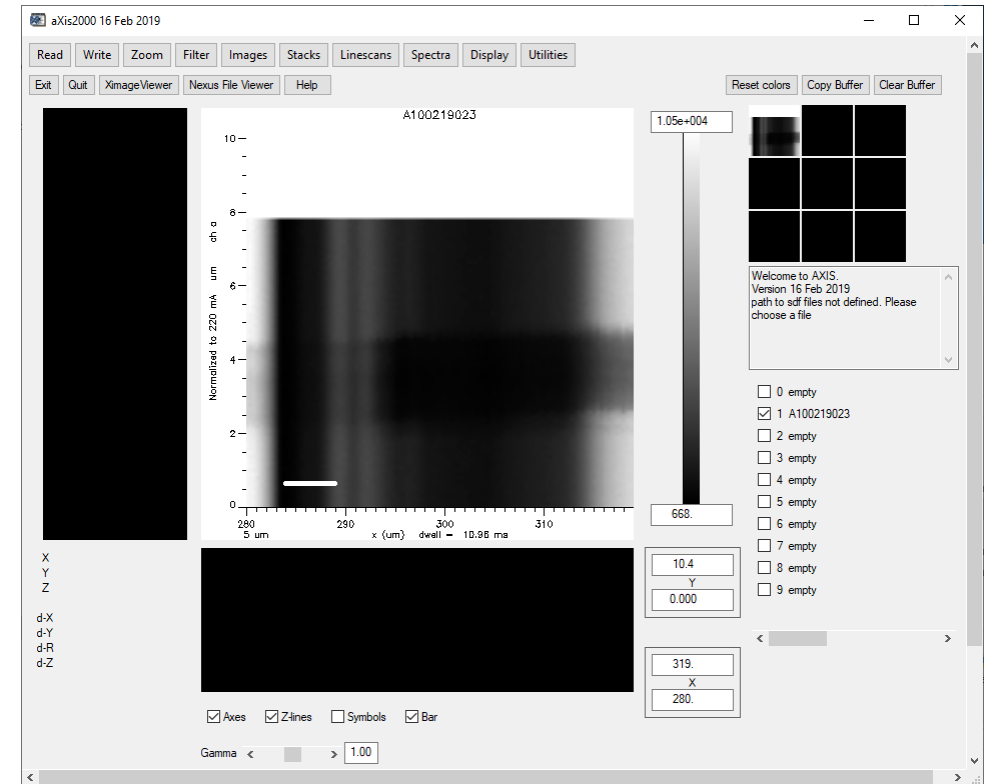
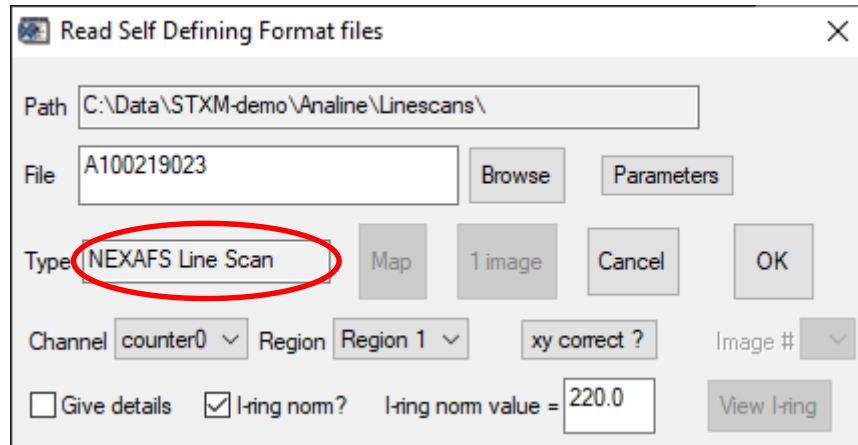
# Linescans



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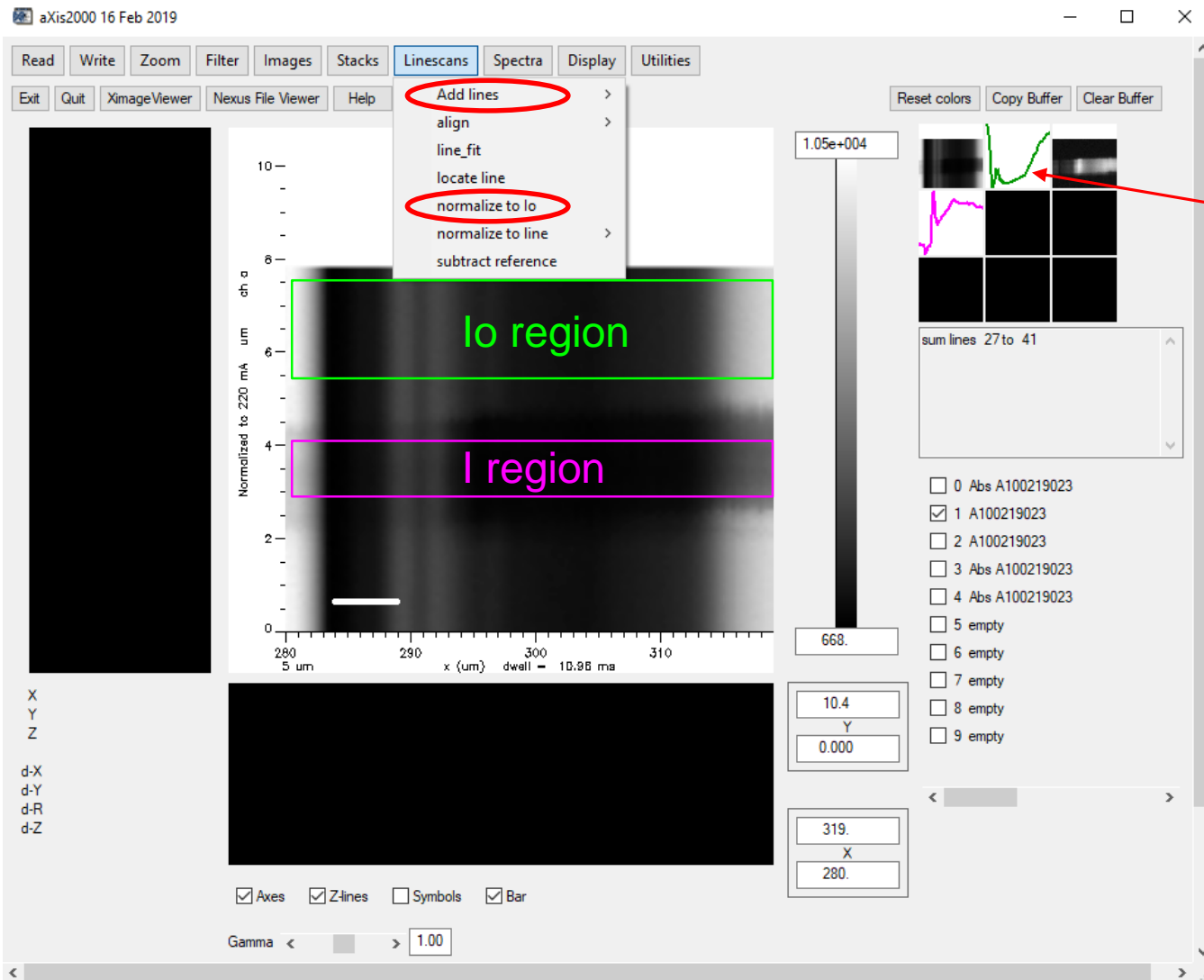
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# aXis2000 – Read Ambient-STXM Linescans



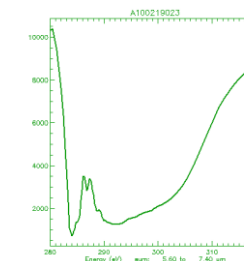
- **First click on spectrum:** select the starting point
- **Second click on spectrum:** select the ending point, then calculate the d-X, d-Y, and d-Z of the two points
- **Third click on spectrum:** clear the selected points

# aXis2000 – Linescans Processing

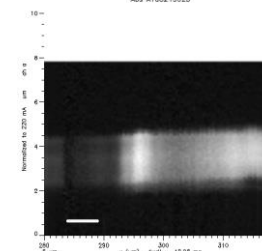


## Some Useful Functions

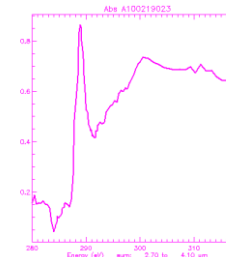
- **Add lines:** define two lines horizontally and average the intensity between the two lines
- **Normalize to lo:** normalize the linescan spectro-image to the lo spectrum



Lo Spectrum



Linescan OD image



OD Spectrum



# Stacks

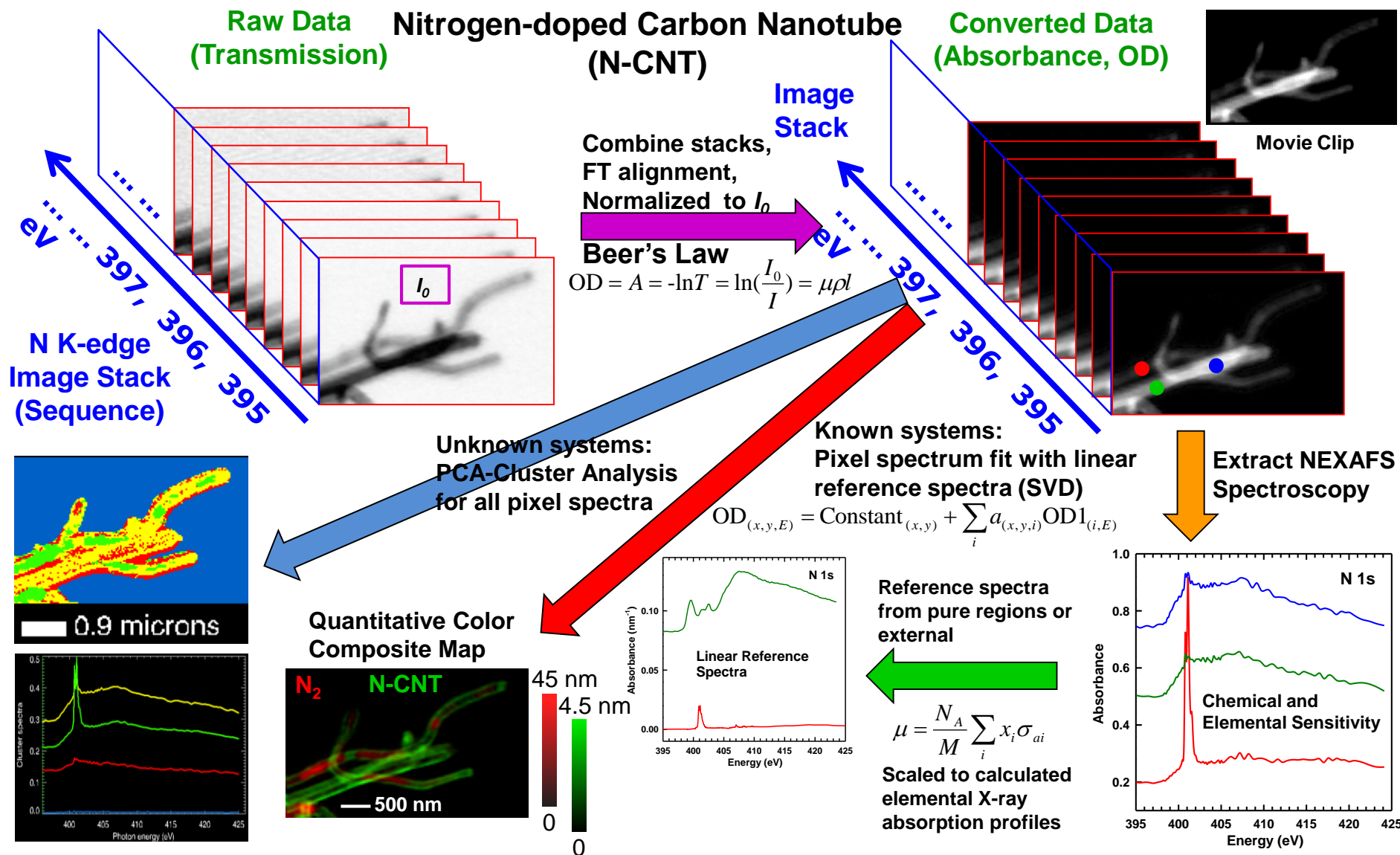


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# STXM Stacks Data Processing



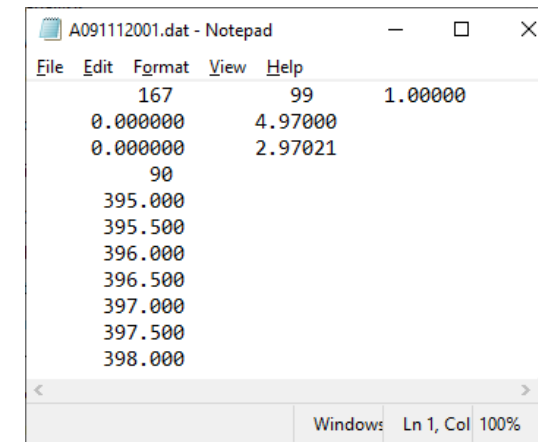
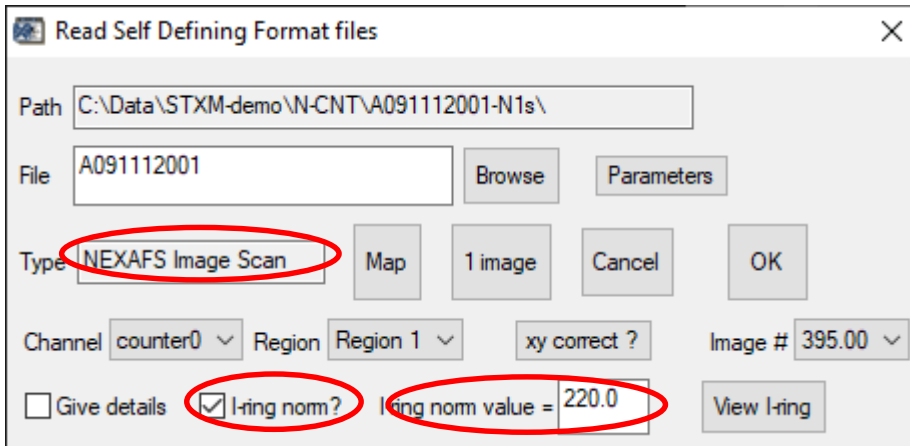


# STXM Data Analysis File Naming Symbols and Rules

| Symbols                 | Description                                | Examples   |
|-------------------------|--|--|
| <b>A</b>                | designate letter for CLS Ambient-STXM data | A161216053.ncb   |
| <b>C</b>                | designate letter for CLS Cryo-STXM data    | C160927034.ncb   |
| <b>only file number</b> | raw transmission data                      | A161216053.ncb   |
| <b>a</b>                | aligned stack                              | A161216053a.ncb  |
| <b>aod</b>              | aligned stack, then converted to od stack  | A161216053aod.ncb                                      |
| <b>avg</b>              | averaged stack image or spectrum           | A161216053aod-avg.ncb                                  |
| <b>c, cali</b>          | energy calibrated                          | A161216053aodc.ncb, or A161216053caod.ncb              |
| <b>cl, clip</b>         | clipped, cleaned                           | A161216053aodc-clip.ncb                                |
| <b>ls, l</b>            | linescan                                   | lsA161216052.txt                                       |
| <b>m</b>                | remeshed                                   | A161216053aodm.ncb                                     |
| <b>map</b>              | chemical map                               | A161216051aod-map.ncb                                  |
| <b>mask</b>             | stack mask                                 | A161216053aod-mask.ncb                                 |
| <b>n</b>                | normalized                                 | A161216053aodn.ncb                                     |
| <b>od</b>               | optical density                            | A161216050od.axb                                       |
| <b>od1</b>              | optical density per nm                     | A161216053od1-FeO.txt                                  |
| <b>oda</b>              | optical density stack, then aligned        | A161216053oda.ncb                                      |
| <b>p</b>                | part of the stack                          | A161216053aodp.ncb                                     |
| <b>sm</b>               | smoothed spectrum, image                   | A161216056od-sm-FeO.txt                                |
| <b>sf</b>               | elemental absorption profile               | FeO-sf-od1.txt   |
| <b>t</b>                | truncated spectrum, stack, clipped stack   | A161216053aodt.ncb                                     |
| <b>x</b>                | point scan                                 | xA161216055od.txt                                      |
| Original File Types     | Derived File Types                         | Naming Rules   |
| <b>Images</b>           | Image                                      | A/C + date + sequence number + symbols (+ sample)      |
| <b>Point Scans</b>      | Spectrum                                   | x + A/C + date + sequence number + symbols (+ sample)  |
| <b>Linescans</b>        | Spectrum                                   | ls + A/C + date + sequence number + symbols (+ sample) |
|                         | Spectrum-Image                             | ls + A/C + date + sequence number + symbols (+ sample) |
| <b>Stacks</b>           | Stack                                      | (A/C + date +) sequence number + symbols (+ sample)    |
|                         | Image                                      | (A/C + date +) sequence number + symbols + sample      |
|                         | Map  | (A/C + date +) sequence number + symbols + sample      |
|                         | Spectrum                                   | (A/C + date +) sequence number + symbols + sample      |

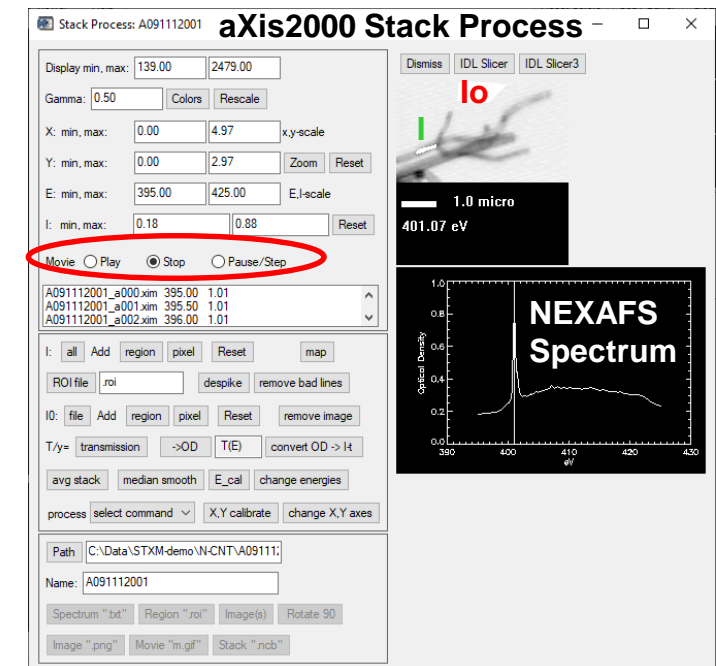


# aXis2000 – Read Ambient-STXM Stacks

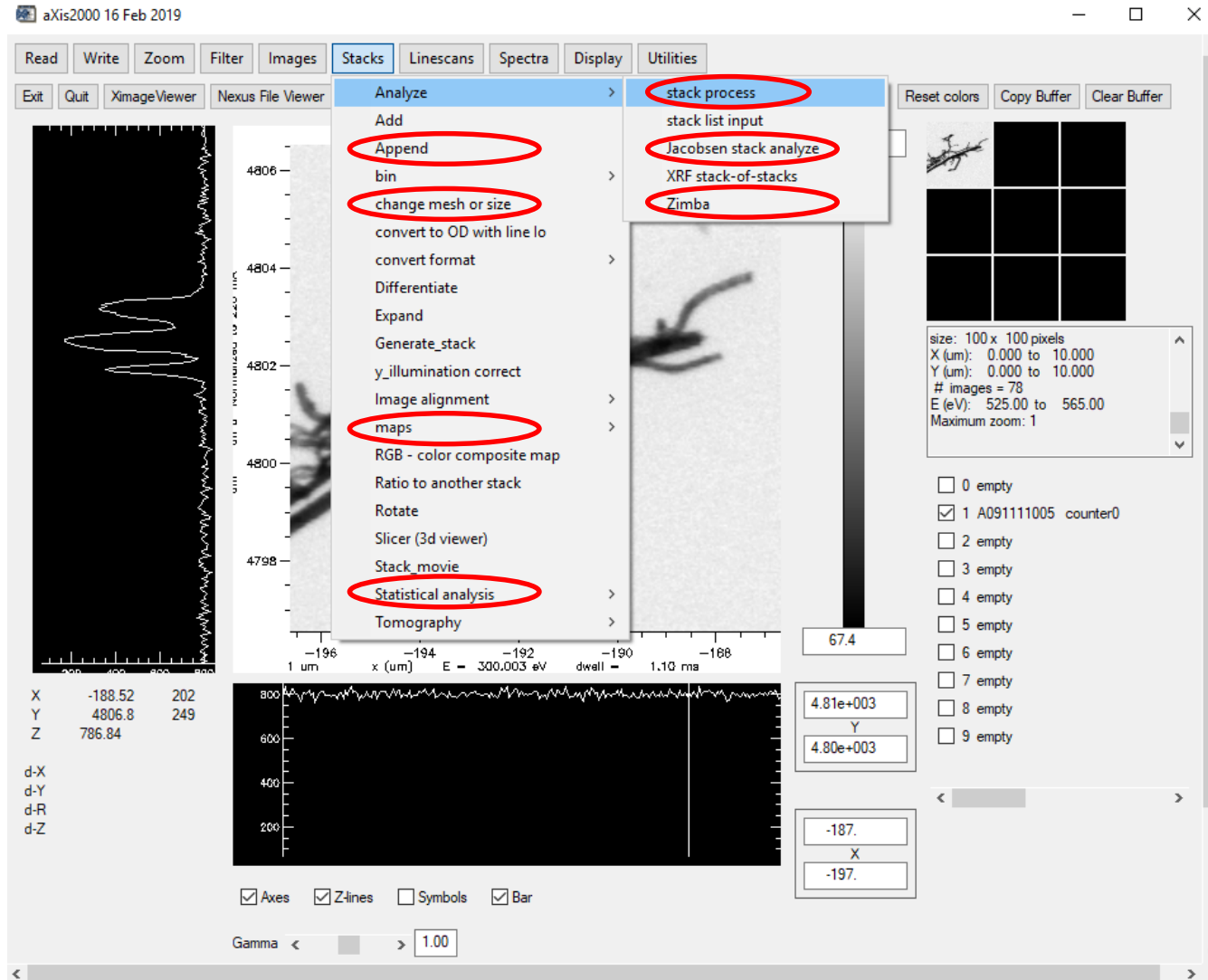


A091111001.dat

- Compile raw Ambient-STXM stack data: aXis2000 → Read → STXM (sdf)
- Give a stack file name, then generate two files:
  - One \*.dat file that has stack dimensions, pixel numbers, and photon energies
  - One \*.ncb binary stack data file
- Uncheck “I-ring norm?” if ring current information is missing or wrong for some images.
- After stack compiling, the aXis2000 Stack Process will be automatically launched with inputting a “suggested zoom” number
- Play movie in “Stack Process” to check if the stack is complete in images/energies.



