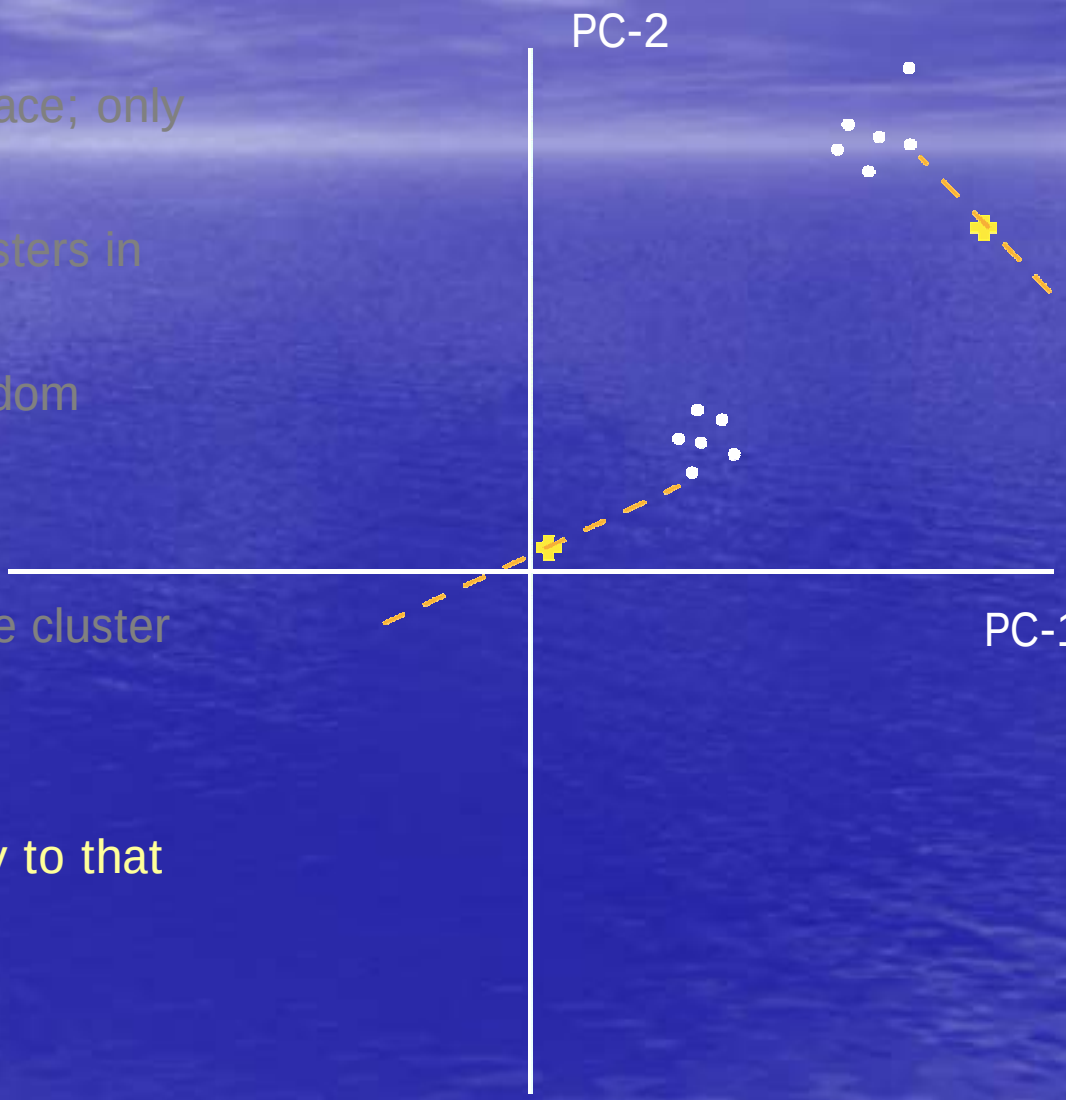
Slide courtesy of
Chris Jacobsen
SUNY Stony Brook

Cluster analysis: Euclidian distance learning algorithm

- Data are in multidimensional space; only 2 dimensions shown here.
- Ideally data are arranged in clusters in this space!
- Put down cluster centers at random positions.
- Iterate:
  - Calculate distances from one cluster center to all data points.
  - Pick shortest distance.
  - Move cluster center partway to that nearest point.



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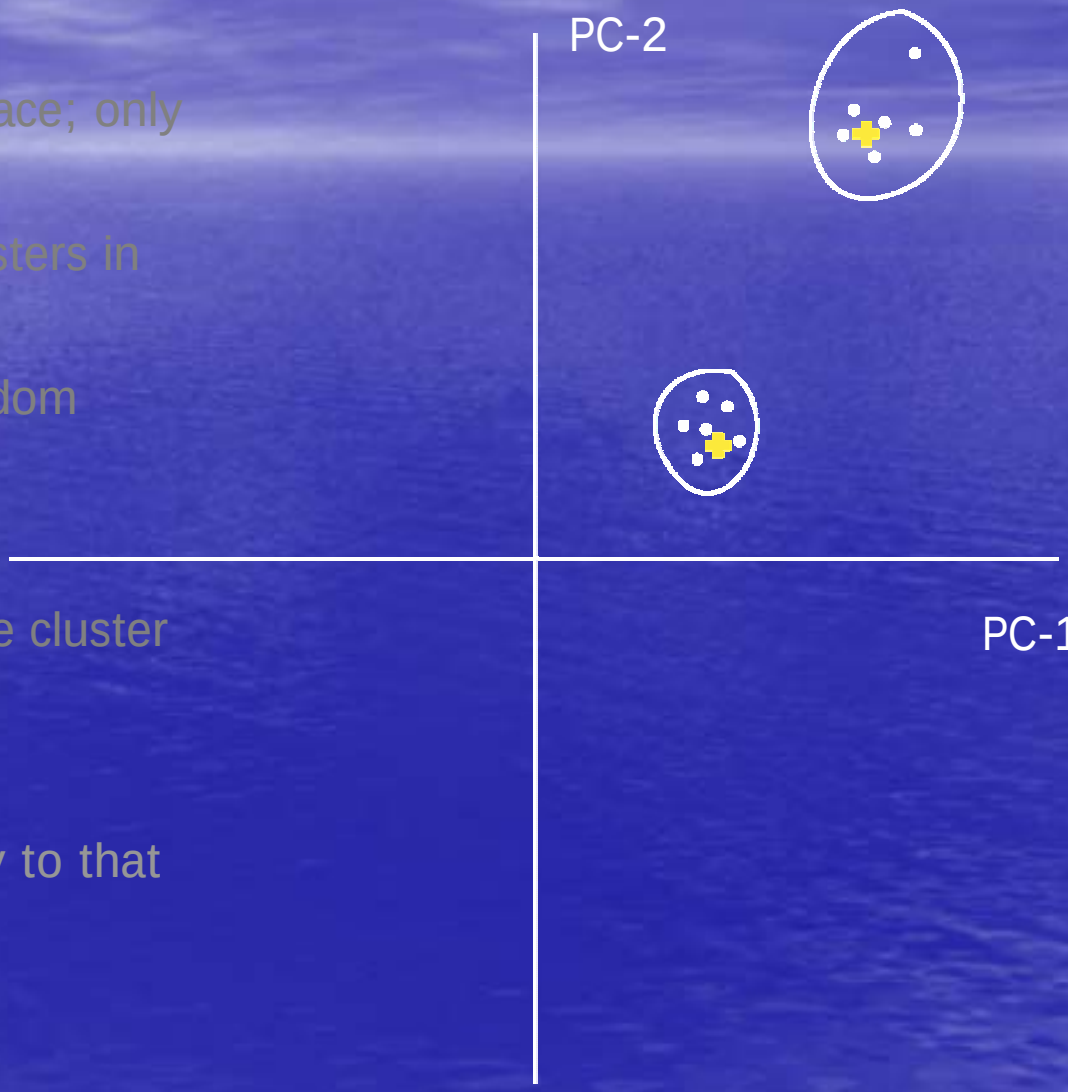
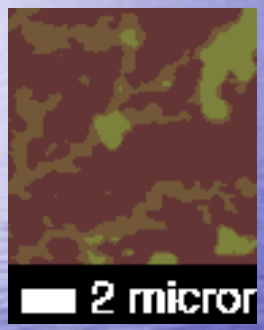
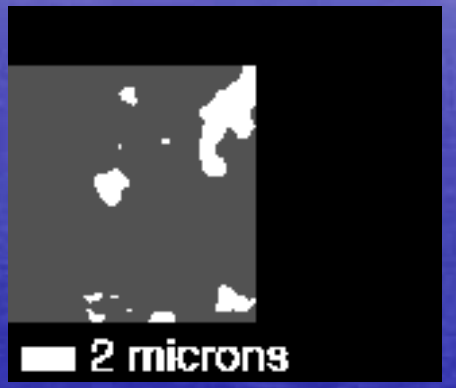


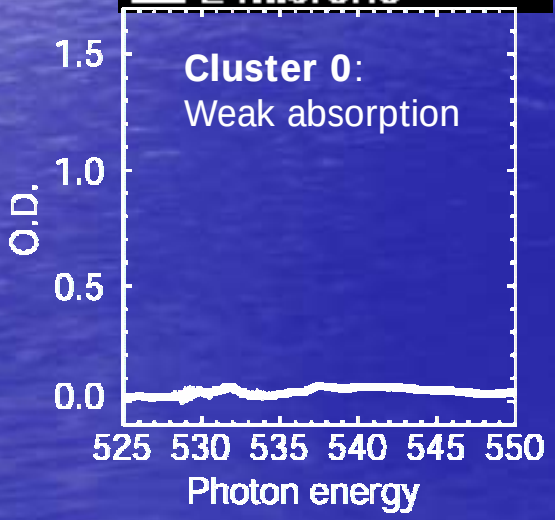
Slide courtesy of
Chris Jacobsen
SUNY Stony Brook

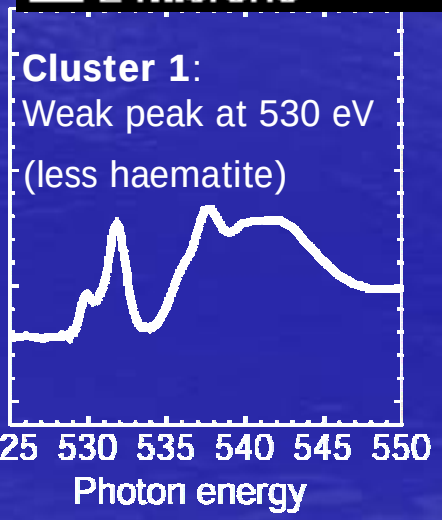
Lu/Haematite structural incorporation

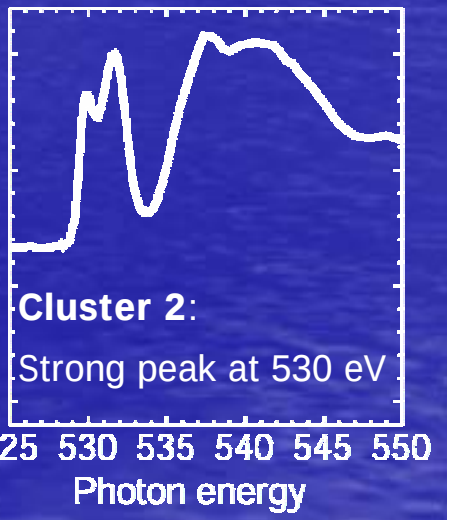
- *T. Schäfer*, INE Karlsruhe
- Lu as homologue for Am, Cm
- 5% Lu in Haematite: transformation in solution, rinsed, dried
- Cluster analysis of O 1s stack ➡ Lu incorporation in Haematite.