# aXis2000 – Stacks

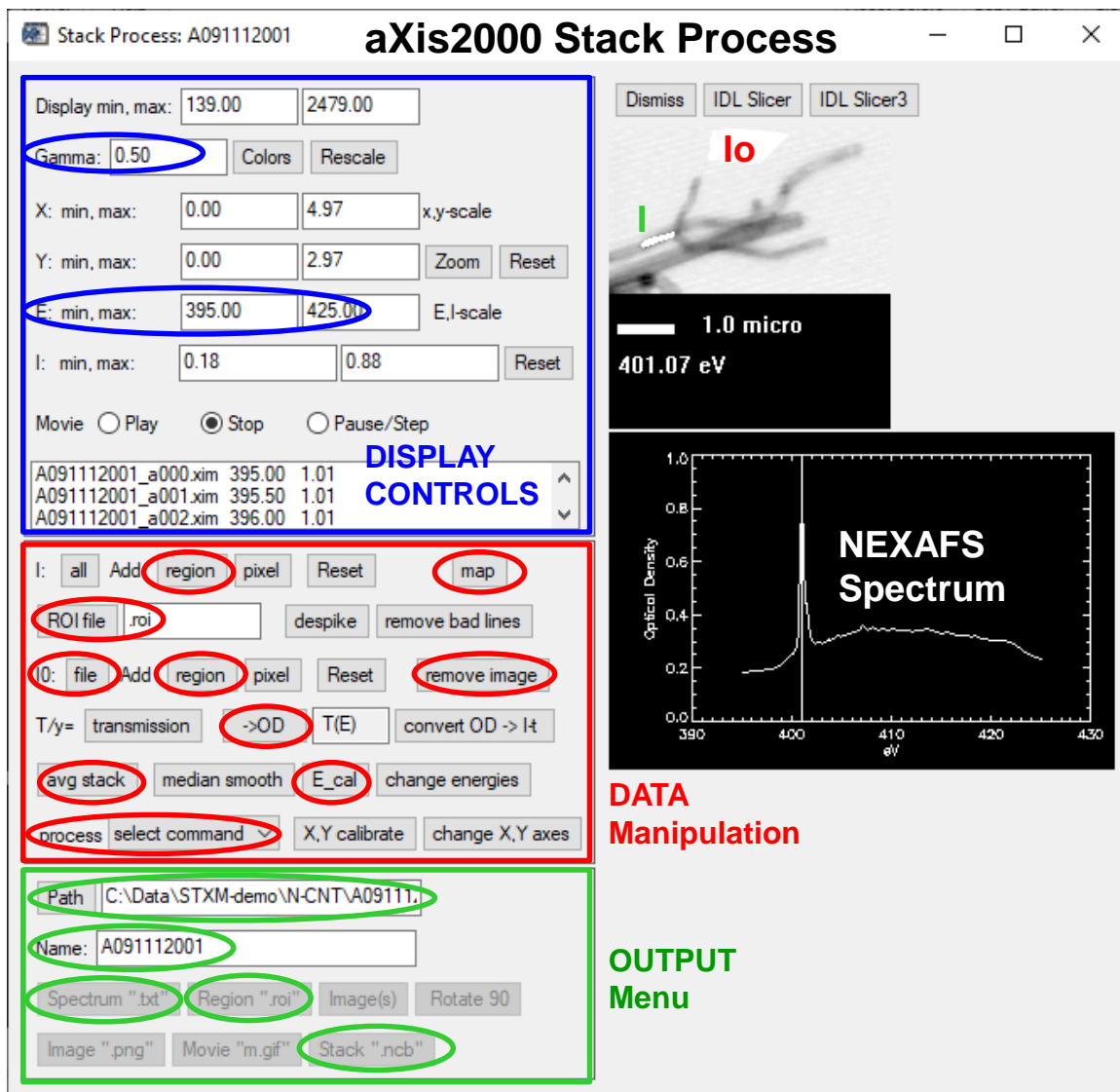


## Some Useful Functions

- **Stack process:** stack data display, manipulation, and output
- **Jacobsen stack analyze:** stack data display, alignment, manipulation, and output
- **Zimba:** stack data build, display, alignment, manipulation, and output
- **Append:** append two stacks with the same pixel and physical dimensions
- **Change mesh or size:** change stack pixel number or physical size
- **Maps:** perform fitting like SVD or Stack fit for the stack, and other fittings
- **Statistical analysis:** PCA analysis



# aXis2000 – Stack Process

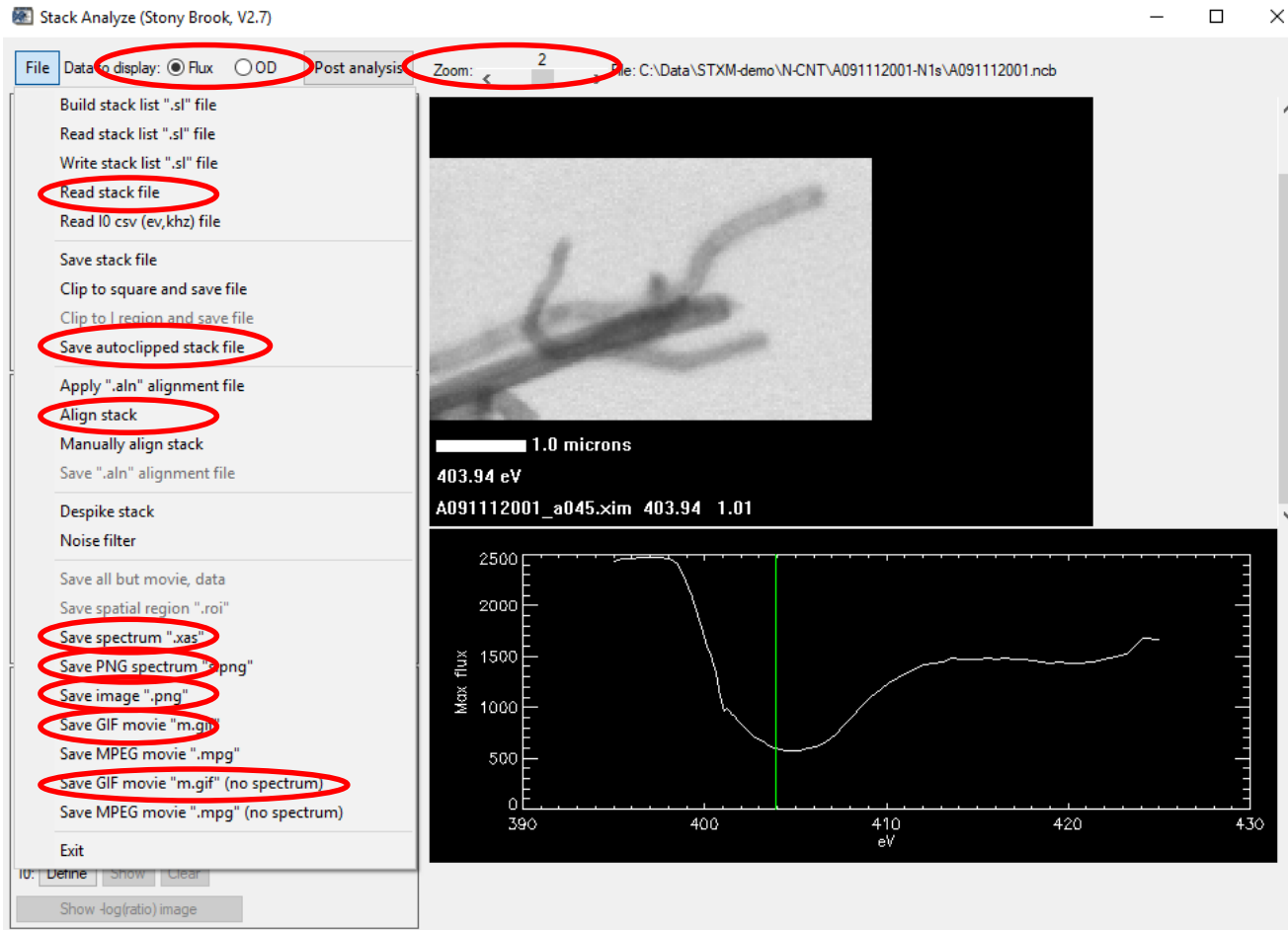


## Some Useful Functions

- **Gamma**: change image Gamma value
- **E**: define stack energy range
- **I: region**: select sample region
- **I: ROI file**: load a sample ROI region file
- **I: map**: generate a two image subtraction map
- **I0: file**: load an I0 file
- **I0: region**: select an I0 region
- **I0: remove image**: delete an image of stack
- **->OD**: convert to OD stack
- **Avg stack**: average all stack images
- **Process**: multiple math process for stack
- **Path**: saving path, no space in folder names
- **Name**: file name for output, click “enter” to activate the output menu buttons
- **Spectrum, Region, Stack**: commonly saved file types



# Stack Analyze (Stony Brook, V2.7)



## Some Useful Functions

- **Flux/OD:** display in flux (transmission) or OD (absorption) format
- **Zoom:** select the zoom factor for the stack images
- **Read stack file:** read a stack and choose \*.ncb format
- **Save autoclipped stack file:** after iterations of alignment, save autoclipped stack file before select lo region.
- **Align stack:** launch the “Stack Align” widget, then process stack alignment
- Save spectrum, image, and movie in formats except the “mpg” format that requires IDL licence

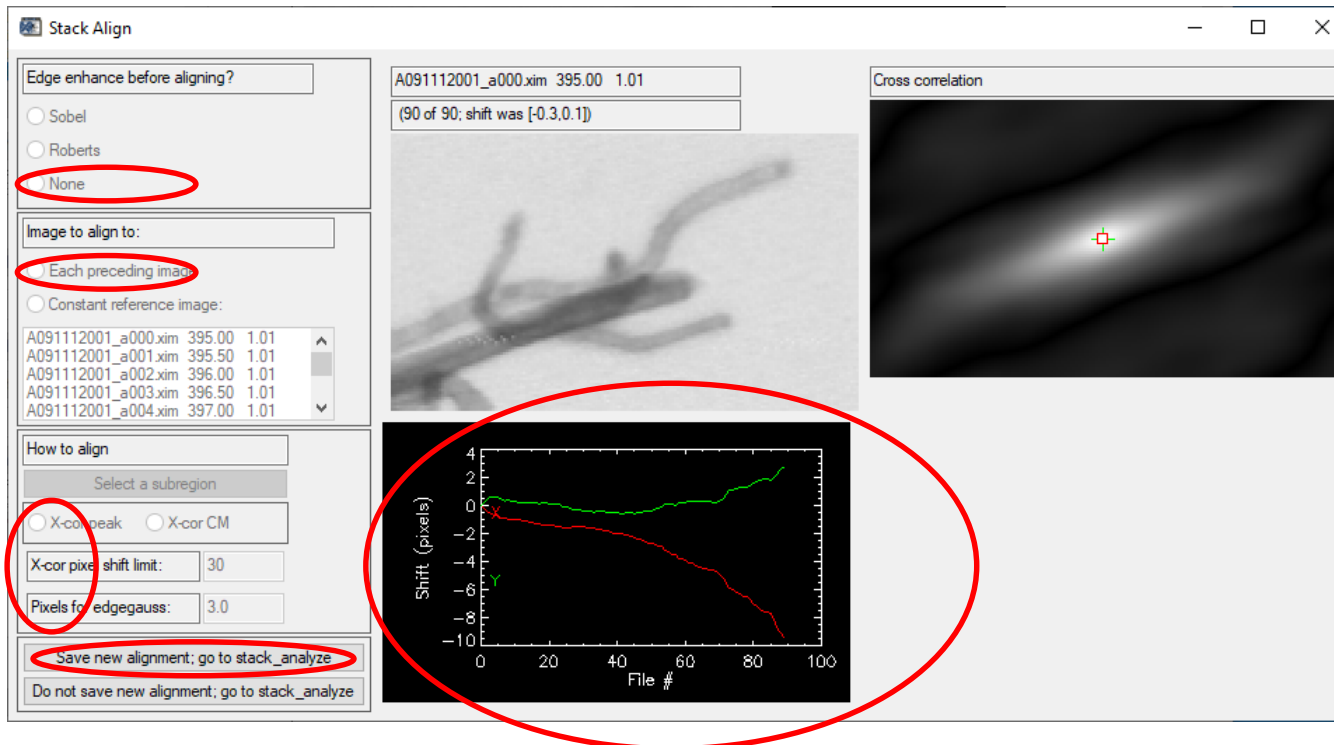




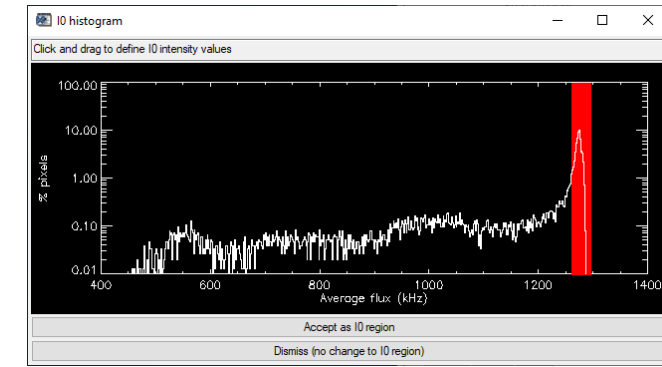
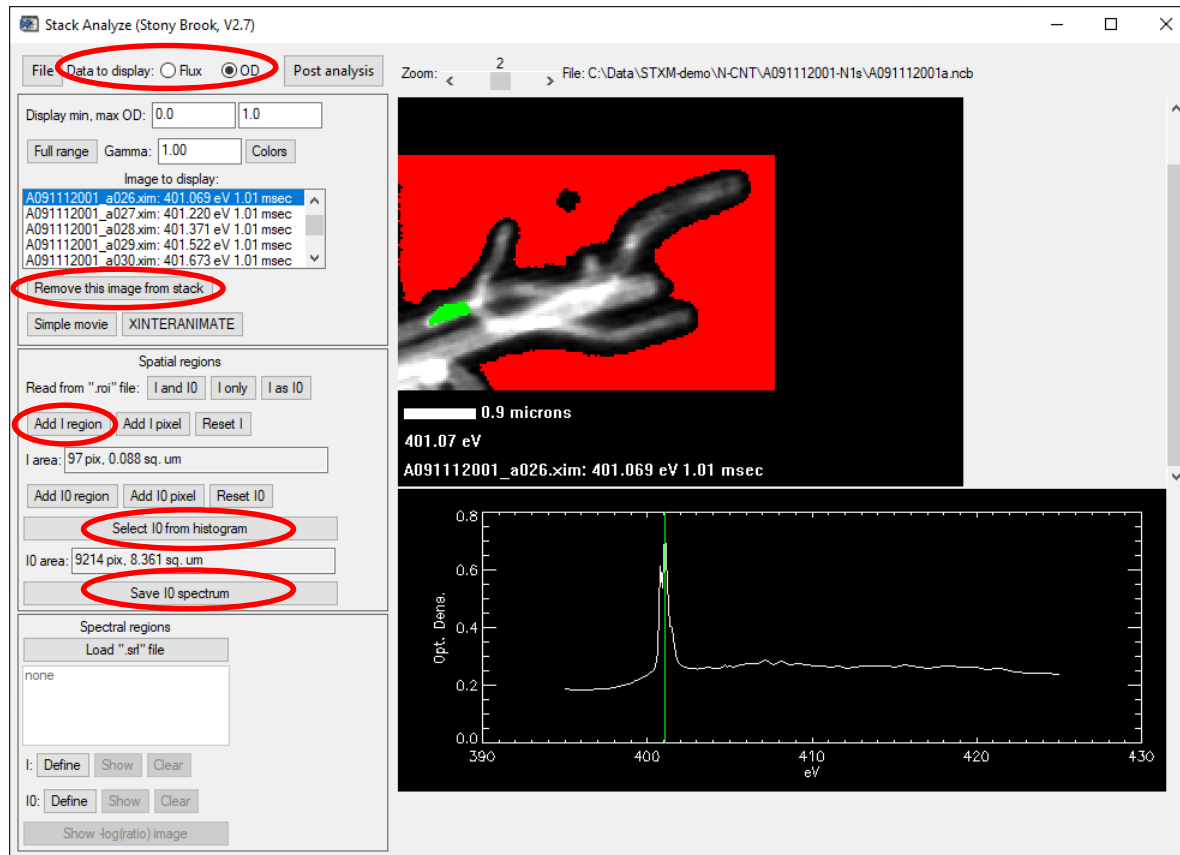
# Stack Analyze (Stony Brook, V2.7) – Stack Align

## Some Useful Functions

- **Edge enhance before aligning:** choose “None” for most cases unless the image contrast is very poor.
- **Image to align to:** choose “Each preceding image” for most cases; or choose a best contrast image for some cases; use the same reference image for all alignment iterations.
- Use other default settings unless the alignment is very challenging.
- **Save new alignment; go to** **stack\_analyze**: after each alignment, save the alignment back to the stack without a separate alignment file.
- Align the stack until the X-Shift and Y-Shift are zero and fully overlapped, or smaller than 1 pixel.



# Stack Analyze (Stony Brook, V2.7)



## Some Useful Functions

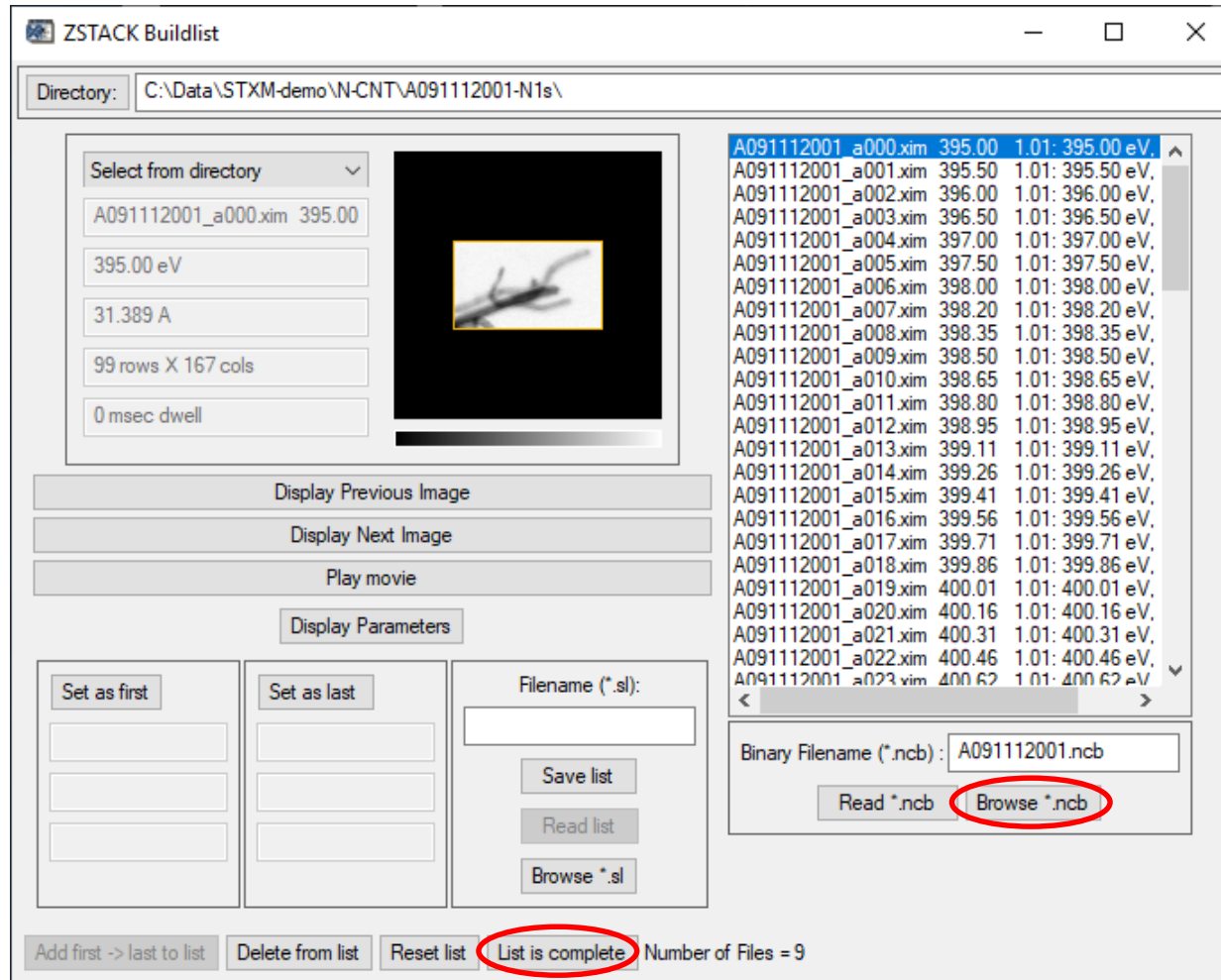
- **Flux/OD:** display in flux (transmission) or OD (absorption) format
- **Remove this image from stack:** delete bad images or unwanted images even before stack alignment
- **Add I region:** select a sample region to check NEAXFS spectroscopy
- **Select IO from histogram:** select the highest intensity peak for IO, as shown in the window above
- **Save IO spectrum:** save the IO spectrum in \*.xas format

**stack\_analyze.sav → File → Read stack file; File → Align stack → Save autoclipped stack file → Select IO from histogram (click-hold-drag) → Save IO spectrum**



# aXis2000 – Stacks – Zimba

aXis2000 → Stacks → Analyze → Zimba



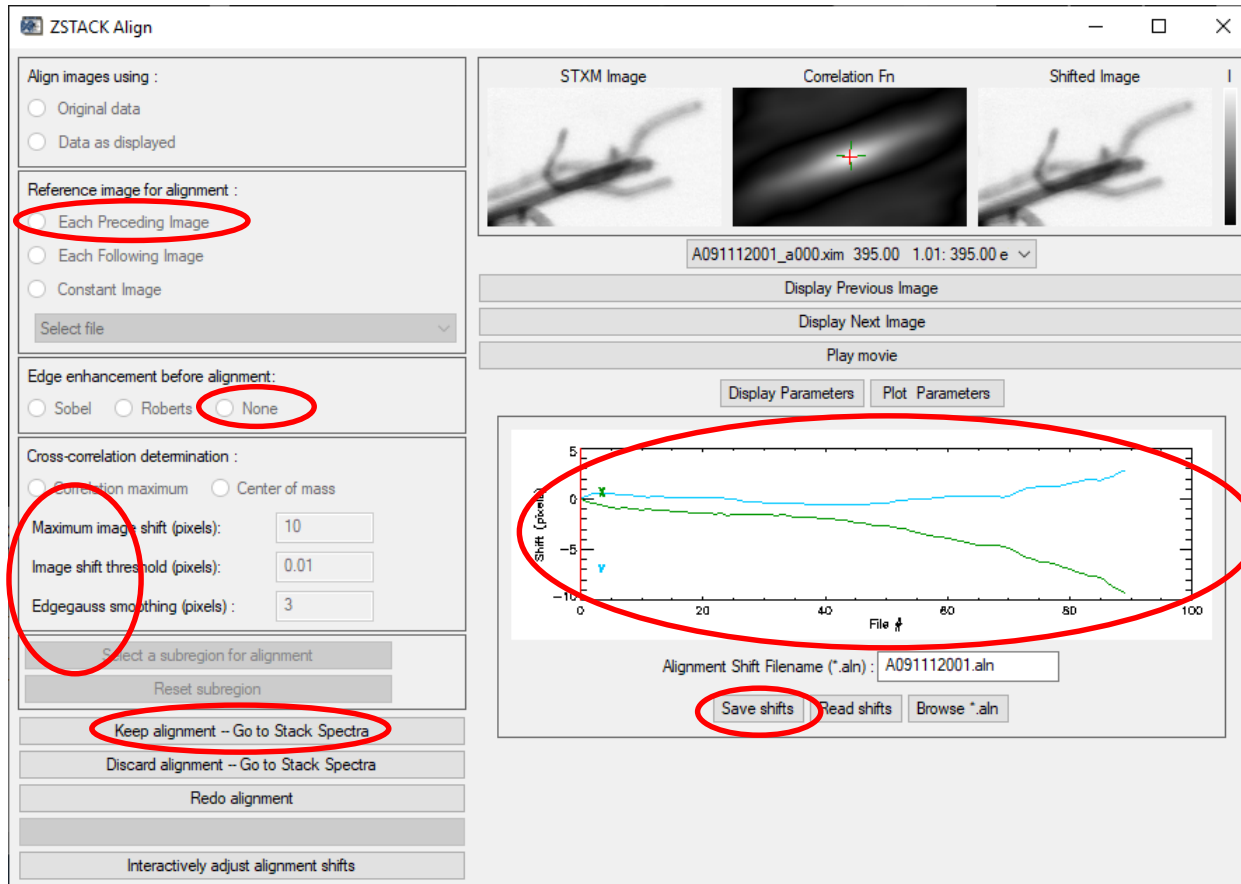
## Some Useful Functions

- **Browse \*.ncb:** browse and open a \*.ncb stack
- **List is complete:** after loading the stack, click “List is complete” to move to the “ZSTACK Align” widget



# aXis2000 – Stacks – Zimba – ZSTACK Align

aXis2000 → Stacks → Analyze → Zimba → ZSTACK Align



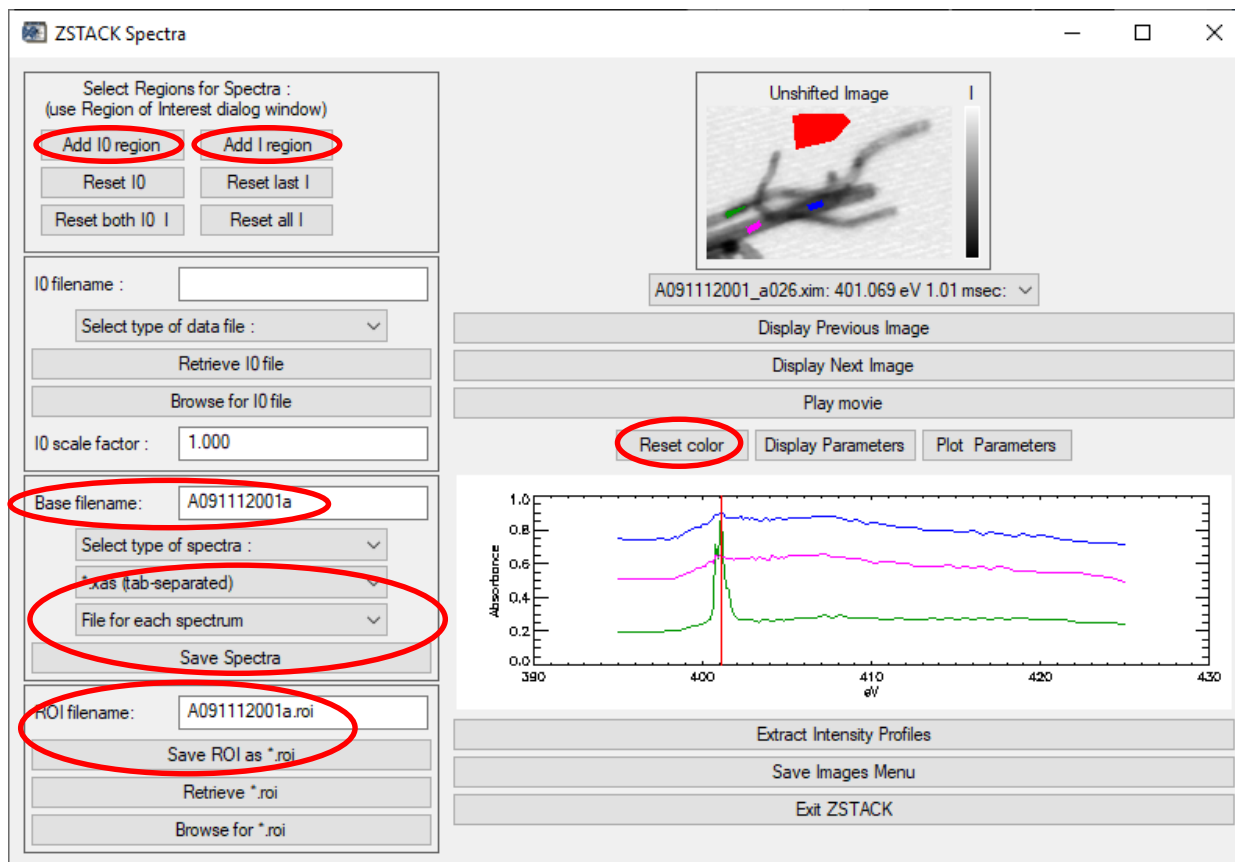
## Some Useful Functions

- **Reference image for alignment:** choose “Each Preceding Image” for most cases; or choose a best contrast image for some cases; use the same reference image for all alignment iterations.
- **Edge enhancement before alignment:** choose “None” for most cases unless the image contrast is very poor.
- Use other default settings unless the alignment is very challenging.
- **Start auto-alignment:** you will see this function before alignment
- **Skip alignment:** you will see this function before alignment; click this button if alignment was done by other software
- **Keep alignment – Go to Stack Spectra:** after alignment, move on to “ZSTACK Spectra”
- **Save shifts:** after each alignment, need to save an alignment file \*.aln
- Align the stack until the X-Shift and Y-Shift are zero and fully overlapped, or smaller than 1 pixel.



# aXis2000 – Stacks – Zimba – ZSTACK Spectra

aXis2000 → Stacks → Analyze → Zimba → ZSTACK Align → ZSTACK Spectra



## Some Useful Functions

- **Add IO region:** select an empty region without sample for IO; if the stack is already OD stack, don't need to select an IO region.
- **Add I region:** can select multiple sample regions
- **Base filename:** for convenience, just use stack file name
- Select **“xas (tab-separated)”** and **“File for each spectrum”**, then click **“Save Spectra”**. Note the saved spectra are transmission spectra including IO spectrum if the stack is transmission stack; and for an OD stack, the saved spectra are OD spectra.
- Give a region of interest (ROI) file name, then click **“Save ROI as \*.roi”** to save the ROI file with extension name \*.roi.
- **Reset color:** if there is display problem, click **“Reset color”** button.



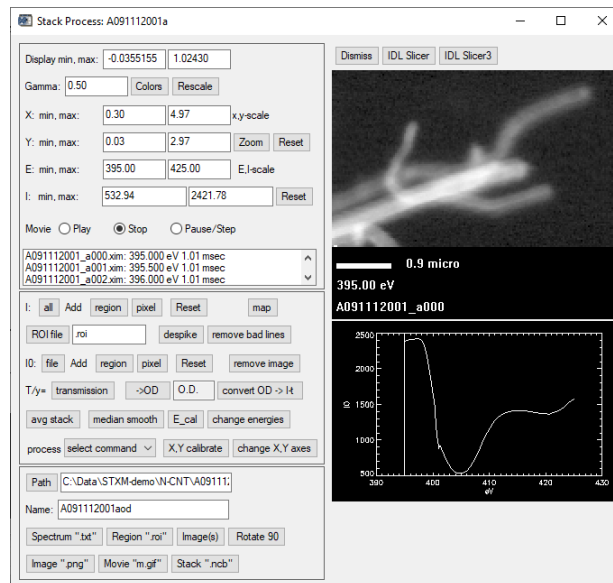


# aXis2000 – Stack Process – Save OD Stack, Stack Average Image, and Spectra

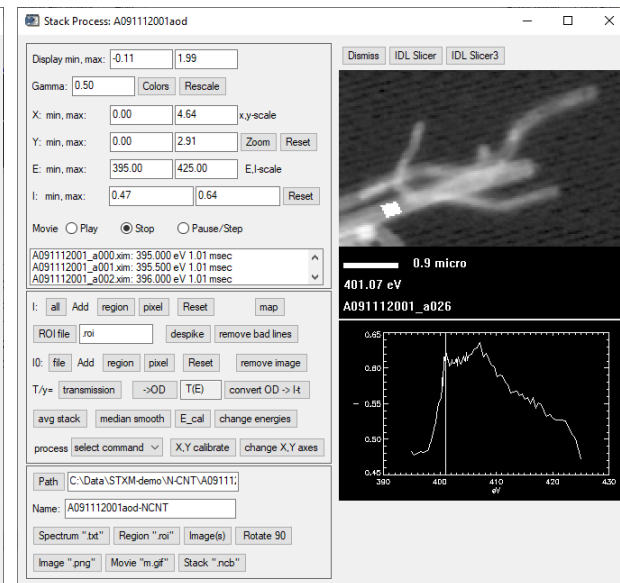
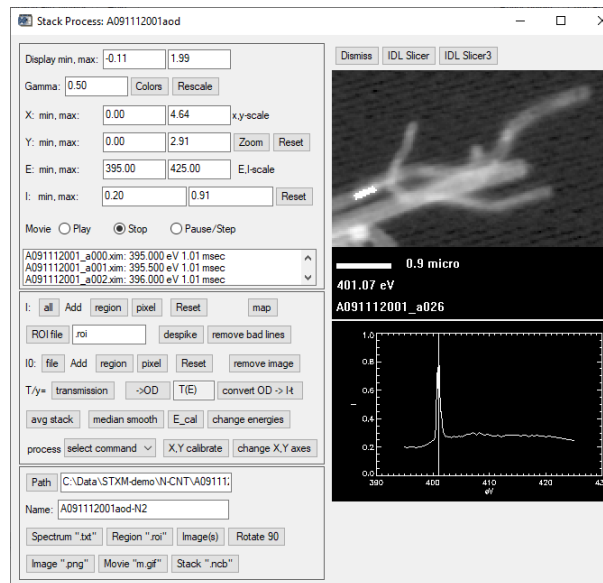
**aXis2000 → Stacks → Analyze → stack process → select an aligned transmission stack → click “No” for alignment file → suggested zoom value → IO file (\*.\*, then choose \*.xas io file) → ->OD → save stack**

**aXis2000 → Stacks → Analyze → stack process → select an aligned OD stack → click “No” for alignment file → suggested zoom value → avg stack → Store average image in an empty buffer, then save the image → select “I: region” → click draw a sample region on the stack → click “ACCEPT region” → give a file name, then hit “enter” → click “Spectrum “.txt”” to save the sample NEXAFS spectrum**

Save OD stack, average stack image

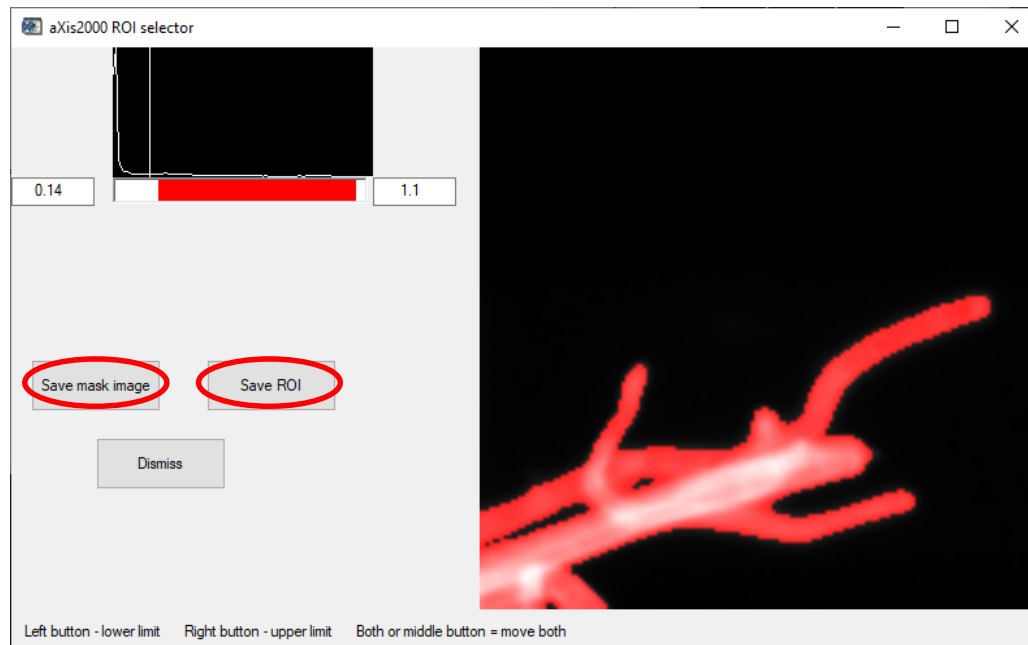


Save Sample Region NEXAFS Spectra



# aXis2000 – Stack Average Image – Generate Mask and Use Mask for Spectrum

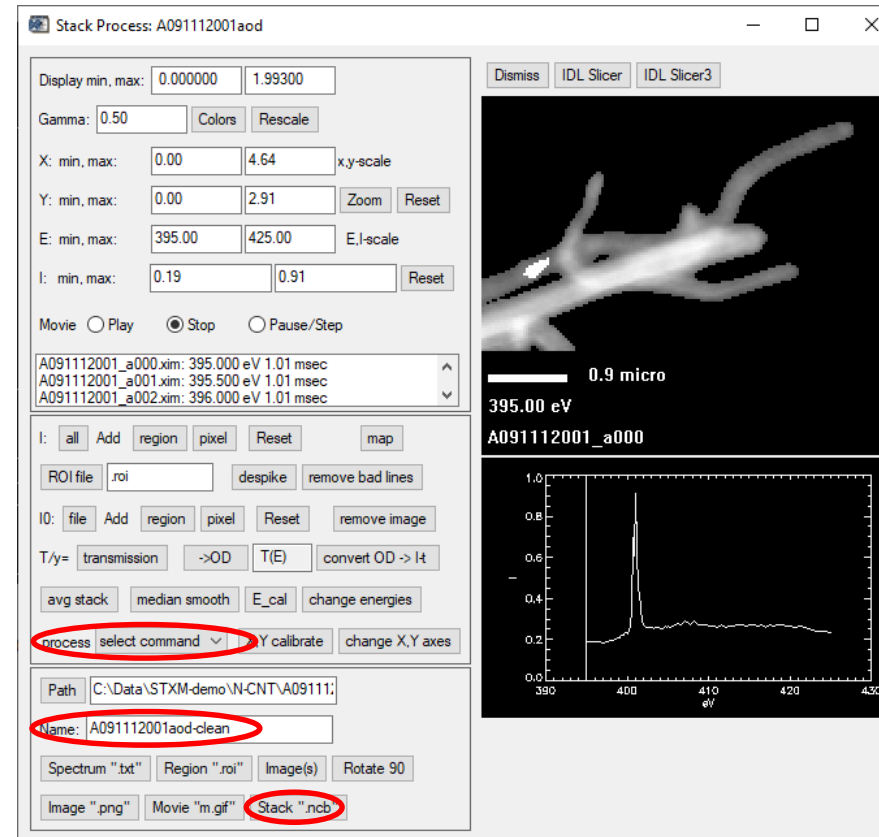
**aXis2000 → Read → Images → AXIS → open a stack average OD image → Images → generate mask → threshold → histogram → adjust lower/upper limit to select desired sample region → Save ROI → (optional) edit mask → Save mask image → Choose Buffer → Write → AXIS → save the mask image in \*.axb format → Images → Delete region → select regions on mask to replace with zero → repeat “generate mask” .....**



**aXis2000 → Stacks → Analyze → stack process → select an aligned OD stack → click “No” for alignment file → suggested zoom value → select “I: ROI file” → load the mask \*.roi file → give a file name, then hit “enter” → click “Spectrum “.txt”” to save the sample NEXAFS spectrum**

# aXis2000 – Stack Average Image – Generate Mask and Use Mask for Stack

**aXis2000 → Stacks → Analyze → stack process →** select an aligned OD stack → click “No” for alignment file → **suggested zoom value → process: select command → \*image →** load a mask image in \*.axb format → **weight by 1 →** select an “I region” to activate the output menu → give a file name, then hit “enter” → click “**Stack “.ncb”**” to save the background cleaned stack

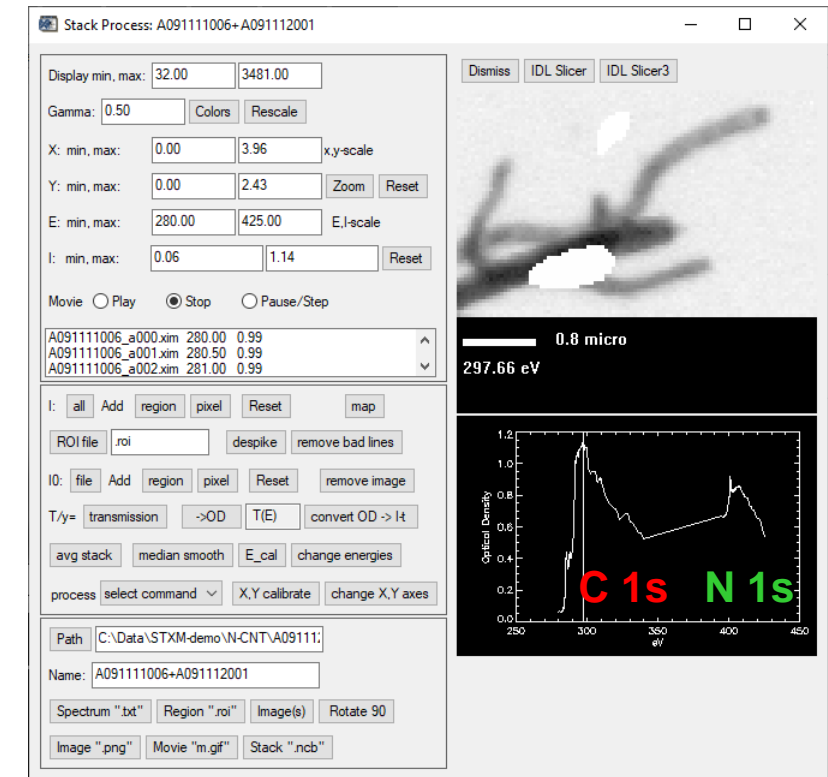


# aXis2000 – Stacks – Change Mesh or Size – Append

- **Stack A091111006**: C 1s stack, 4  $\mu\text{m}$  x 2.5  $\mu\text{m}$ , 100 pixel x 63 pixel, step size: 40 nm
- **Stack A091112001**: N 1s stack, 5  $\mu\text{m}$  x 3.0  $\mu\text{m}$ , 167 pixel x 99 pixel, step size: 30 nm
- **Appending stacks procedure**
  - Cut A091112001 X-dimension 33 pixels and Y-dimension 17 pixels to have the same physical size as A091111006
  - Change mesh for the cut A091112001 to 100 pixel x 63 pixel, then append the two stacks together

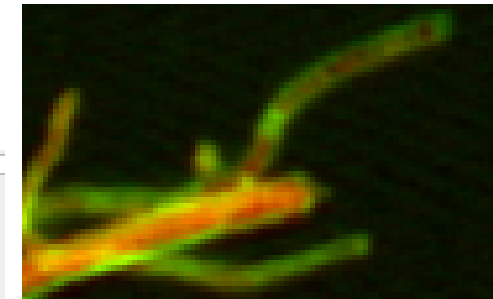
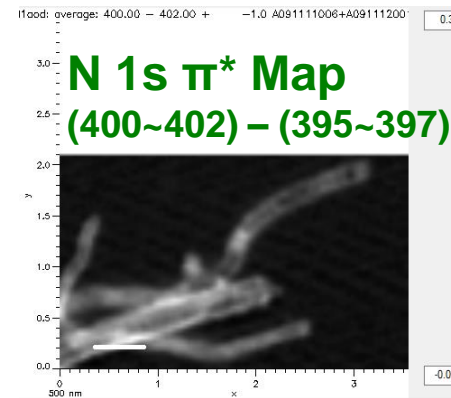
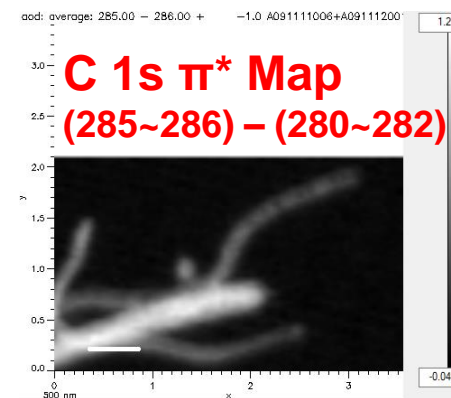
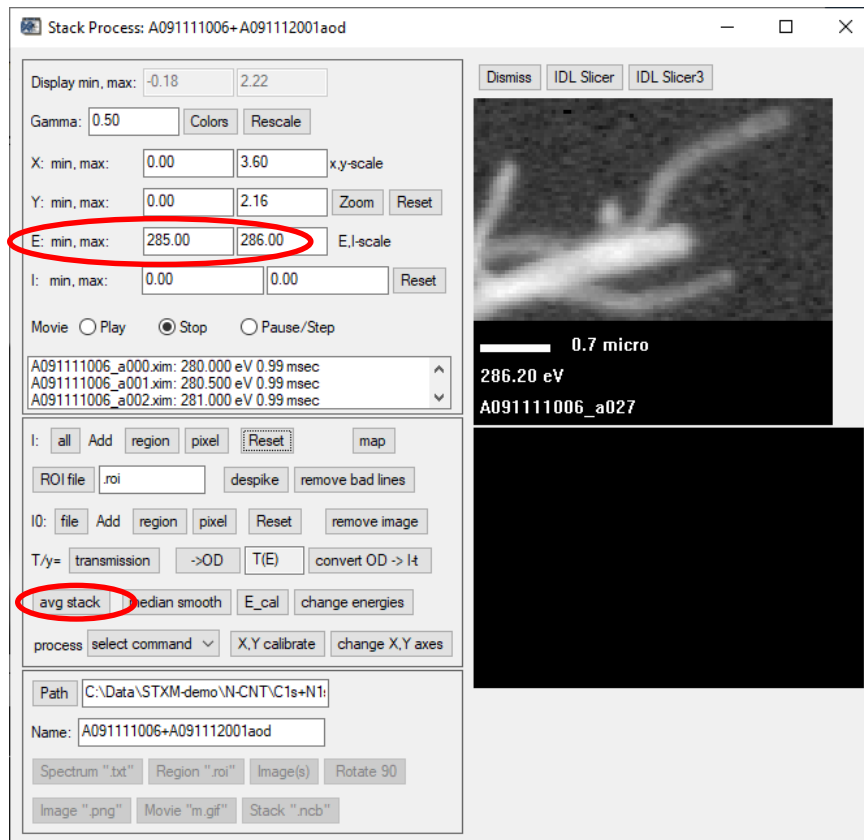
**aXis2000 → Stacks → Analyze → stack process → select a raw transmission stack → click “No” for alignment file → suggested zoom value → select an “I region” to activate the output menu → give a file name, then hit “enter” → click “Stack “.ncb”” → keep columns(x) > 33 → keep columns(x) < 166 → keep rows(y) > 17 → keep rows(y) < 98**