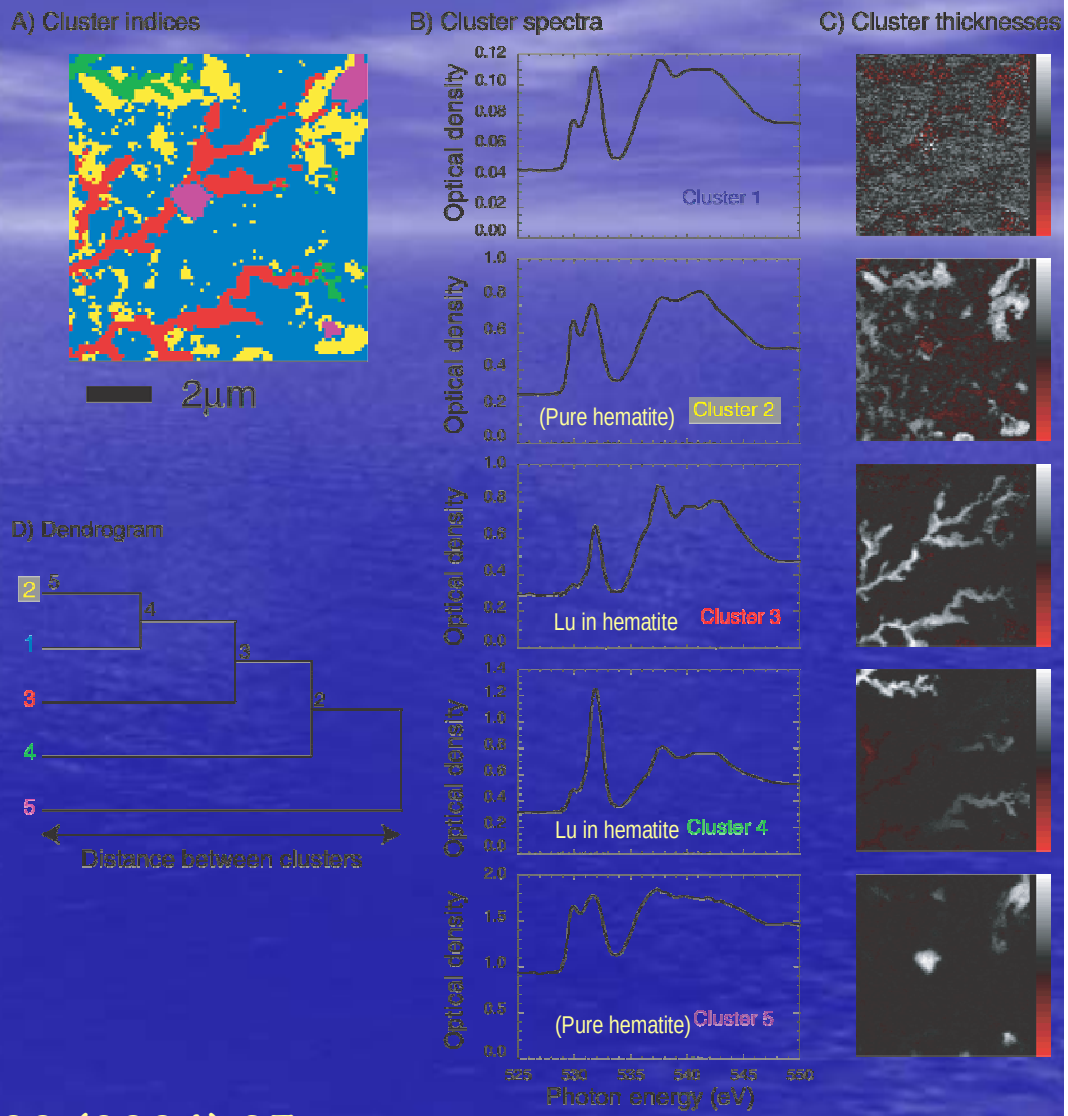




Slide courtesy of
Chris Jacobsen
SUNY Stony Brook

Cluster analysis of spectromicroscopy data

- Study of Lu (stand-in for Am) incorporation in hematite (groundwater transport). T. Schäfer *et al.*, INE Karlsruhe
- Oxygen near-edge spectra: molecular orbital availability, occupancy. Acquire ~150 images across edge.
- Cluster analysis: reveals spectroscopic themes even with a complex, unknown specimen.

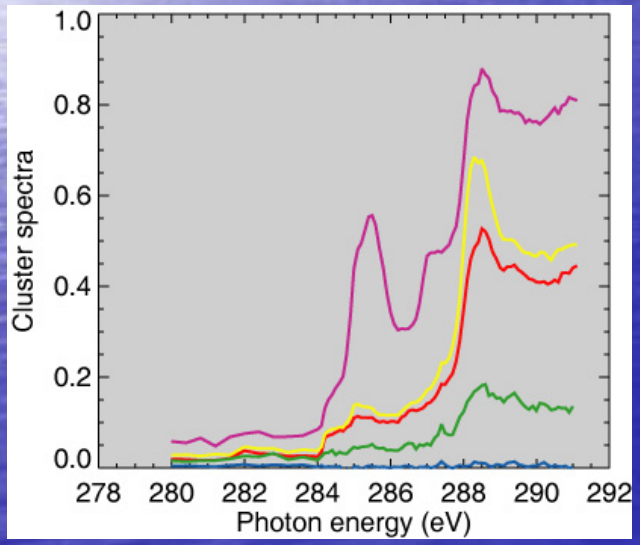


M. Lerotic *et al.*, *Ultramicroscopy* 100 (2004) 35

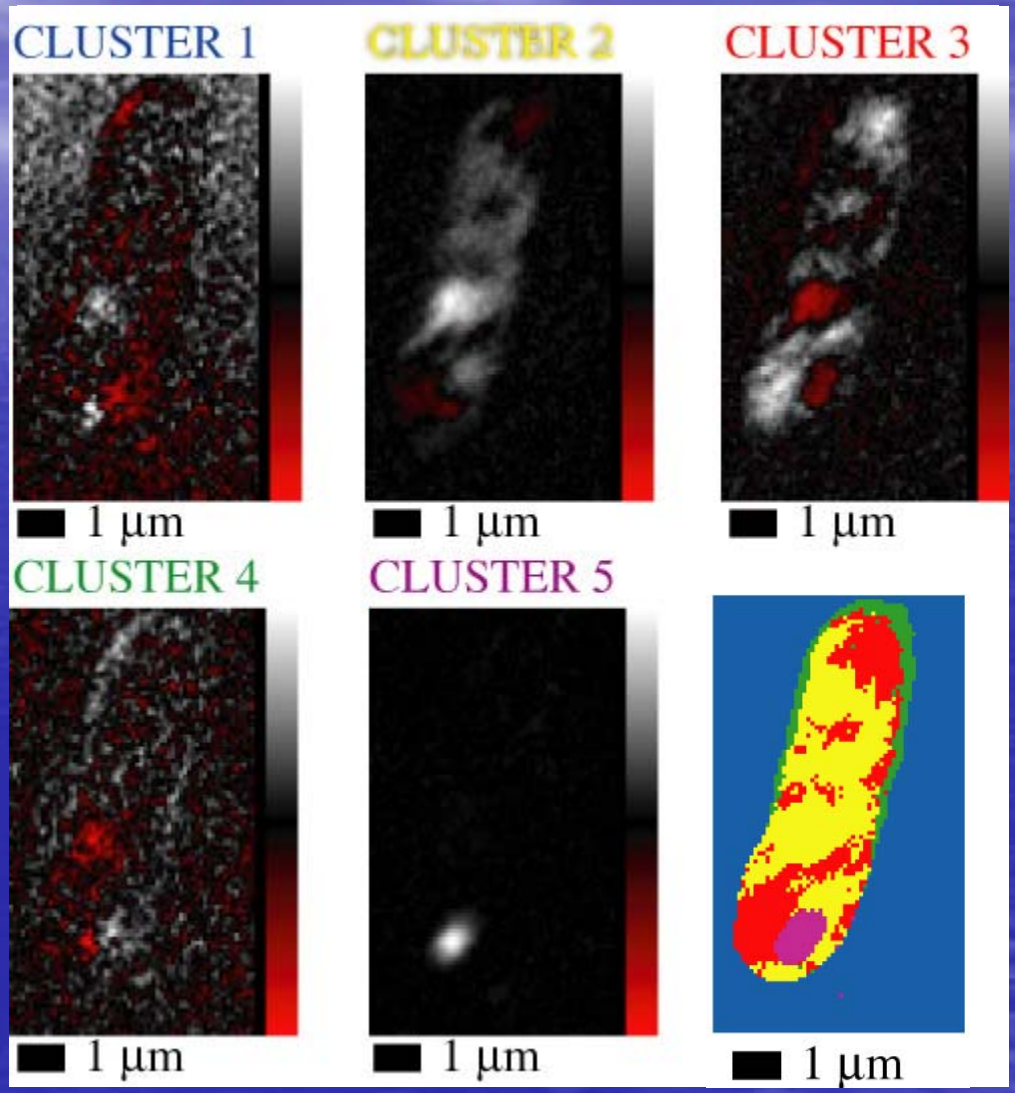
Slide courtesy of
Chris Jacobsen
SUNY Stony Brook

Angle metric improves classification

- Problem: Euclidean clustering confuses composition and thickness information
- Recent advances: use **angle distance measure** to classify based on compositional variations only (insensitive to thickness)
- **Specimen: a spore in a uranium-reducing bacterium (J. Gillow, A.J. Francis, BNL)**
- Use PCA and angle metric clustering to find representative spectra



- SVD with these internal spectra used to derive thickness mapds

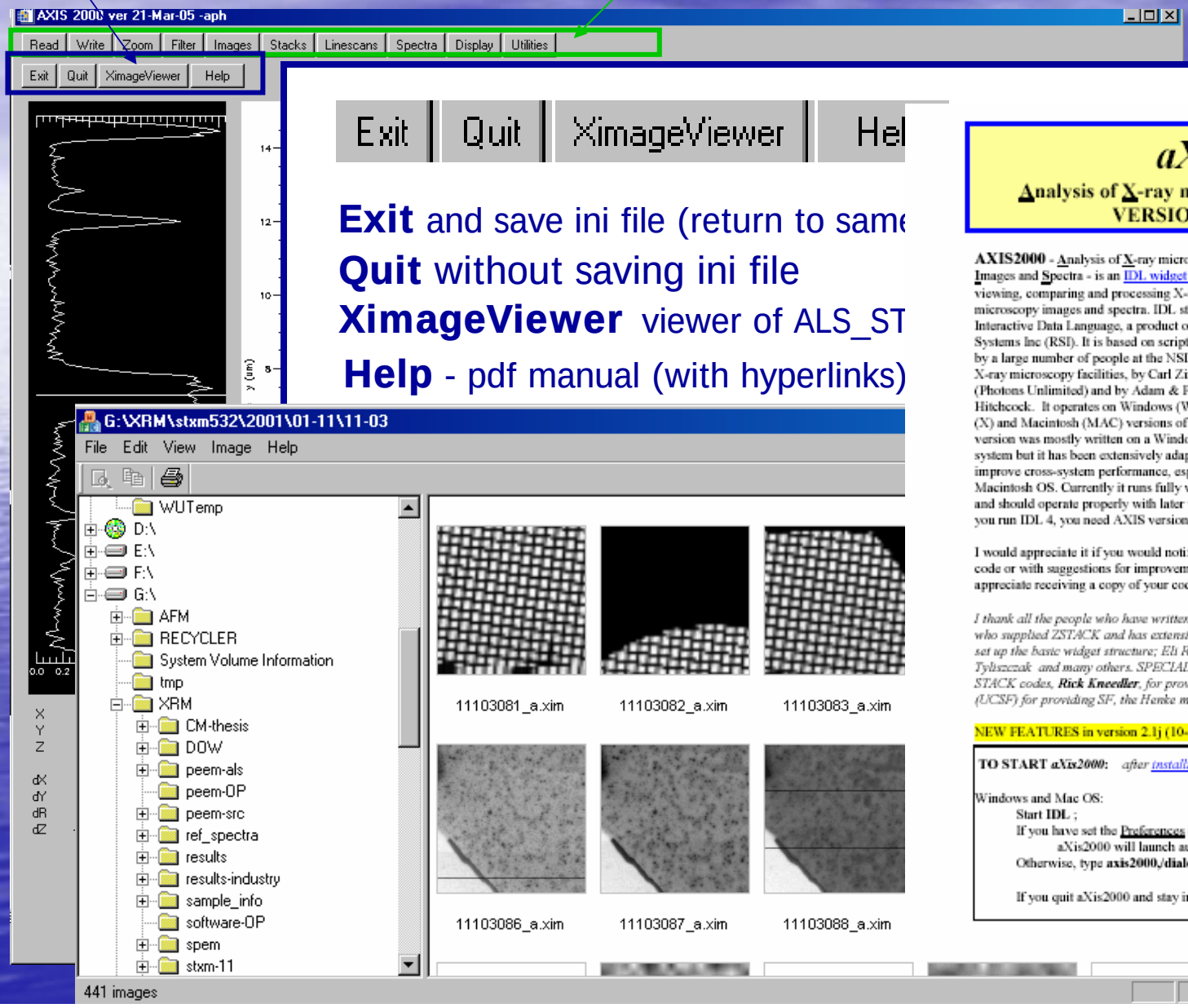


Details: **M. Lerotic** and C. Jacobsen, J .Electron Spectrosc.144 (2005) 1137

Features of aXis2000 widget (1)

single action menus

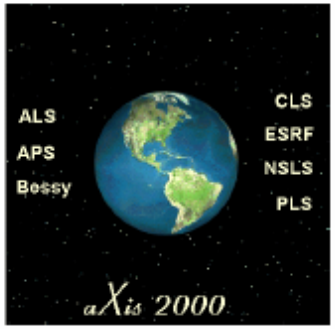
Pull-down menus



aXis 2000

Analysis of X-ray microscopy Images and Spectra
VERSION 2.1k (12-May-02)

AXIS2000 - Analysis of X-ray microscopy Images and Spectra - is an IDL widget for viewing, comparing and processing X-ray microscopy images and spectra. IDL stands for Interactive Data Language, a product of Research Systems Inc (RSI). It is based on scripts developed by a large number of people at the NSLS and ALS X-ray microscopy facilities, by Carl Zimba (Photons Unlimited) and by Adam & Peter Hitchcock. It operates on Windows (WIN), Unix (X) and Macintosh (MAC) versions of IDL. This version was mostly written on a Windows-98 system but it has been extensively adapted to improve cross-system performance, especially for Macintosh OS. Currently it runs fully with IDL 5.2 and should operate properly with later versions If you run IDL 4, you need AXIS version 1.6a or earlier.