**aXis2000 → Stacks → change mesh or size → click “Yes” for change MESH (and keep same image size) → input “# of X pixels” as 100 → input “# of Y pixels” as 63 → save the re-meshed stack → Stacks → Append → select **STACK1**: A091111006.ncb and **STACK2**: A091112001tm.ncb → save the appended stack file name as **A091111006+A091112001.ncb****



# aXis2000 – Stacks – Elemental/Chemical On/Off Mapping

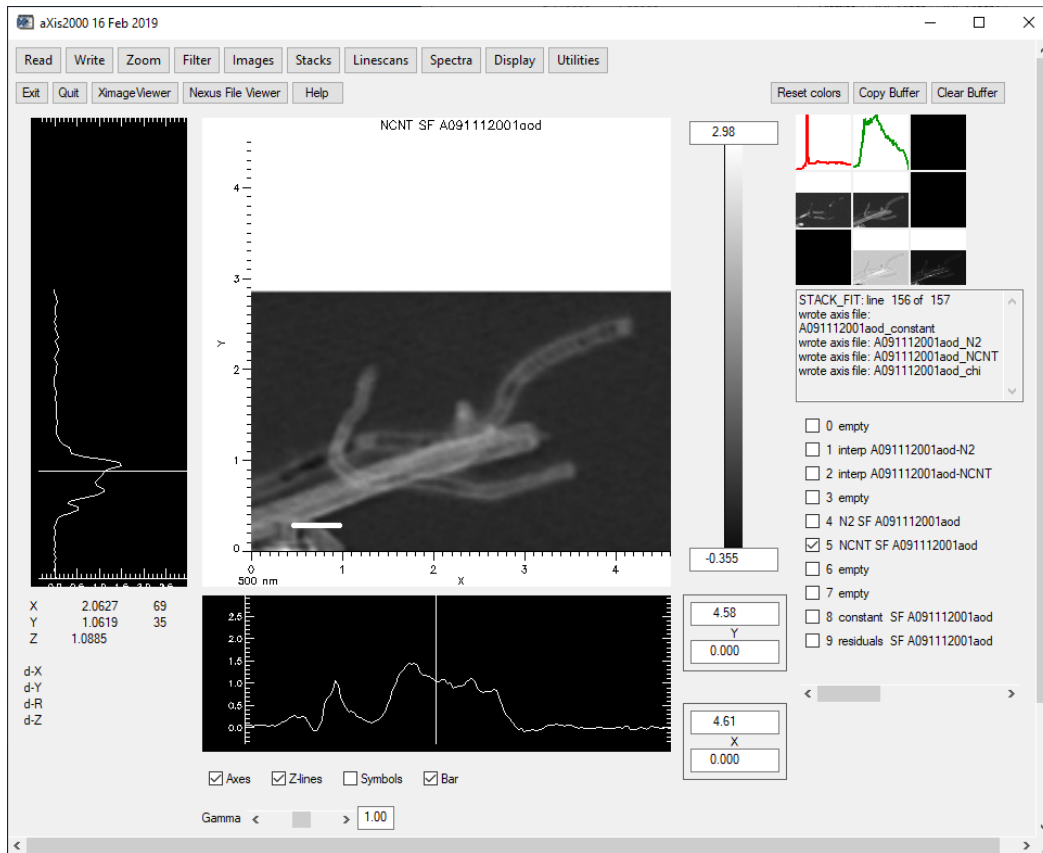
**aXis2000 → Stacks → Analyze → stack process** → select an aligned OD stack, e.g. A091111006+A091112001aod.ncb → click “No” for alignment file → **suggested zoom** value → change the “**E: min, max**” for pre-edge or post-edge → **avg stack** → **Store average image in** an empty buffer, then save the image → change the “**E: min, max**” again and generate other images → click a post-edge image → **Images → Add → Buffer** → choose the pre-edge image → **scaled by -1** → **Write** → **AXIS** → save map





# aXis2000 – Stacks – Maps – Stack Fit / SVD

**aXis2000 → Stacks → maps → Stack fit or SVD → select an aligned OD stack → click “No” for parameter file → input “# of components (1-8)” → choose “Spectrum of component 0” → give a very short “Name for component 0” → choose the rest component(s) spectrum → give a Name of fit parameter file → then click “enters” for the rest default settings → result is saved and displayed in buffers**



## Output of Stack Fit / SVD

- **Buffer 1:** reference spectrum of **Component 0**, in this case it is N2 spectrum obtained from the stack directly, i.e. internal reference
- **Buffer 2:** reference spectrum of **Component 1**, in this case it is NCNT spectrum obtained from the stack directly, i.e. internal reference
- **Buffer 4: Component 0** distribution map, in this case it is N2 distribution map
- **Buffer 5: Component 1** distribution map, in this case it is NCNT distribution map
- **Buffer 8: Constant** map (only for Stack Fit)
- **Buffer 9: Residuals** map



# aXis2000 – Stack Fit / SVD – Color Composite Map

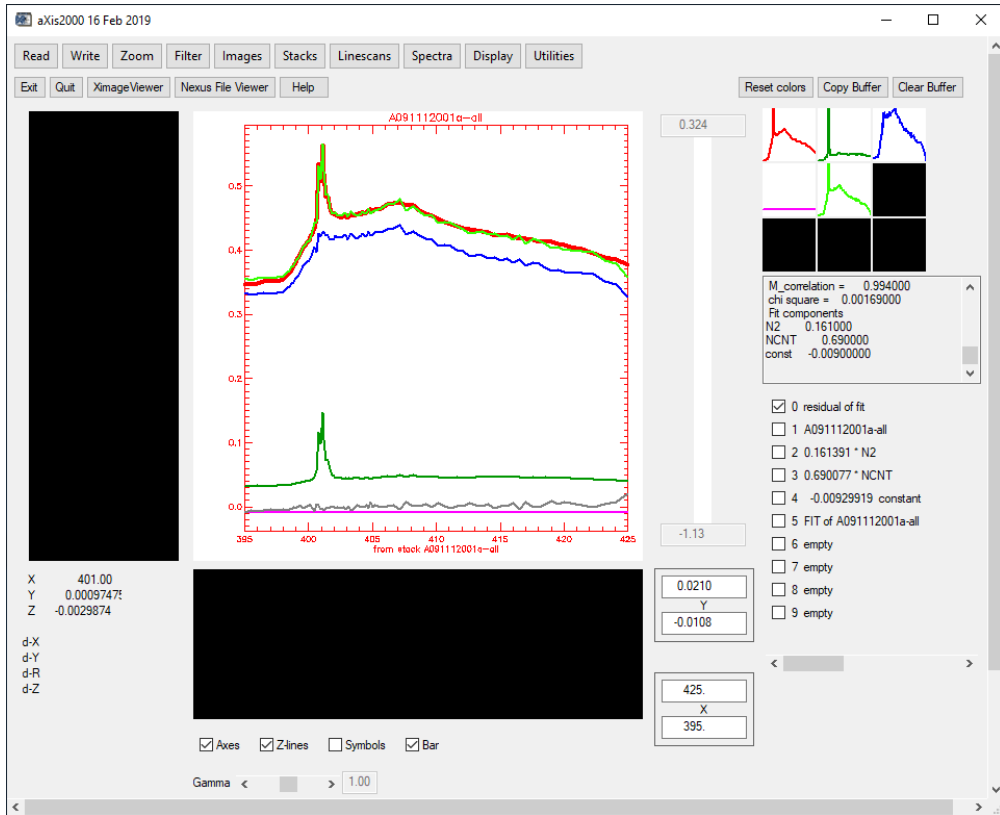
Click “**Component 0 map**” → **Images** → **Clip signal** → **histogram** → click “**around 0**” and “**highest visible intensity**” → **Copy Buffer**, and place it to **Buffer 1** → repeat the procedure for “**Component 1**” and place it to **Buffer 2** → in this case of only two components, a third blank image of zero intensity needs to be created → click any component image → **Images** → **Gain** → **Multiply by 0** → place the blank image to **Buffer 3** → click a blank buffer like **Buffer 7** → **Display** → **RGB composite** → select **RED**, **GREEN**, and **BLUE** images from **Buffer 1** to **3** respectively → click “**Yes**” for Autoscale each component → save the image in \*.tif format



- **Buffer 0:** color composite map
- **Buffer 1:** high contrast image of **Component 0**
- **Buffer 2:** high contrast image of **Component 1**
- **Buffer 3:** blank image with zero intensity

# aXis2000 – Spectra Curve Fit – Stack Fit / SVD

**aXis2000** → **Read** → **Spectra** → **AXIS** → open a spectrum for all sample regions like A091112001aod-all.txt → click the spectrum → **Spectra** → **Curve fit** → **linear regression (stack fit)** or **SVD** → click “**No**” for parameter file → input “**Number of components**” → choose “**Spectrum of component 0**” → give a very short “**Name for component 0**” → choose the rest component(s) spectrum → give a **Name of fit parameter file** → result is displayed in buffers → save spectra by → **Write** → **AXIS**

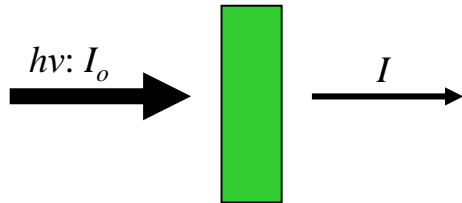


## Output of Curve Stack Fit / SVD

- **Buffer 1:** the original sample spectrum
- **Buffer 2:** fitting coefficient times reference spectrum of **Component 0**, i.e. N2 spectrum
- **Buffer 3:** fitting coefficient times reference spectrum of **Component 1**, i.e. NCNT spectrum
- **Buffer 4: Constant** (only for Stack Fit)
- **Buffer 5:** simulated fit spectrum

# Principles of STXM Quantitation

## Beer's Law



$$T = I/I_0$$

$$OD = \text{Abs.} = \ln(I_0/I) = \mu \rho l$$

OD: optical density

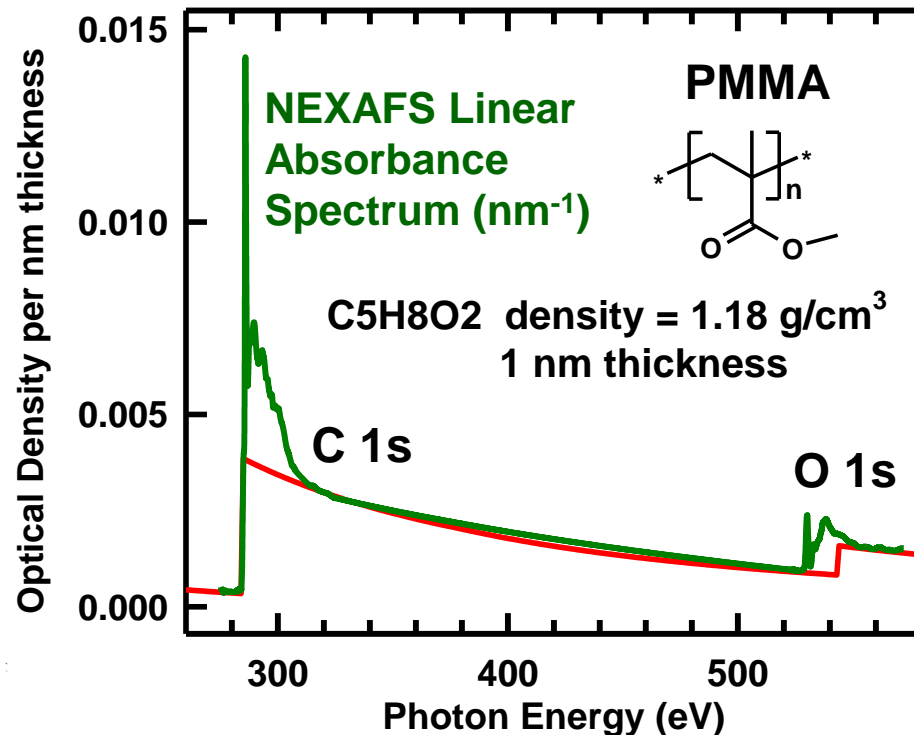
$\mu$ : mass absorption coefficient

$\rho$ : material density

$l$ : thickness

## Optimal STXM Sample Transmission:

$$0.1 \sim 1 \sim 2 = OD = \ln(I_0/I) = -\ln(T) = -\ln(90\% \sim 37\% \sim 14\%)$$



## Mass Absorption Coefficient for the Elements

ATOMIC DATA AND NUCLEAR DATA TABLES 54, 181-342 (1993)

X-RAY INTERACTIONS: PHOTOABSORPTION, SCATTERING, TRANSMISSION,  
AND REFLECTION AT  $E = 50\text{--}30,000$  eV,  $Z = 1\text{--}92$

B. L. HENKE,\* E. M. GULLIKSON, and J. C. DAVIS

Center for X-Ray Optics  
Lawrence Berkeley Laboratory  
Berkeley, California 94720

The primary interactions of low-energy x rays within condensed matter, viz. photoabsorption and coherent scattering, have been described for photon energies outside the absorption threshold regions by using atomic scattering factors. Atomic scattering factors may be accurately determined



## Calculated Elemental Mass Absorption Coefficient for Compounds

$$\mu = \frac{N_A}{M} \sum_i x_i \sigma_i$$

$N_A$ : Avogadro's number

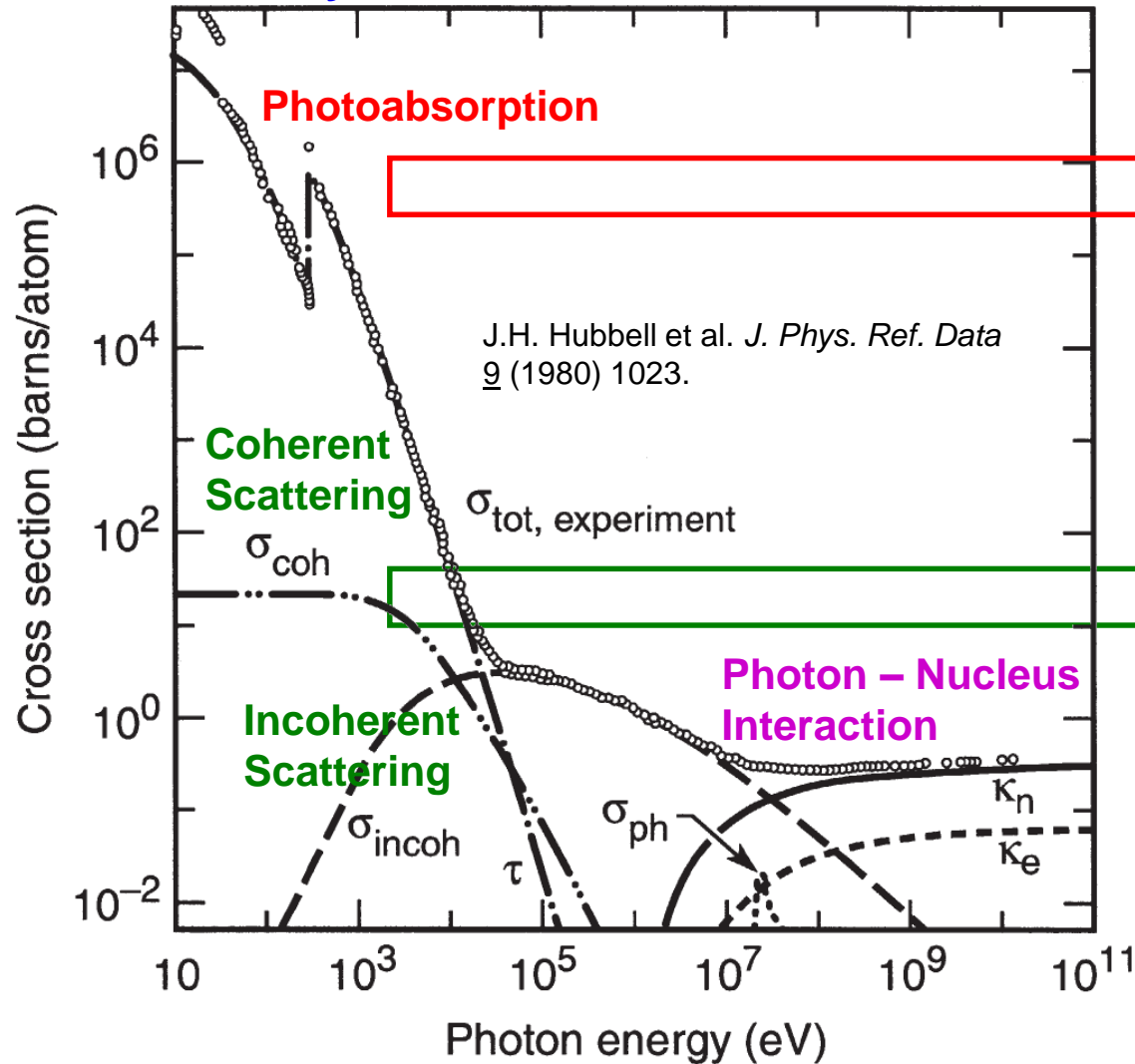
$M$ : molecular weight

$x_i$ : number of atom  $i$

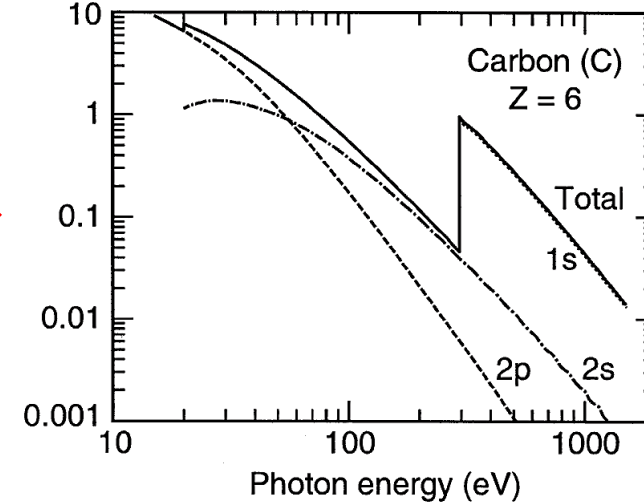
$\sigma_i$ : atomic photoabsorption cross section

# X-ray – Matter (Atomic) Interaction

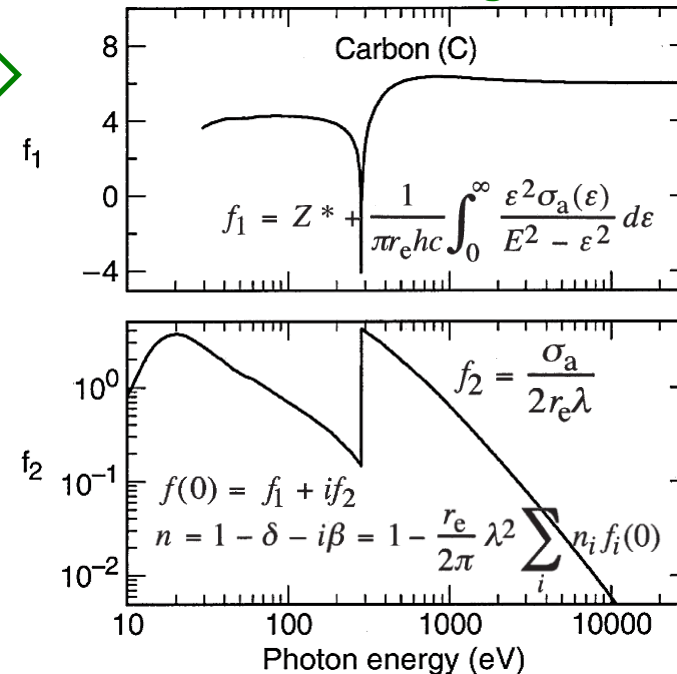
## X-ray Interaction with Carbon Atoms



## Atomic Cross Section

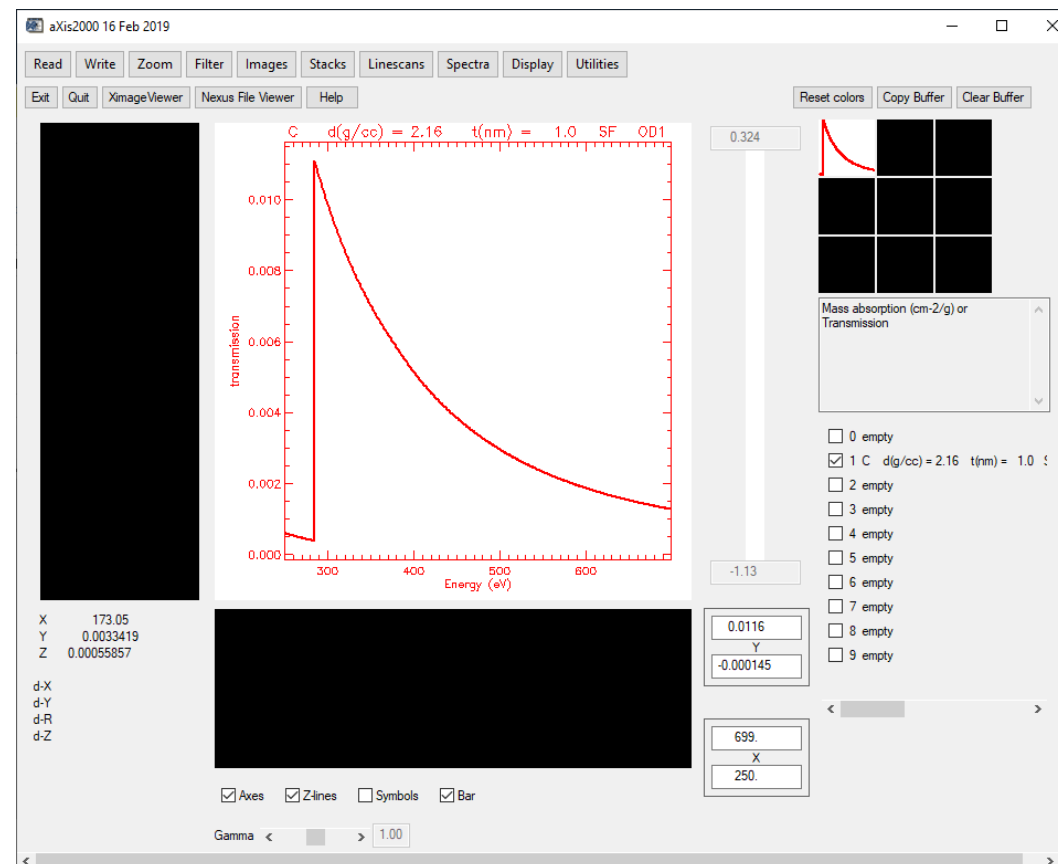


## Atomic Scattering Factors



# aXis2000 – Utilities – Calculate X-ray Parameters (SF)

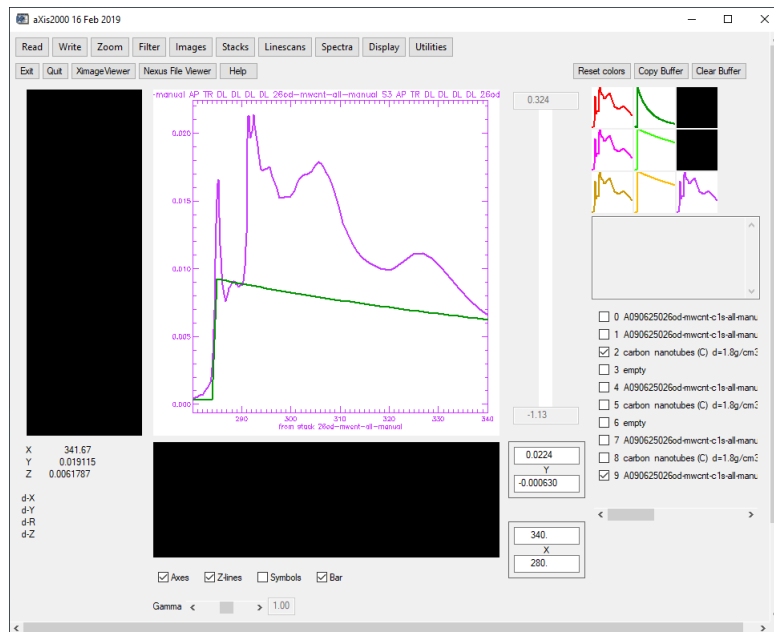
**aXis2000 → Utilities → Calculate X-ray parameters (SF) → Formula, e.g. C → minimum energy → maximum energy → transmission → density (g/cc), e.g. 2.16 (graphite) → thickness (μm): 0.001 → click “Yes” to “Convert to OD” → accept or update “Header for output file” → Write → AXIS → give a file name and save file**