I would appreciate it if you would notify me by email (aph@mcmaster.ca) about problems with the code or with suggestions for improvements. If you make extensions or corrections, I would appreciate receiving a copy of your code revisions to 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 has extensively improved the package overall; my son, **Peter** who helped set up the basic widget structure; Eli Rotenberg, Jonathan Denlinger, Stefano Cerasari, Tolek Tyliszczak and many others. SPECIAL thanks to **Chris Jacobsen** (Stony Brook, nsls) for sharing his STACK codes, **Rick Kneedler**, for providing the basis for the **stack-fit** routine, and **Billy Loo** (UCSF) for providing SF, the Henke mass absorption routine.*

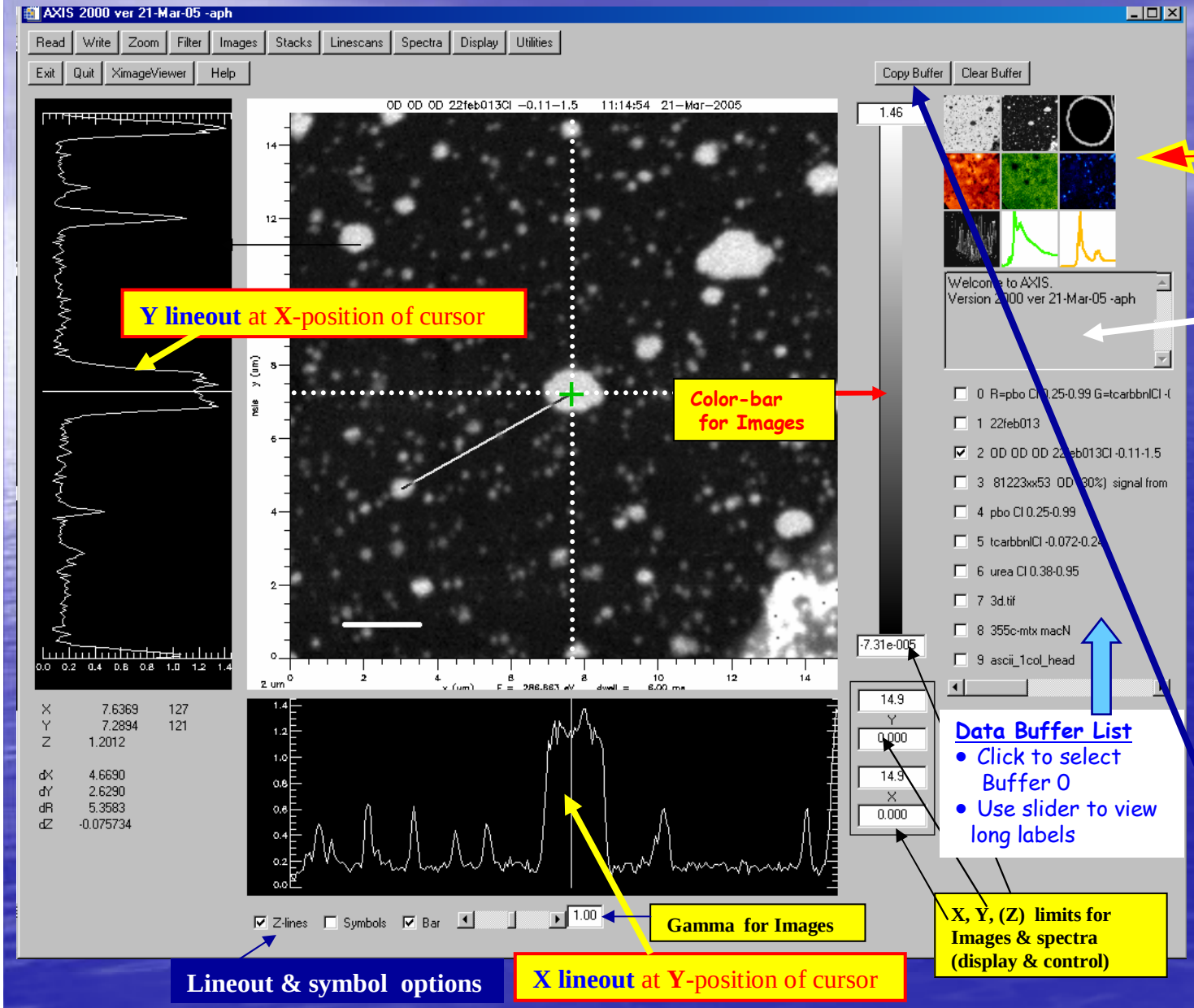
NEW FEATURES in version 2.1j (10-may-02) since 2.1j (28-Feb-02) are HIGHLIGHTED

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,/dialog** on the IDL command line.

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

Features of aXis2000 widget (1)



Concept

9 'permanent' data buffers

any process that modifies data places the result in buffer 0 (the 'working' buffer)

if you want to SAVE that result you must Copy it to a permanent buffer

Features of aXis2000 widget (2)

Main Image

- Displays currently selected image or selected spectrum (or groups of either 4 or 9 buffers, if Display~Thumbnails used)
- Size of AXIS can be adjusted from **0.5 to 2.0** of its nominal size (360x360 pixels in Main Image) by size parameter in **axis.ini**

Mouse

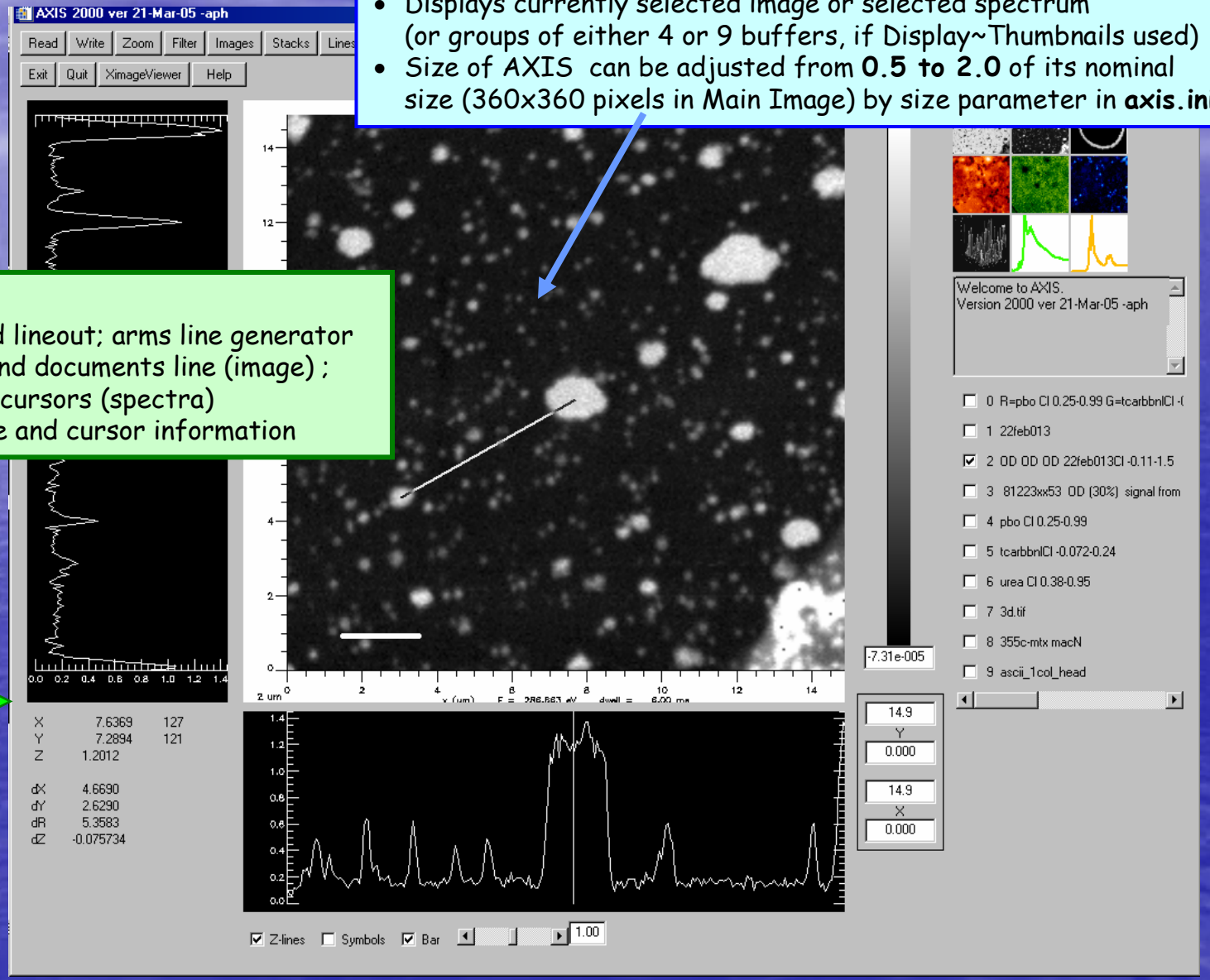
- First click – cursor and lineout; arms line generator
- Second click – draws and documents line (image) ; - reports difference in cursors (spectra)
- Third click – clears line and cursor information

Cursors

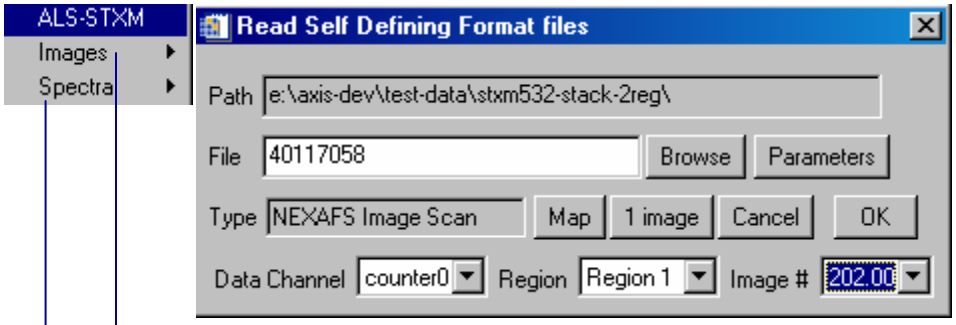
(X,Y,Z) – at cursor pixel indices

(dX,dY,dZ) – change over line (images) or between cursors (spectra)

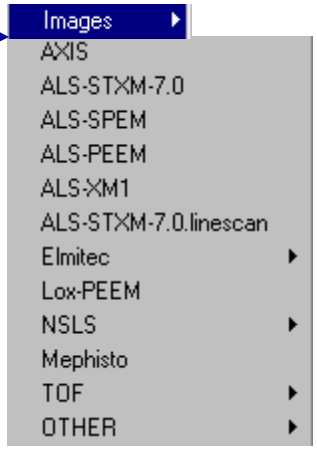
dR – distance along line (images only)



Pull-down menus (1 of 6)

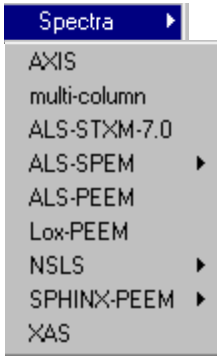


reads all types of ALS STXM files
(images, spectra, stacks, motors, DAQ …)



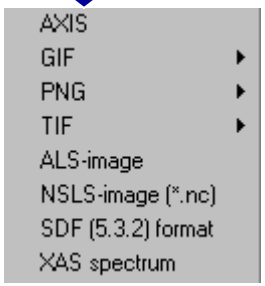
reads image data of many other types of X-ray microscopes
- Axis - internal format
- ALS - PEEM, SPEM, XM1
- SRC - PEEM (Sphinx, Mephisto)
- CLS, SLS, SRC - Elmitec
- CLS - TOF (time-of-flight)

and standard image types
(BMP, PNG, GIF, TIF)



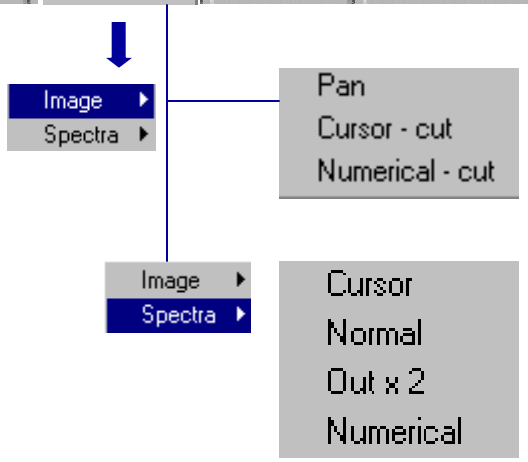
reads many other types of spectral data
- Axis - internal format
- ALS - PEEM, SPEM
- SRC - PEEM (Sphinx, Mephisto)
- CLS - Lox (acq. program for Elmitec)
- CLS - TOF (time-of-flight)
- NSLS - STXM

Pull-down menus (2 of 6)



writes various types of data files

- Axis - internal format (spectra = ascii; images = binary)
- GIF, PNC, TIF - standard image formats
- ALS-image - old (77.0.1) format
- NSLS-image - old and current formats for X1a STXM
- SDF - self defining format used for ALS STXM
- XAS spectrum - fully documentable spectral file (for reference standards)



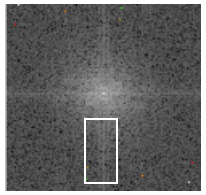
expanded views of currently displayed buffer

Numerical option allows precision extraction of identical regions of images or spectra

Pull-down menus (3 of 6)

- Smooth
- Median
- Lee Filter
- Convol
- Clean (FT image filter)

4 different smoothing routines with adjustable parameters
(apply to both images and spectra)