# aXis2000 – Quantitative Scaling Reference Spectra

**aXis2000 → Read → Spectra → AXIS →** open a pure sample spectrum, i.e. **MWCNT** at **Buffer 1**, and a **sf** file for MWCNT at **Buffer 2** → click **Buffer 1** → **Spectra** → **Calibrate** → **Y** → **1 point** → click pre-edge baseline, and set “**New Y**” to zero → **Copy Buffer**, and place it at **Buffer 4** → click **Buffer 2** and change the X display limits to **280 – 340 eV** → **Spectra** → **Truncate**, and click 280 and 340 eV positions → **Copy Buffer**, and place it to **Buffer 5** → calibrate pre-edge to zero and place it to **Buffer 8** → click **Buffer 4** → **Spectra** → **Gain** → **divide by 14** → **Display** → **Over Plot** → **No Rescale**, and choose **Buffer 8**, until the spectrum and the sf file overlap in both pre-edge and post-edge → place the scaled spectrum to **Buffer 7** → check **Buffer 5** pre-edge **Y value**, and use this value to calibrate **Buffer 8** pre-edge **Y value** → place the calibrated and scaled spectrum to **Buffer 9** → **Write** → **AXIS**

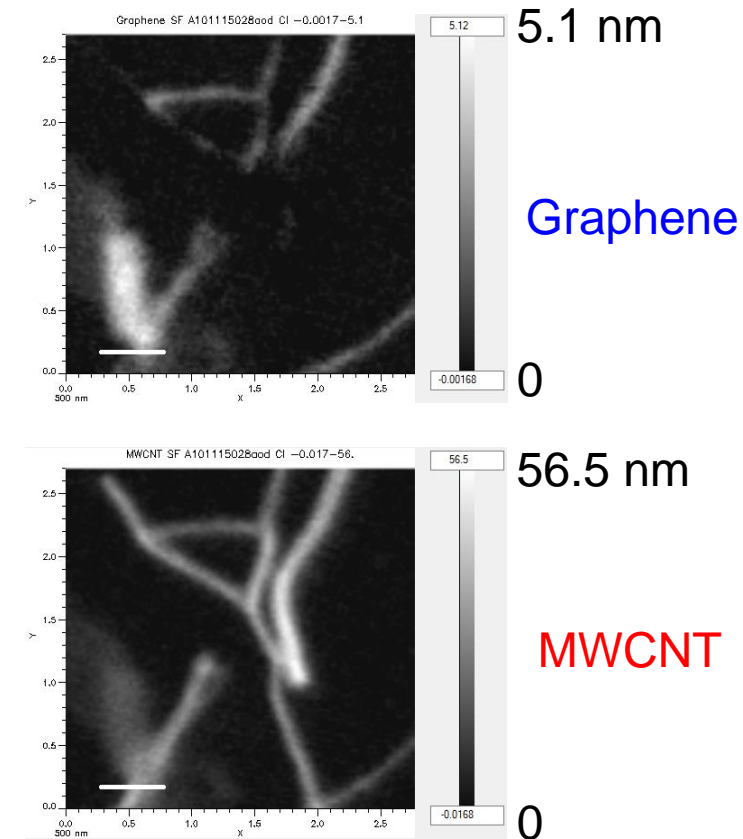
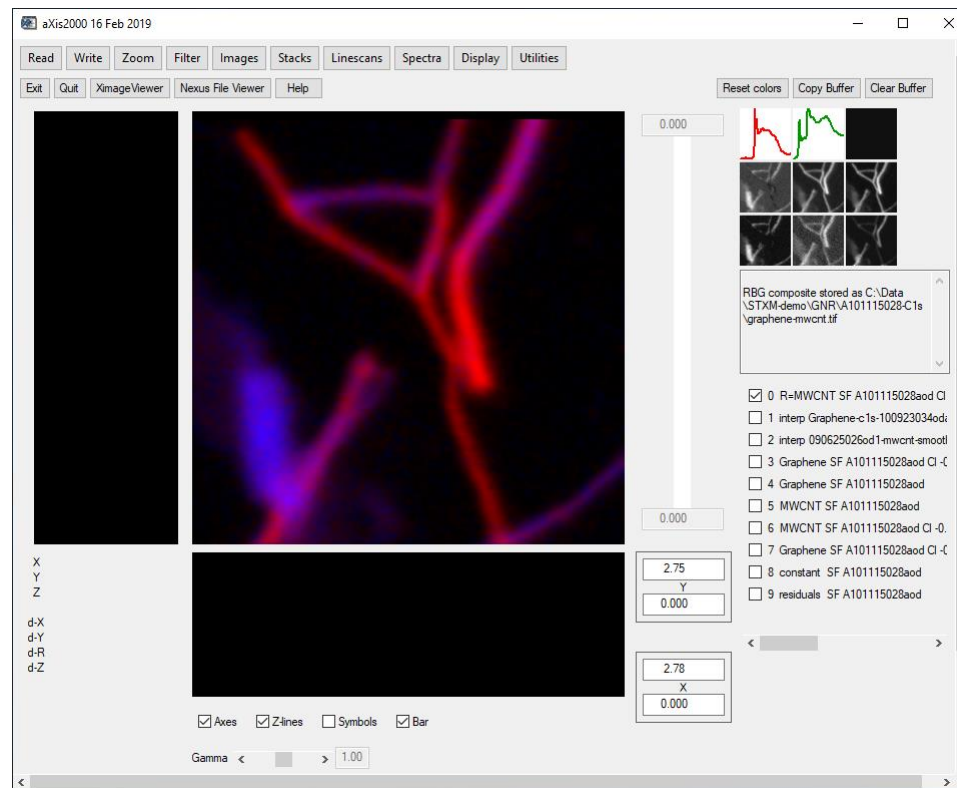


## Process of Quantitative Scaling Reference Spectra

- **Buffer 1:** the original MWCNT sample spectrum
- **Buffer 2:** sf file of MWCNT, i.e. 1 nm thick elemental X-ray absorption profile
- **Buffer 4:** pre-edge zeroed MWCNT sample spectrum
- **Buffer 5:** truncated sf file, i.e. 280-340 eV
- **Buffer 7:** pre-edge zeroed and scaled MWCNT spectrum
- **Buffer 8:** pre-edge zeroed and truncated sf file
- **Buffer 9:** pre-edge calibrated and scaled MWCNT spectrum, i.e. 1 nm thick MWCNT NEXAFS spectrum

# aXis2000 – Stacks – Quantitative Stack Fit / SVD

**aXis2000 → Stacks → maps → Stack fit or SVD → select an aligned OD stack → click “No” for parameter file → input “# of components (1-8)” → choose “Spectrum of component 0”, i.e. 1 nm thick graphene spectrum → give a very short “Name for component 0” → choose the rest component(s) spectrum, i.e. 1 nm thick MWCNT spectrum → give a Name of fit parameter file → then click “enters” for the rest default settings → result is saved and displayed in buffers**



# Summary: Typical Measure & Analysis of a STXM Stack

## MEASURE

## Typical Steps:

1. FIND A SUITABLE AREA
2. Check it has suitable properties (based on prior knowledge)
3. Measure **stack maps** (few images → few components) or **stacks** (good to look for surprises)
4. Check for **damage**
5. make sure you have a **valid lo** - **measure at SAME TIME (2<sup>nd</sup> area if needed)**
6. Check **energy calibration**

## ANALYSIS - STACKS

- Convert from raw data to a binary stack
- Align - Jacobsen stack\_analyze or Zimba
- Convert to OD
  - (best to use built-in lo; otherwise, measure lo (point or stack) just before or after)
- Inspect → Zimba
- Identify suitable reference spectra - external or **internal**
- Convert ref. spectra to OD1
- FIT - Singular Value Decomposition (SVD) versus Stack Fit (SF)
- Clean component maps (remove outliers)
- Display - non-rescale versus rescale RGB
- CHECK critical aspects: residuals, residual stacks; extract spectra of component-map-masked regions & fit to the reference spectra & inspect QUALITY of FIT
- Perform Multivariate Statistical Analysis (PCA\_GUI, Mantis) & compare

# Cryo-STXM

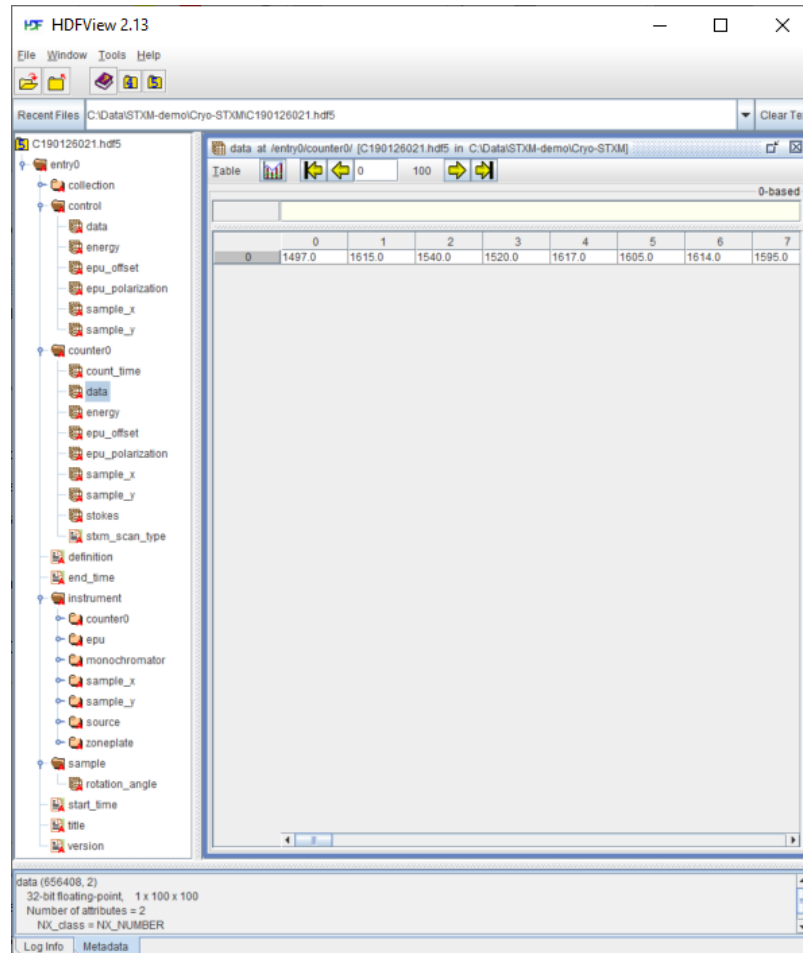


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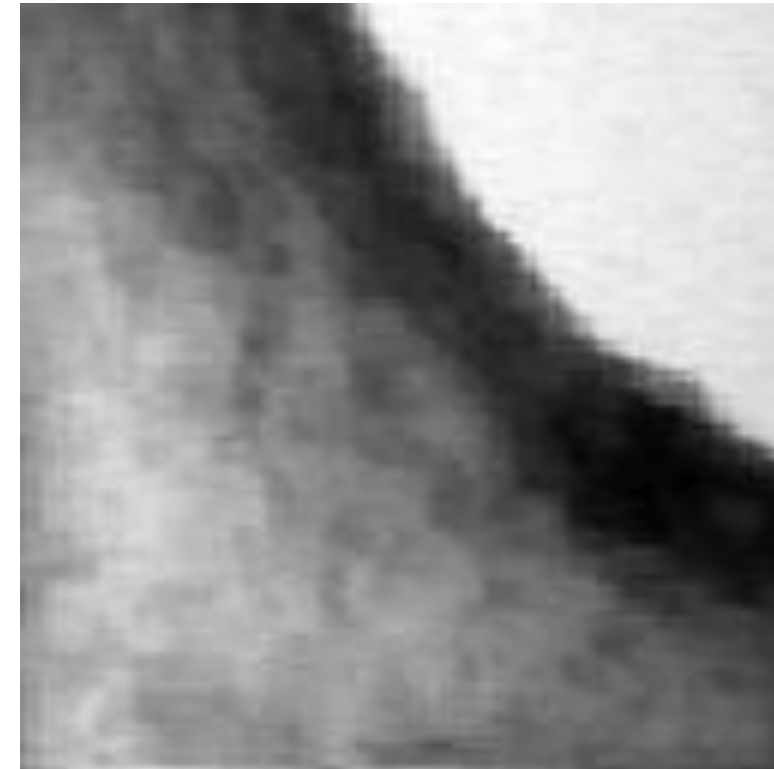
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# Cryo-STXM Data Format

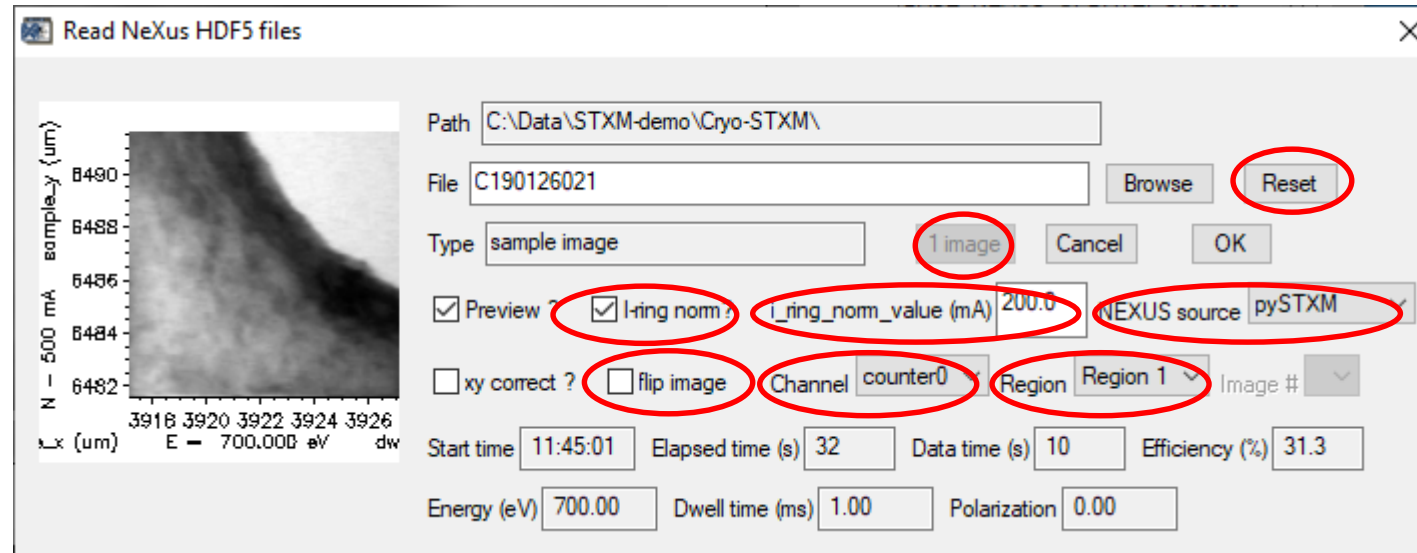
**HDF5 File:** e.g. **C190126021.hdf5**,  
Scans, STXM, and Beamline settings



**Image Preview File:**  
e.g. **C190126021.jpg**



# aXis2000 – Read Cryo-STXM Images

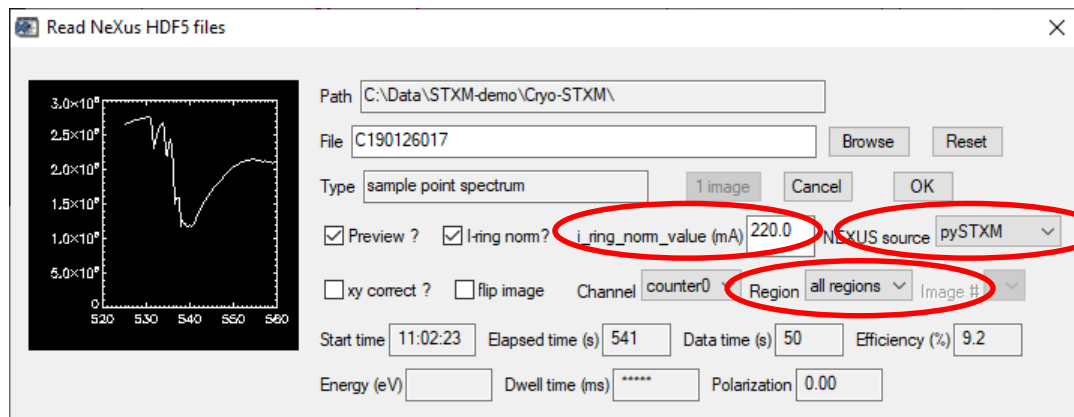


- **Reset:** clear loaded image and information
- **1 image:** read an image from a selected photon energy for a stack
- **I-ring norm?:** normalization to I-ring
- **I\_ring\_norm\_value:** CLS 220 mA
- **NEXUS source:** CLS pySTXM
- **Flip image:** flip image up and down
- **Channel:** select data channel if more than one detector is used
- **Region:** select sample region if more than one image region is defined

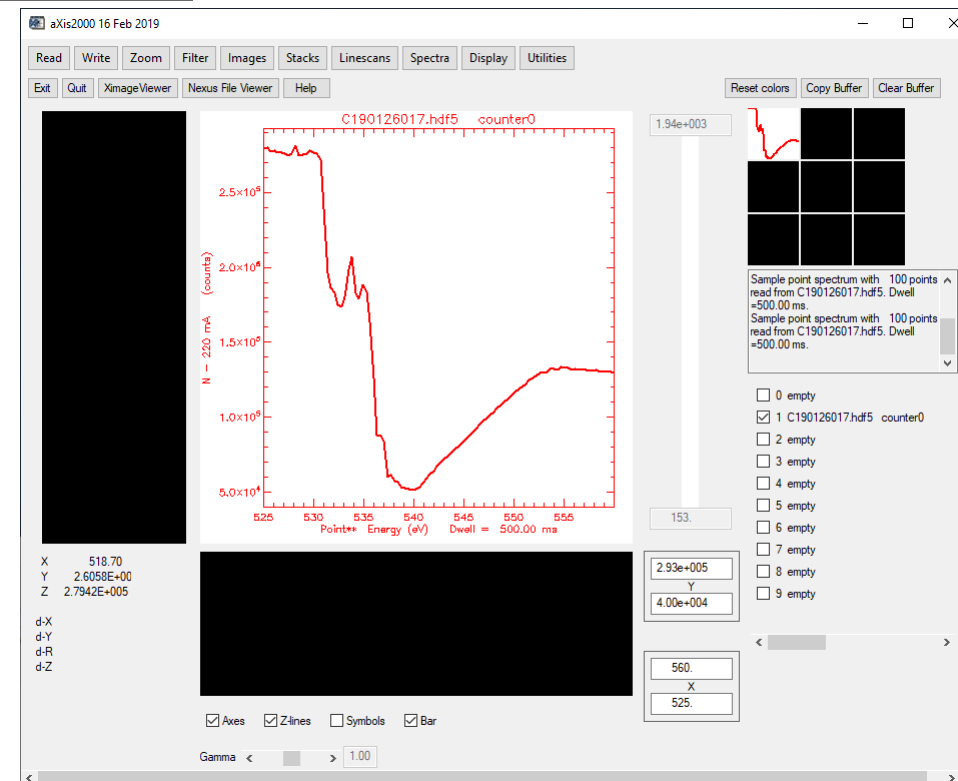




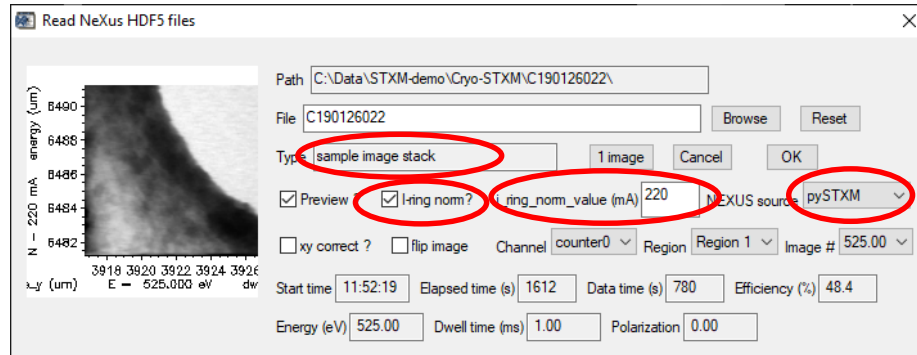
# aXis2000 – Read Cryo-STXM Point Spectra