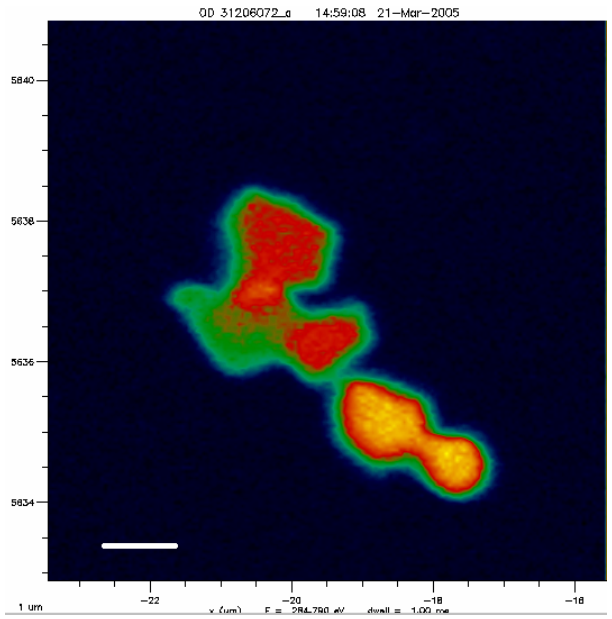


box used to identify signals in 2d FT to be removed. Systematic noise is generally sharp lines)

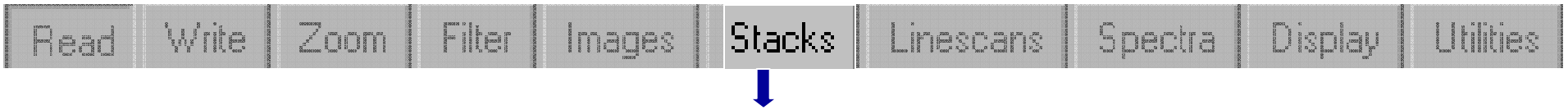
many procedures useful to manipulate images

see manual (accessed by **Help** command in aXis2000) for details

- Add
- Average pixels
- Calibrate XY
- Clip signal
- Convert_to_OD
- Cross-link density
- Deglitch
- Delete region
- Distort XY scale
- exp(Z)
- Fix rollover
- Gain
- histogram
- ln(Z)
- log10(Z)
- generate mask
- Modify one point
- Multiply buffers
- Particle analyze
- Pixels only
- Profiles
- Ratio to
- Remove zeros
- Replace line
- Resize
- RGB composite
- Rotate
- Set XY scale
- Warp

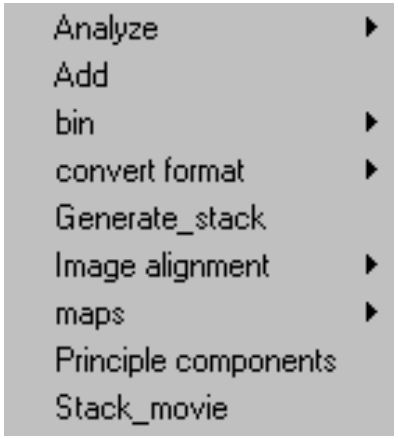


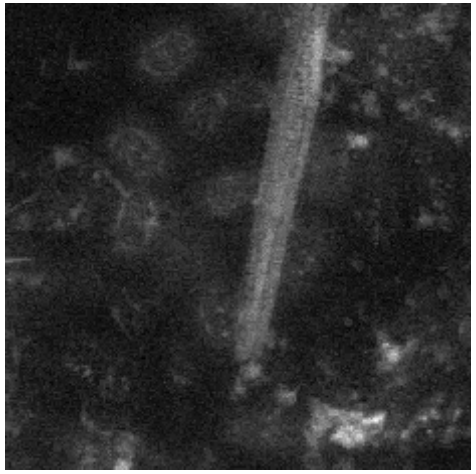
Pull-down menus (4 of 6)

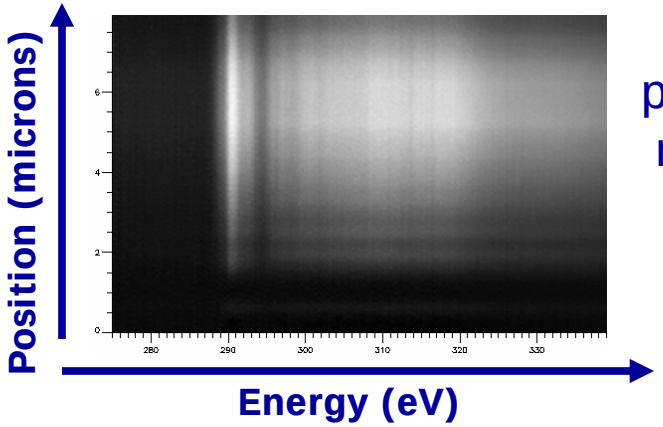


manipulation of image sequences ("STACKS")

see Help file in aXis2000 for details

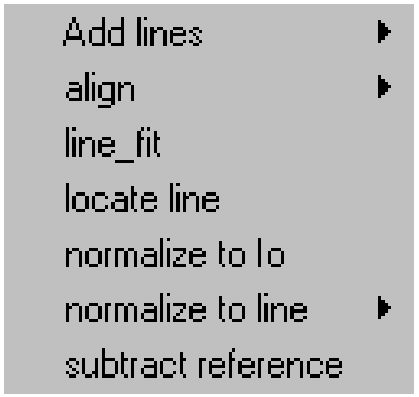




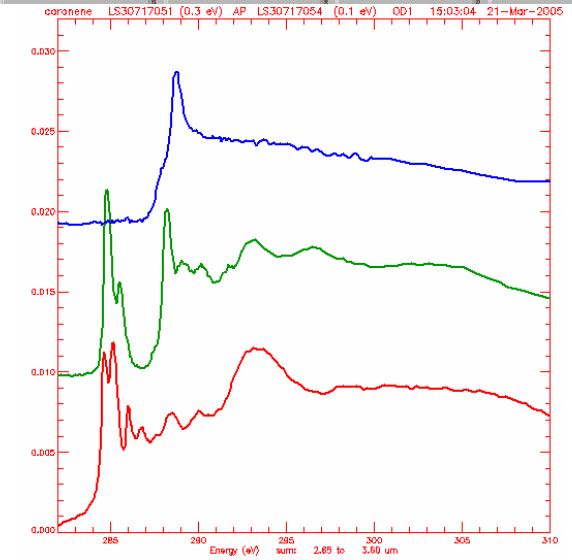


procedures useful to manipulate linescan spectra

see Help file in aXis2000 for details



Pull-down menus (5 of 6)



manipulation of spectra

see Help file in aXis2000 for details

- Absolute value
- Add ▸
- Calibrate ▸
- Curve fit ▸
- Delete
- Differentiate
- Gain ▸
- E_to_Wavelength
- exp(Y)

- Integrate
- ln(Y)
- log10(Y)
- Linear Background
- Modify one point
- Multiply
- Peak area
- Ratio_to
- Reverse values
- Split
- Truncate