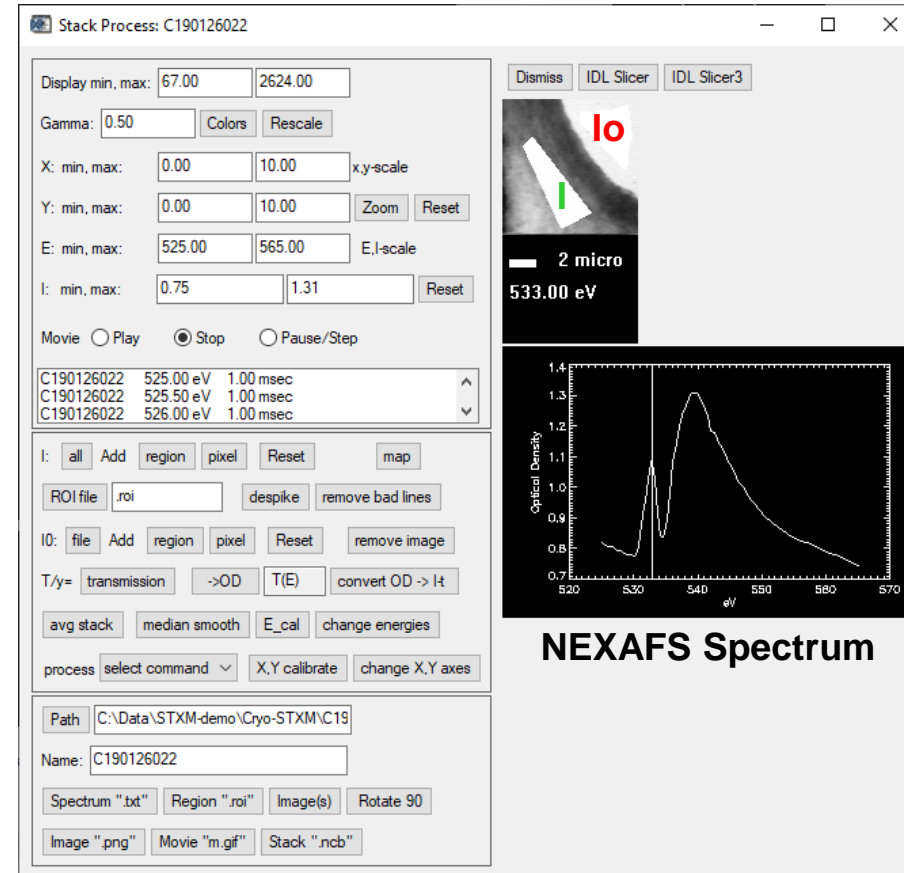
- **Note:** even select all regions, only one spectrum can be loaded into aXis2000



# aXis2000 – Read Cryo-STXM Stacks



- Compile raw Cryo-STXM stack data:  
aXis2000 → Read → STXM (NeXus)
- Other steps are the same as Ambient-STXM



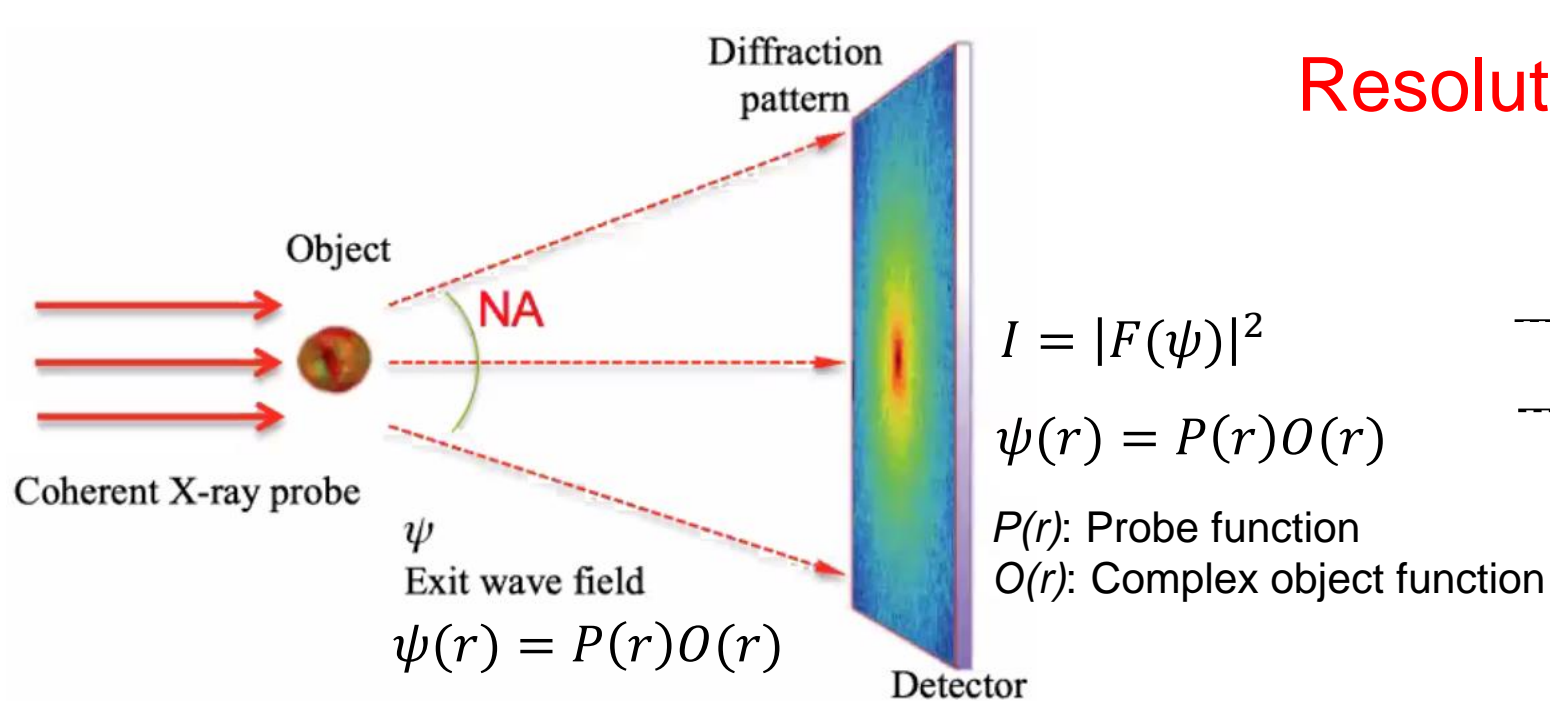
# STXM-Ptychography



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# Coherent Diffractive Imaging (CDI)



$$\text{Resolution: } \sigma_t = \frac{\lambda Z}{S}$$

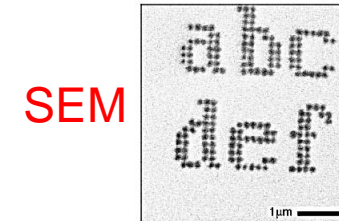
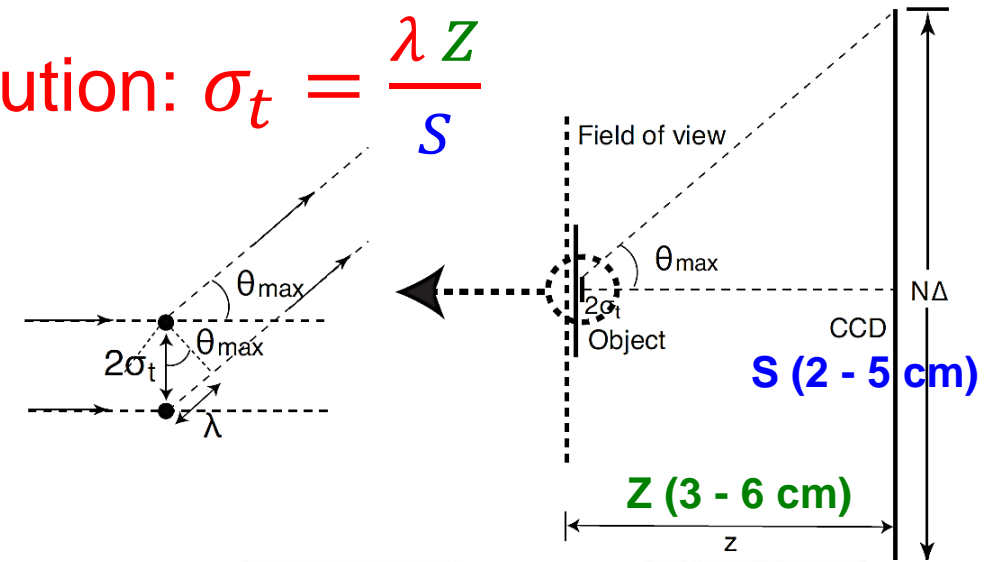


Figure 1 A scanning electron microscope image of the specimen. The specimen was fabricated by depositing gold dots, each ~100 nm in diameter and 80 nm thick, on a silicon nitride membrane.

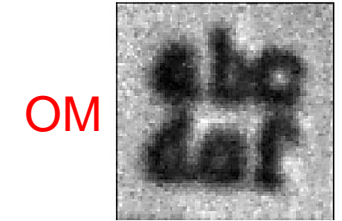


Figure 3 An optical microscope image of the specimen.

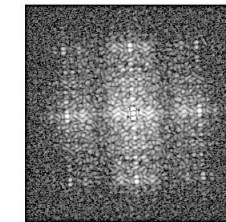


Figure 2 A diffraction pattern of the specimen (using a logarithmic intensity scale). The central 15-pixel-radius circular area is supplied by the squared magnitude of the Fourier transform of the optical microscope image (Fig. 3).



Figure 4 The specimen image as reconstructed from the diffraction pattern of Fig. 2.

Complex Refractive Index:  $n = 1 - \delta - i\beta = 1 - \alpha\lambda^2(f_1 + if_2)$

Complex Wavefield of Light:  $P(r) = Ae^{ikt}$

Complex Object Function:  $O(r) = e^{iknt} = e^{ik(1-\delta-i\beta)t} = e^{k\beta t} \times e^{-ik\delta t}$

Absorption:  $|O(r)| = e^{-k\beta t}$  Phase:  $\text{Arg}\{O(r)\} = -k\delta t$

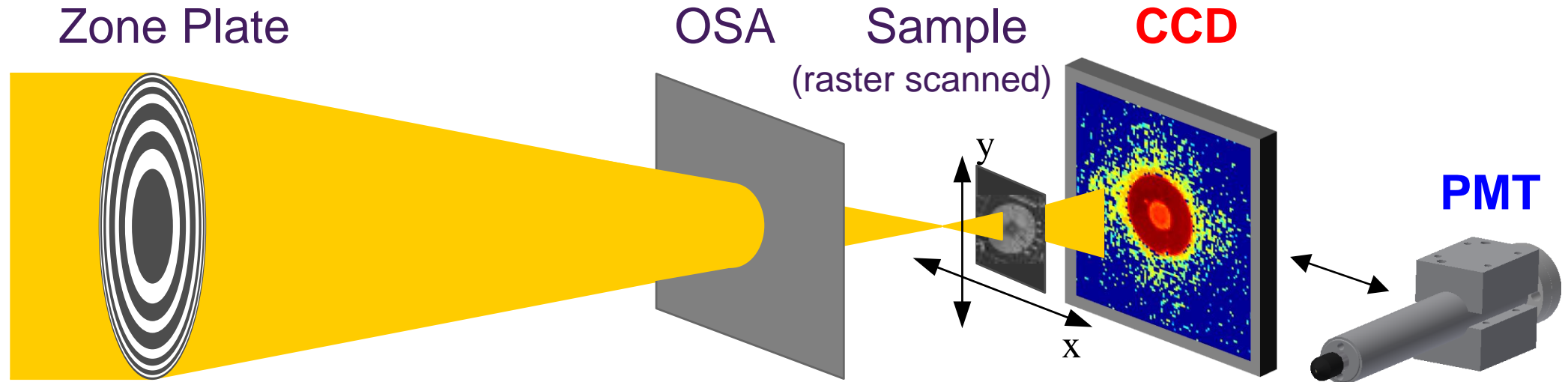
**Diffraction Pattern: Fourier Transform of Product of Probe and Object. Inverse Fourier Transform and Phase Retrieval to solve Object.**



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# From Conventional STXM to STXM-Ptychography



## Conventional STXM

- Sample in-focus
- Point (0D) detector: Scintillator+PMT or PD
- Real-space images
- Diffraction/spot size limited spatial resolution ( $1.22 \cdot \Delta r_n$ : ~30 nm)

## STXM-Ptychography

- Sample in-focus or out-of-focus
- 2D detector: X-ray CCD
- Reciprocal-space images
- Wavelength limited spatial resolution (1 - 2 nm by soft X-rays)
- Large computation in data process



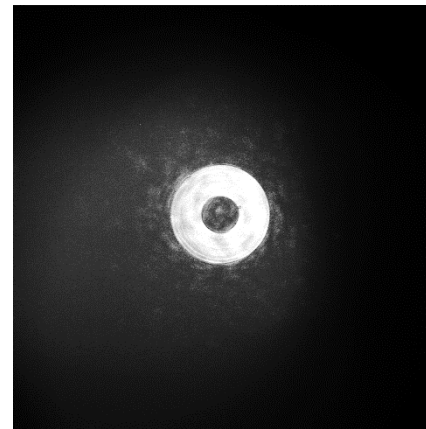
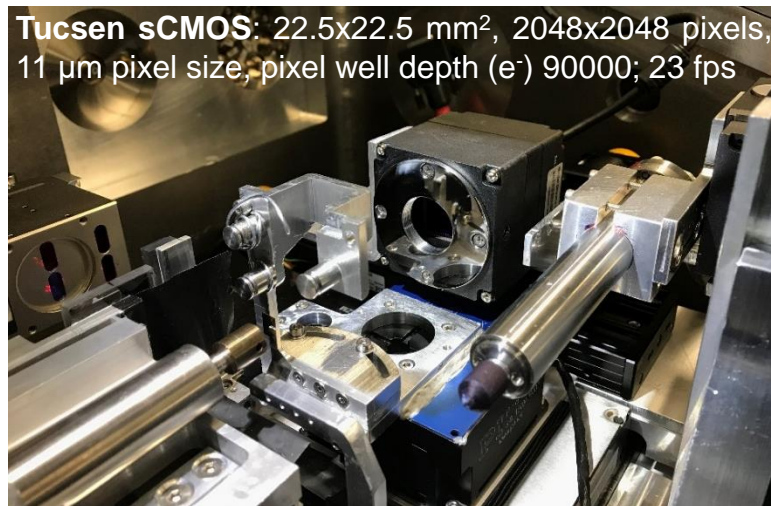
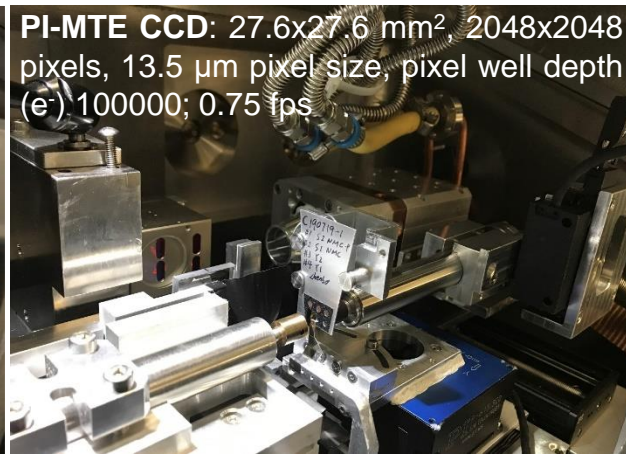
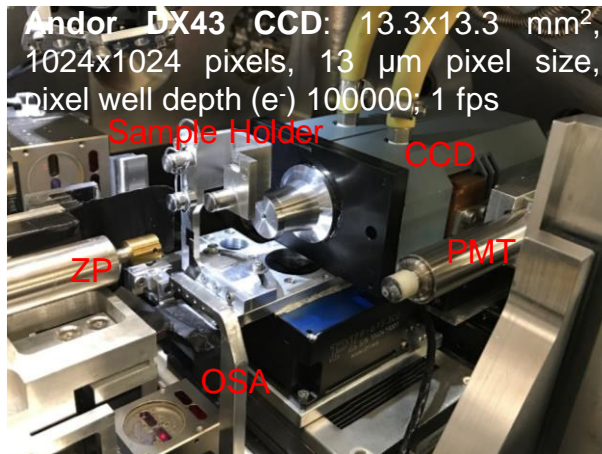


# CLS-SM STXM Instrumentation Development Highlights

## – STXM-Ptychography

### Ambient-STXM

### Cryo-STXM



Diffraction from Au/Pd nanoparticles captured by sCMOS



**Goal: sub-10 nm spatial resolution  
Cryo-Spectro-Ptycho-Tomography !**

Future AXIS-SXR: 4 MPixel Soft X-ray sCMOS camera



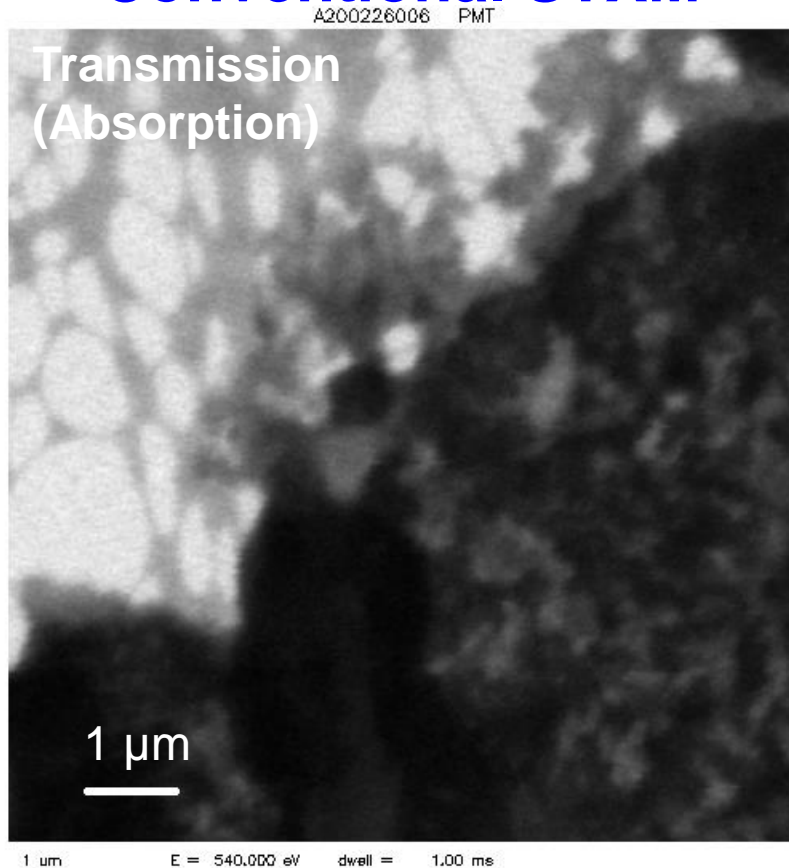
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# Recent STXM Spectro-Ptychography of LIB Cathode

## Conventional STXM



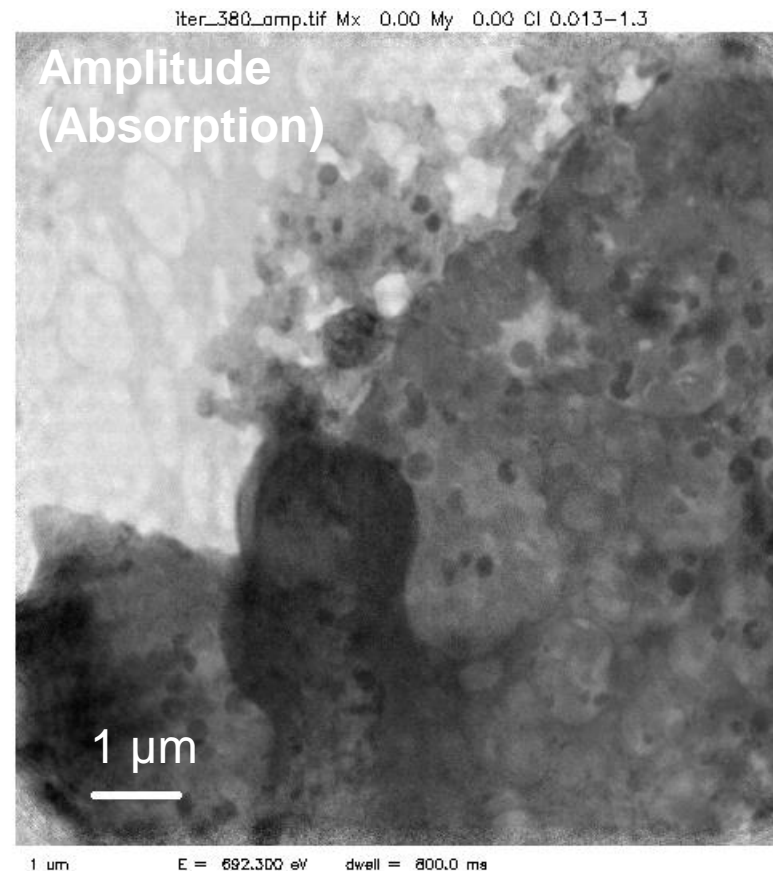
**Pixels: 300 x 300**  
**Resolution: ~40 nm**



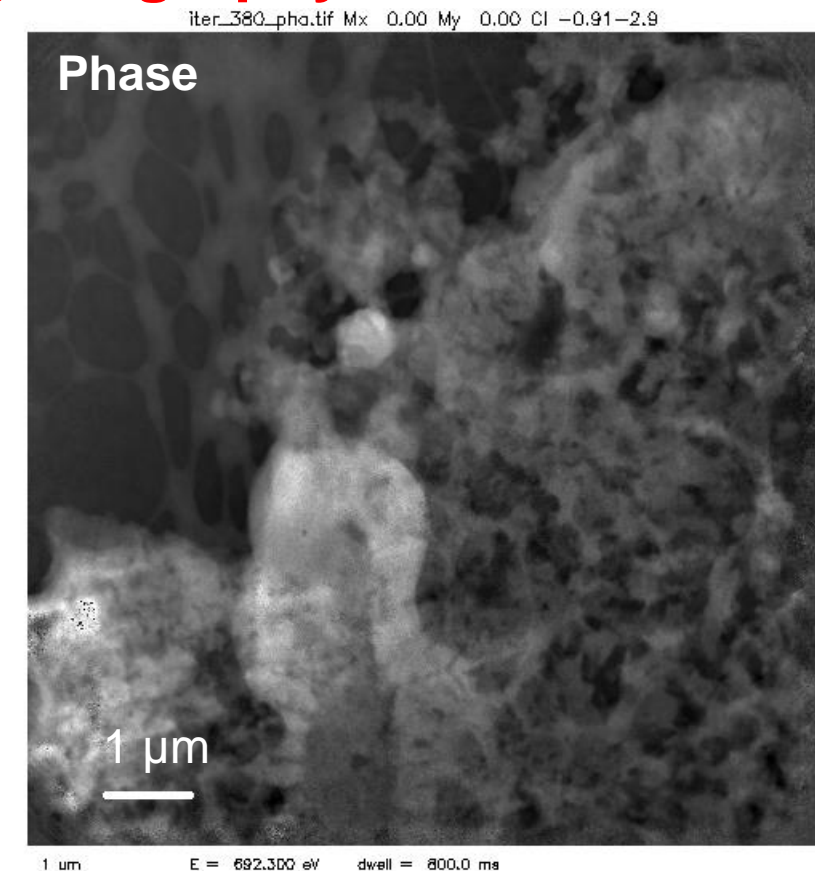
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## STXM-Ptychography

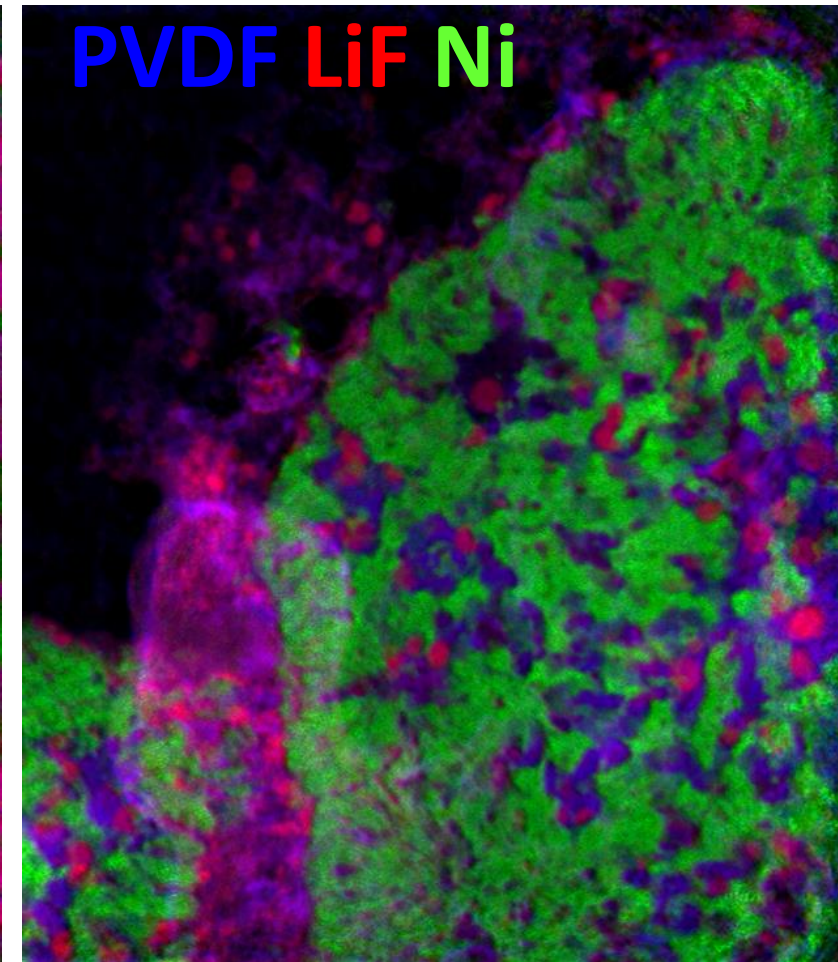
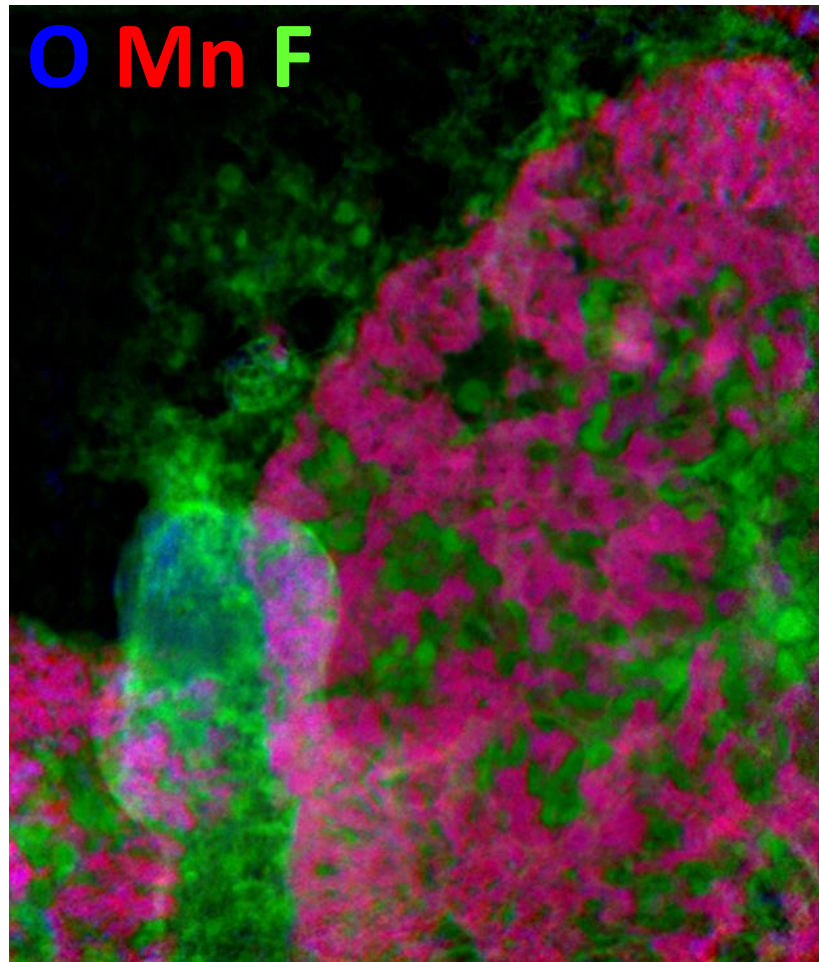
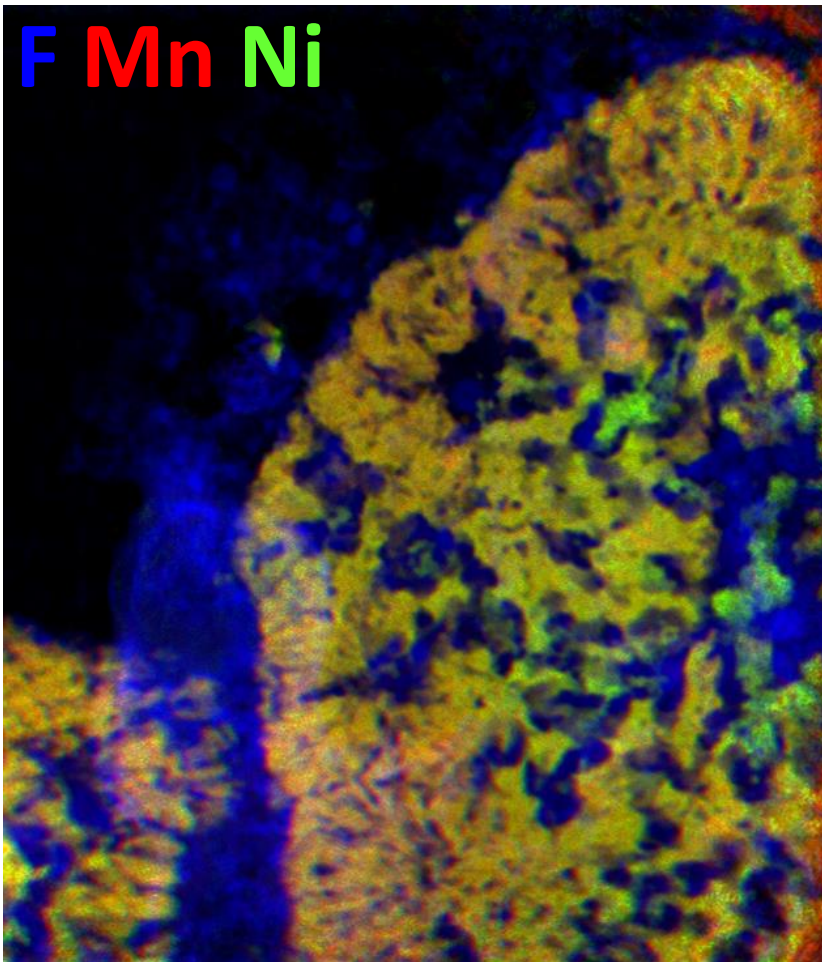


**Pixels: 2426 x 2426**  
**Resolution: ~8 nm**





# Recent STXM Spectro-Ptychography of LIB Cathode



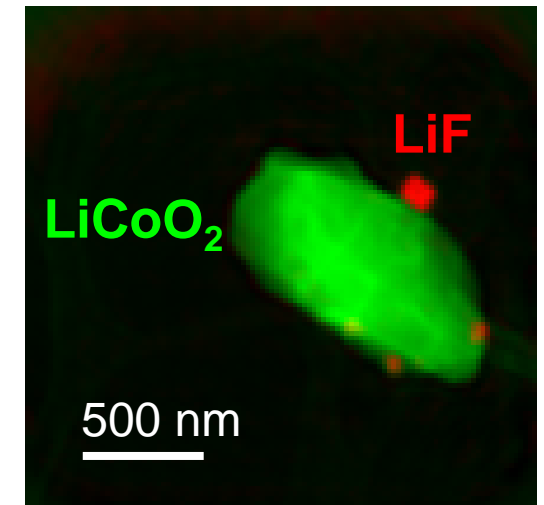
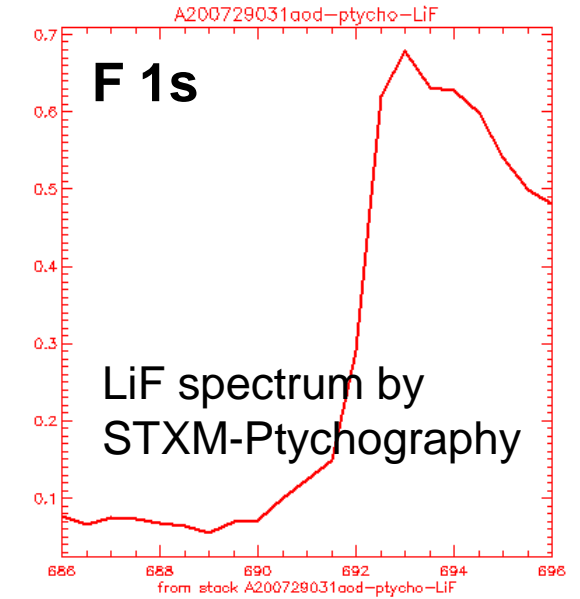
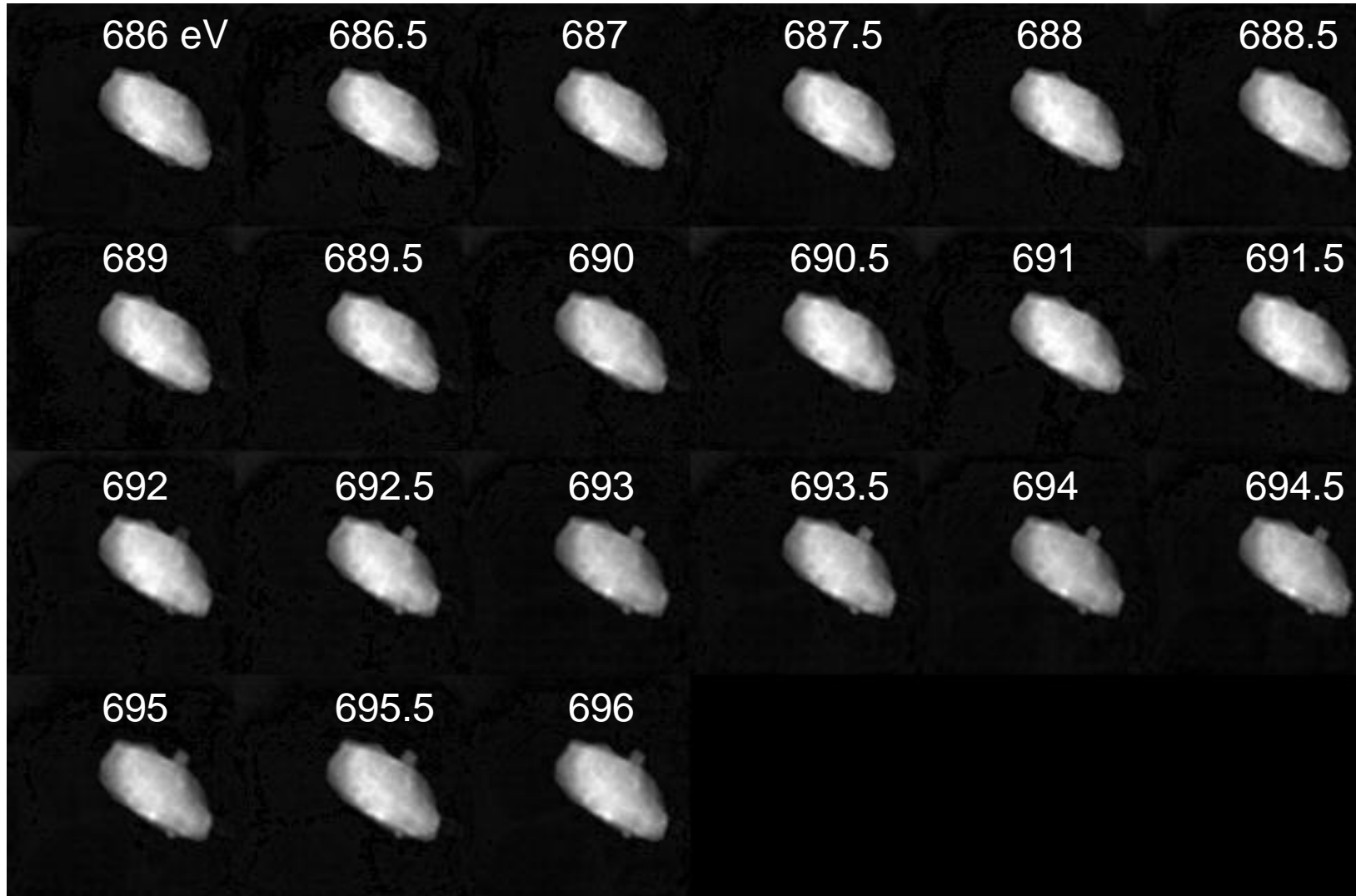
**Spatial Resolution: ~8 nm**



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# Recent STXM Spectro-Ptychography of LIB Cathode





# PyPIE – Single Energy Data Reconstruction

**1. Set root directory**

**2. Select a data file (\*.fits), \*bg\* file auto detected**

**3. Select the data file (\*.fits)**

**4. Display the file**

**5. Click-drag to zoom the zone plate center region, or click the double-arrow for additional options**

**6. Check the center pixel position**

**7. Center pixel position displayed here**

**8. Update the center pixel position**

PyPIE v3.3.0

File Format Hardware Settings Calculation

Open... Ctrl+O

Image Viewer Ctrl+I

Root directory Ctrl+R

Reset All Alt+.

Reset Root path Alt+.

Help Ctrl+H

Exit Alt+F4

05.fits

Intensity

30000

25000

20000

15000

10000

5000

400 600 800 1000

0 200 400 600 800 1000

Data Folder C:/Users/wangj.CORP/Desktop/STXM-data-analysis-webinar-4Dec2020/STXM-Ptychography/Andor-CCD-data/A200905105/A200905105.fits

Energy 853.2 Col Num 16 Col Step 0.25

Spot Size 1.25 Row Num 16 Row Step 0.25

Col Center 498 Row Center 536 Iter Number 1000

Single Energy ☒ Stack Analysis ☐

More

Extra Cfg

View Port

Load .hdr

Start Stop

PyPIE v3.3.0

File Format Hardware Settings Calculation

Home Back Forward

A200905105.fits

Intensity

30000

25000

20000

15000

10000

5000

400 450 500 550 600 650

400 450 500 550 600 650

Data Folder C:/Users/wangj.CORP/Desktop/STXM-data-analysis-webinar-4Dec2020/STXM-Ptychography/Andor-CCD-data/A200905105/A200905105.fits

Energy 853.2 Col Num 16 Col Step 0.25

Spot Size 1.25 Row Num 16 Row Step 0.25

Col Center 515 Row Center 523 Iter Number 1000

Single Energy ☒ Stack Analysis ☐

More

Extra Cfg

View Port

Load .hdr

Start Stop

Show C:/Users/wangj.CORP/Desktop/STXM-data-analysis-webinar-4Dec2020/STXM-Ptychography/Andor-CCD-data/

PyPIE v3.3.0

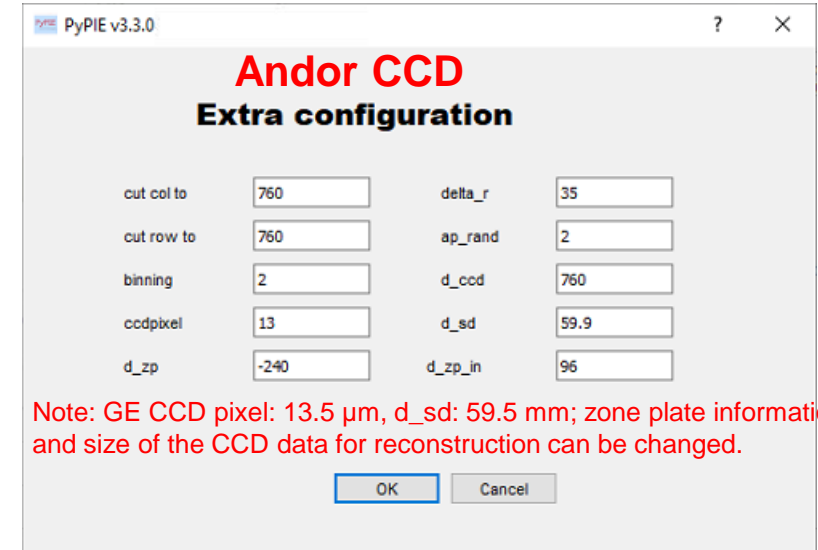
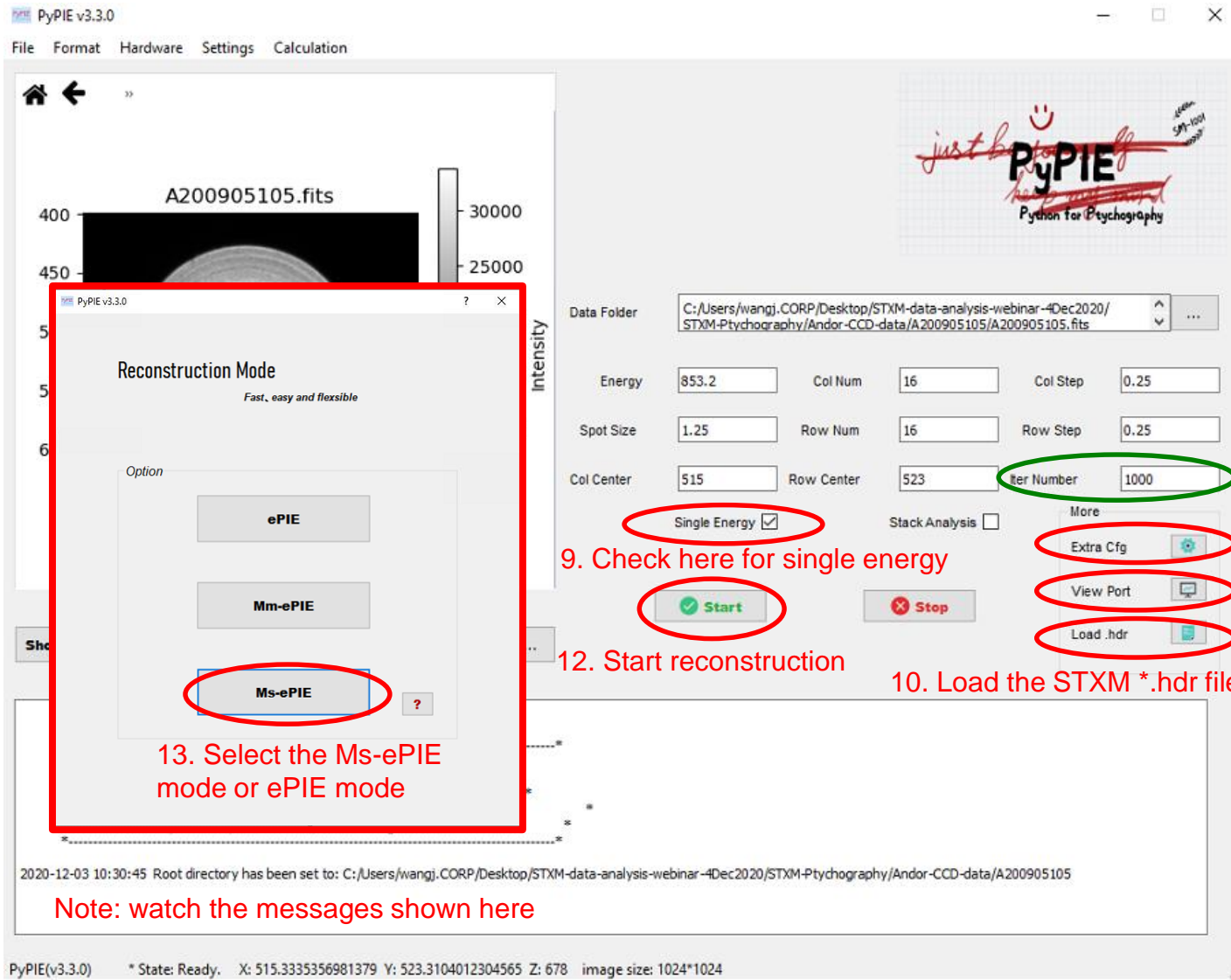
\*State: Ready X: 515.3335356981379 Y: 523.3104012304565 image size: 1024\*1024

2020-12-03 10:30:45 Root directory has been set to: C:/Users/wangj.CORP/Desktop/STXM-data-analysis-webinar-4Dec2020/STXM-Ptychography/Andor-CCD-data/A200905105

Set a root workspace.



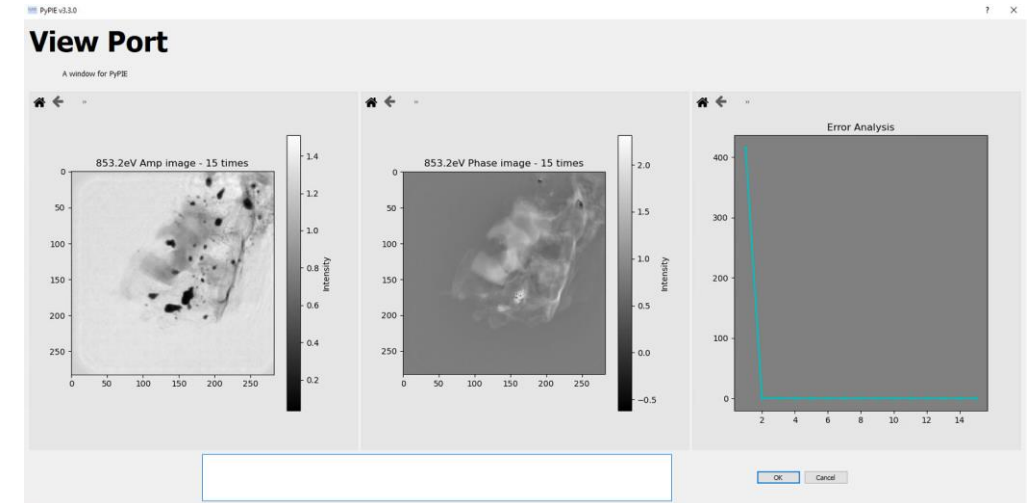
# PyPIE – Single Energy Data Reconstruction



Note: GE CCD pixel: 13.5  $\mu\text{m}$ , d\_sd: 59.5 mm; zone plate information and size of the CCD data for reconstruction can be changed.