Utilities

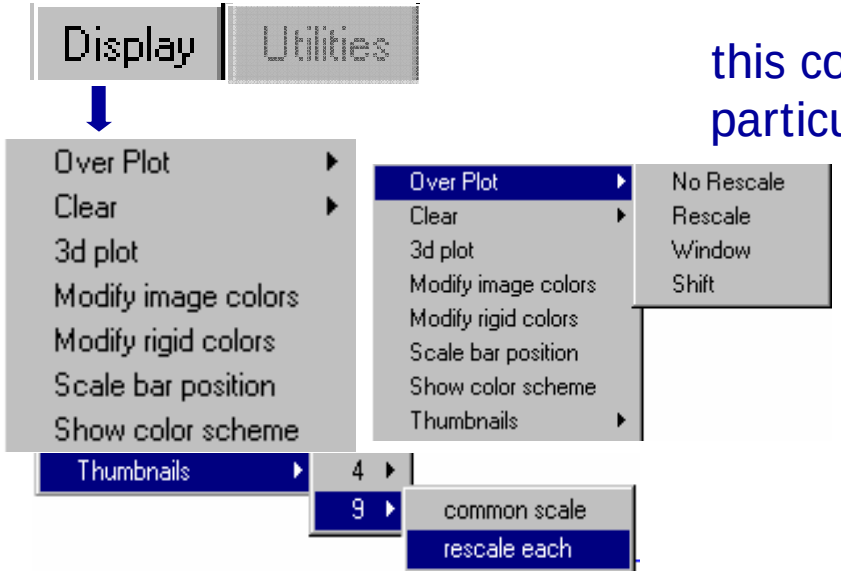
- Print ▸
  - Logbook
  - Annotated
- Change label

miscellaneous procedures

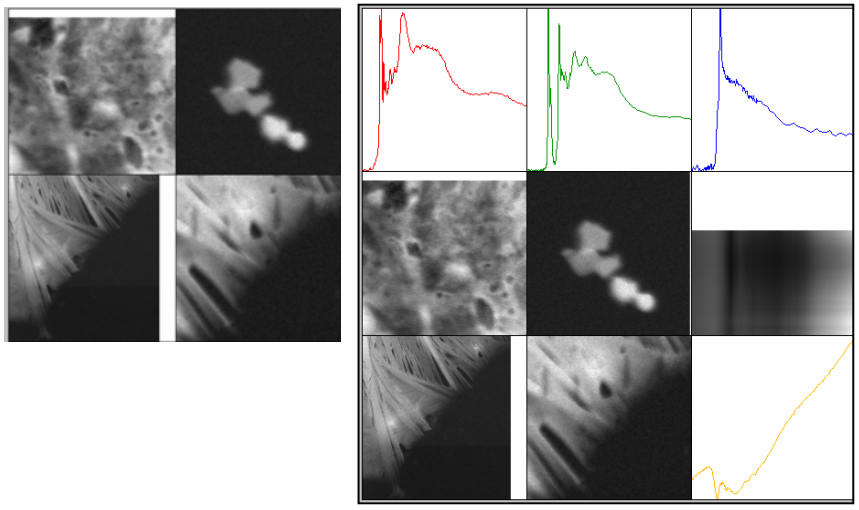
see Help file in aXis2000 for details (modify rigid colors does not yet work)

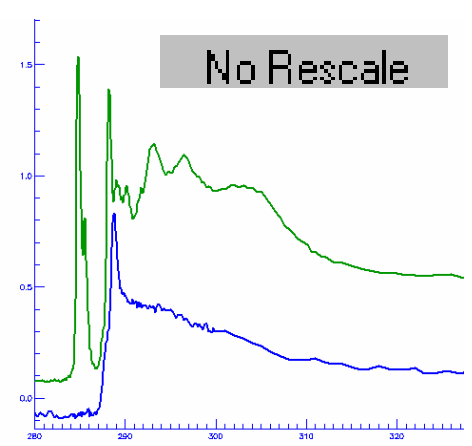
- Print ▸
- Change label
- Change mesh
- Calculate X-ray parameters (SF)
- Execute macro
- Set energy
- Set preferences
- Print SysVar
- Write image ascii ▸

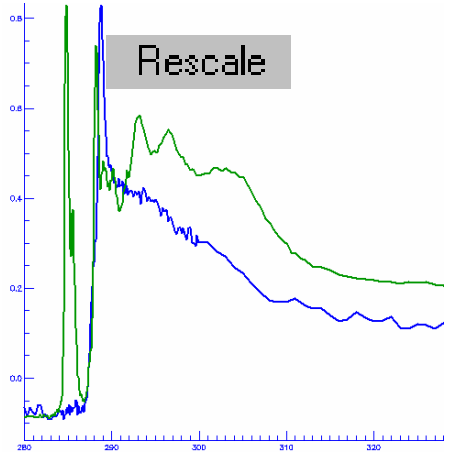
Pull-down menus (6 of 6)

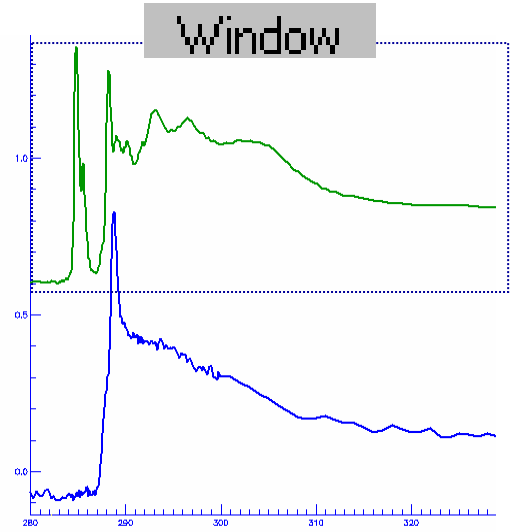


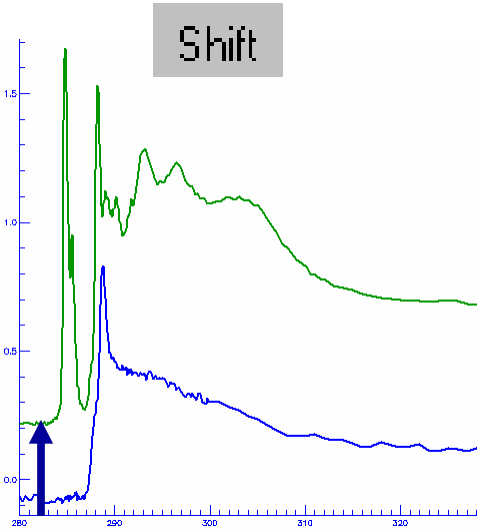
this command menu is used EXTENSIVELY, particularly **OverPlot** and **Thumbnails**











Discussion of possible applications of STXM or X-PEEM