11. Check the extra configuration file

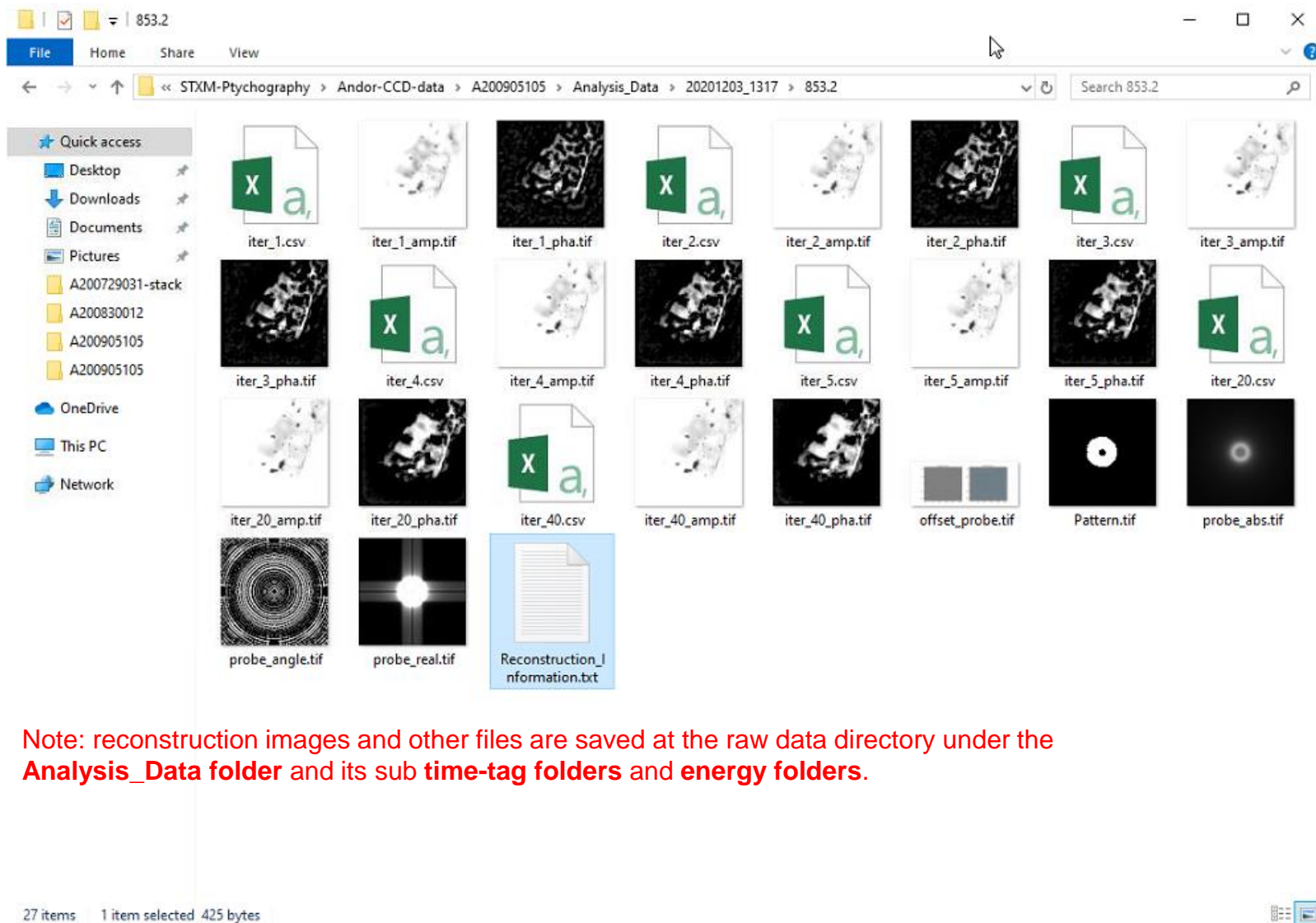
14. Click the View Port to check reconstruction result; reconstruction finishes at the set iteration number, default 1000.



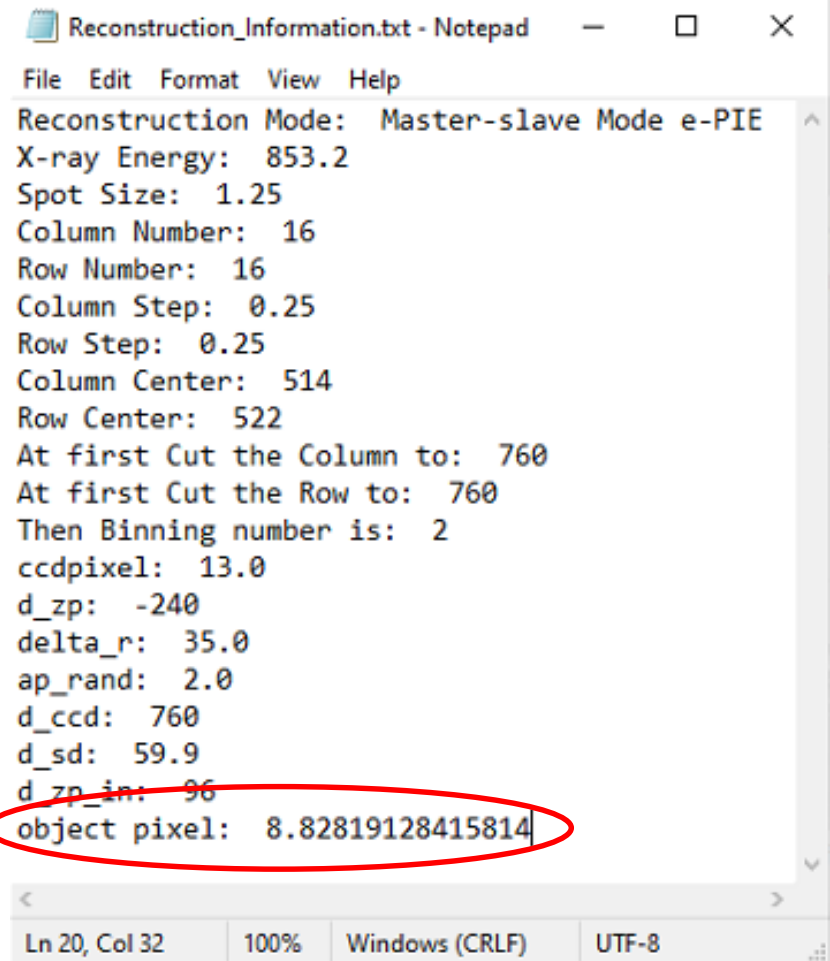
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# PyPIE – Reconstruction Output



Note: reconstruction images and other files are saved at the raw data directory under the **Analysis\_Data** folder and its sub **time-tag** folders and **energy** folders.



Note: object pixel size times total reconstructed pixels in each dimension to produce the actual physical size. But sometimes the object pixel size is half of the actual size due to data binning.



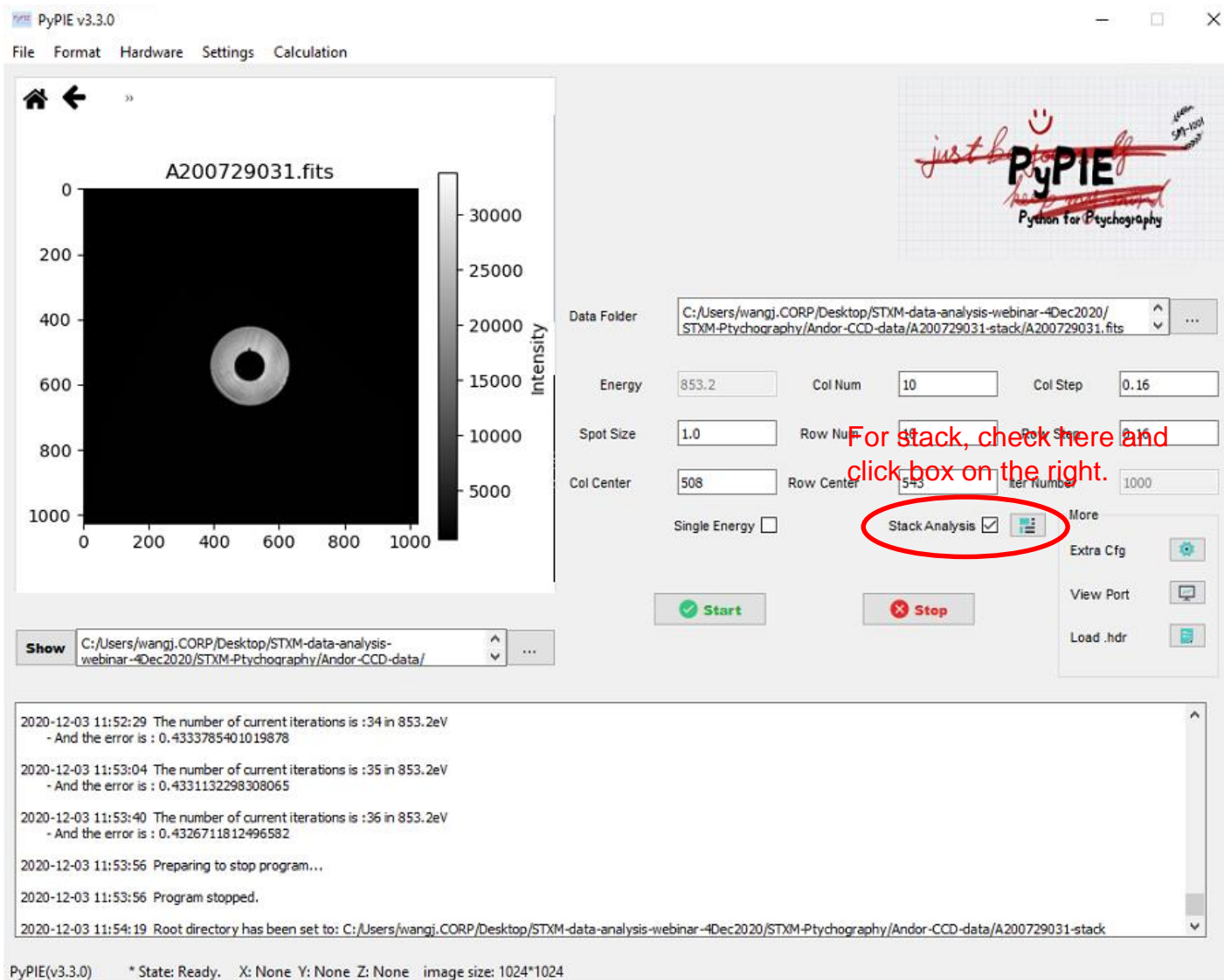
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# PyPIE – Stack Data Reconstruction



The 'Stack Analysis Configurator' dialog box is shown. It includes fields for Start Image (0), Segment (1), Appendix (checked), Files (2), and Total (2). A table displays energy parameters:

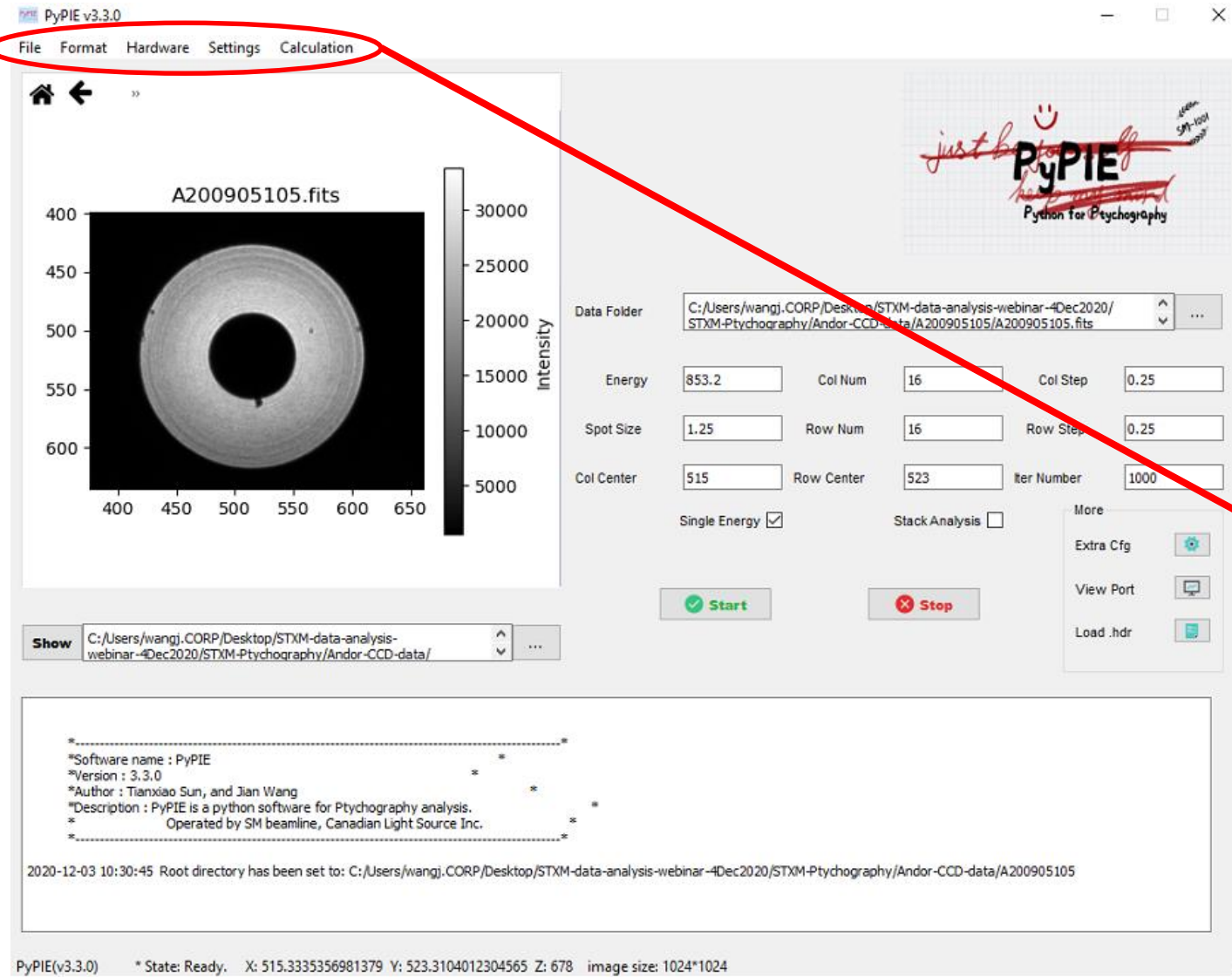
|   | Start Energy(eV) | End Energy(eV) | Energy Step(eV) | Iteration Number |
|---|------------------|----------------|-----------------|------------------|
| 1 | 686              | 696            | 0.5             | 200              |

The 'Iteration Number' field is circled in red. A note in red text states: 'Note: If the energies are evenly distributed, you will see the energy information in the configurator automatically; otherwise, click Load Definition. Finally, you can change the iteration number for a quick analysis or a high-quality reconstruction.' The 'Load Definition' button is also circled in red. The dialog box has 'OK' and 'Cancel' buttons at the bottom.

Note: reconstruction images and other information files are saved at the raw data directory under the **Analysis\_Data** folder and its sub **time-tag** folders and **energy** folders.



# PyPIE – Other Useful Functions



## File

|                 |        |
|-----------------|--------|
| Open...         | Ctrl+O |
| Image Viewer    | Ctrl+I |
| Root directory  | Ctrl+\ |
| Reset All       | Alt+`  |
| Reset Root path | Alt+.  |
| Help            | Ctrl+H |
| Exit            | Alt+F4 |

## Format

|                    |        |
|--------------------|--------|
| Convert Fits 2 Tif | Ctrl+3 |
| Convert Tif 2 Fits | Ctrl+4 |
| Convert Tif 2 Tiff | Ctrl+5 |

## Hardware

|               |                  |
|---------------|------------------|
| CCD type      | Andor Camera     |
| CCD customize | Greateyes Camera |

|               |  |
|---------------|--|
| CCD type      |  |
| CCD customize | <ul style="list-style-type: none"> <li>Flipud</li> <li>Fliplr</li> <li>Rot90</li> <li>Rot180</li> <li>Rot270</li> <li>PathX reverse</li> <li>PathY reverse</li> <li>Probe phase reverse</li> </ul> |

## Settings

|                  |  |
|------------------|--|
| Data file format | <ul style="list-style-type: none"> <li>Reconstruct in Fits</li> <li>Reconstruct in Tiff</li> </ul> |
|------------------|--|

## Calculation

|                  |        |
|------------------|--------|
| Image Calculator | Ctrl+A |
|------------------|--------|

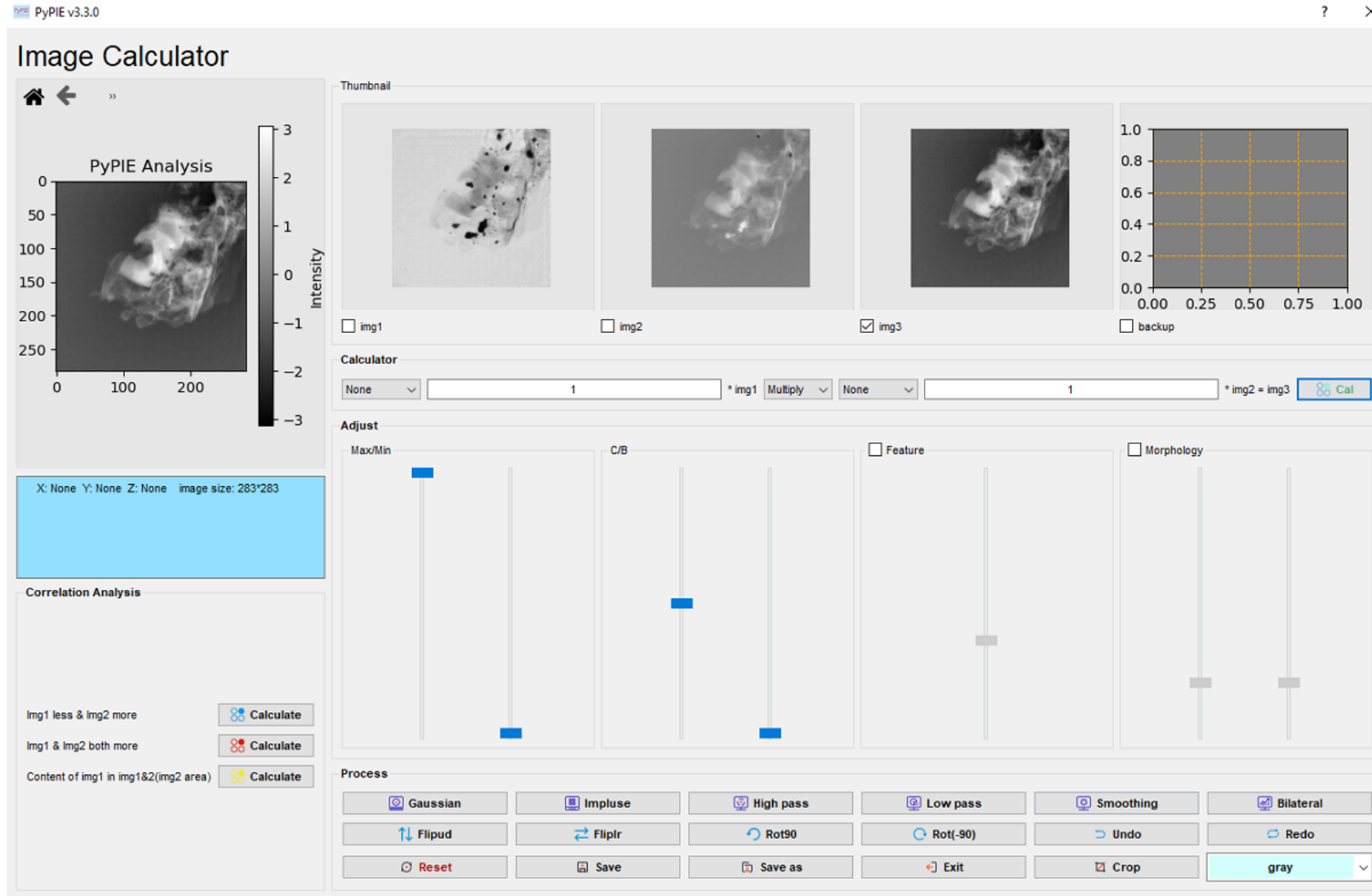


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# PyPIE – Other Useful Functions



# aXis2000 – Generating Ptycho Stacks

Convert a set of tif files to a stack starting from ptycho images reconstructed by PyPIE or SHARP (extracted from the \*.cgi file using e.g. recon\_result\_grey.py, on CLS-SM-ptycho workstation)

1. Read ~ Images ~ Graphics ~ tiff ~ data

(aXis2000~Zoom, Numerical cut)

2. Images~set xy scale

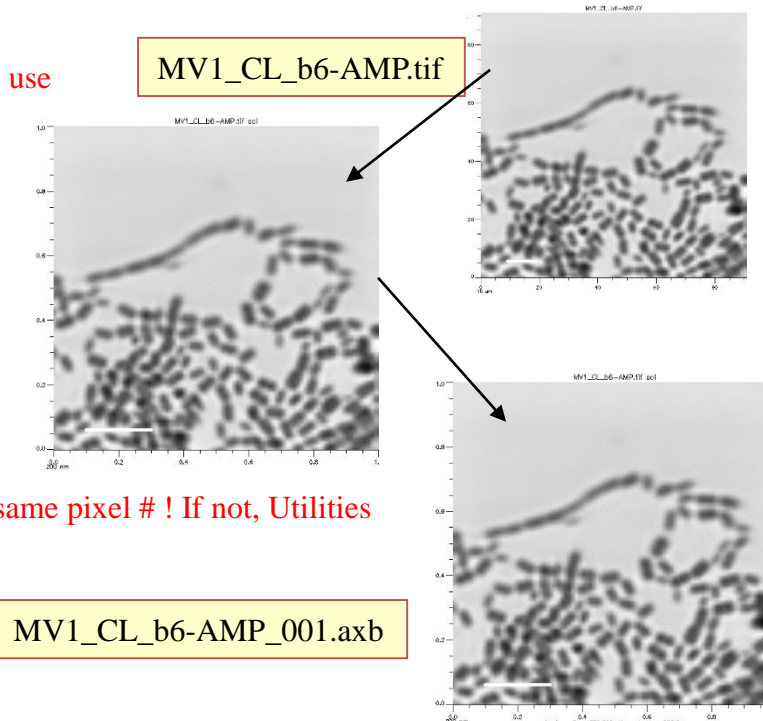
(Use Images ~ Modify X,Y aXes, use object pixel to scale to the image default pixel size of 1 $\mu$ m/pixel)

3. Utilities ~ change energy

4. Utilities ~ change dwell

Make sure all images have the same pixel # ! If not, Utilities ~ Change mesh

5 Write~axis



6. Do the above for each tif file in the stack

7. Prepare a \*.sl (stack list file)

8. Stacks ~ Analyze ~ stack list input

9. Write out as a stack (\*.dat, \*.ncb)

10. Process as required (alignment, convert to OD, etc, etc)

```
E:\data\XRM\Soleil\2019\19-06\06-17\30\  
SS30_1.axb  
SS30_2.axb  
SS30_3.axb  
SS30_4.axb  
SS30_5.axb  
SS30_6.axb  
SS30_7.axb  
SS30_8.axb  
SS30_9.axb  
SS30_10.axb  
SS30_11.axb
```



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