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The MicroAnalysis Toolkit: X-ray Fluorescence Image Processing Software

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Abstract. The MicroAnalysis Toolkit is an analysis suite designed for the processing of x-ray fluorescence microprobe data. The program contains a wide variety of analysis tools, including image maps, correlation plots, simple image math, image filtering, multiple energy image fitting, semi-quantitative elemental analysis, x-ray fluorescence spectrum analysis, principle component analysis, and tomographic reconstructions. To be as widely useful as possible, data formats from many synchrotron sources can be read by the program with more formats available by request. An overview of the most common features will be presented.

Keywords: X-ray fluorescence, analysis, software
PACS: 07.85.Tt, 87.59.-e, 07.05.Kf, 07.05.Rm

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INTRODUCTION

The MicroAnalysis Toolkit was designed and written at the Stanford Synchrotron Radiation Lightsource to handle data processing and analysis from the x-ray fluorescence (XRF) imaging beamlines. It originally was written to take the place of a small suite of scripts that had been used to visualize data, but was unfortunately not flexible enough for user operations. The Toolkit covers basic data visualization and analysis, math operations, dead-time corrections, complex processing, integration and fitting of raw x-ray fluorescence data, chemical speciation mapping analysis, semi-quantitative concentration analysis, and tomography analysis. It is ever expanding to meet user needs and keep pace with experimental progress and data analysis needs. The MicroAnalysis Toolkit is written in Python and makes use of the Python Imaging Library (PIL).

While designed specifically for SSRL data sets and to dovetail with SSRL XAS data collection in many ways, the Toolkit has grown to utilize other data formats. This is important, since many synchrotron imaging users collect data at multiple beamlines from multiple synchrotrons. The MicroAnalysis Toolkit reads data files from an ever-expanding number of data formats, which are listed on the software website: http://microtoolkit.sams-xrays.com. Although other microprobe data viewers and data processors exist in the scientific community (see PyMCA [1] MAPS [2], aXis200 [3], and GeoPIXIE [4] as excellent examples), the MicroAnalysis Toolkit combines many of the disparate features provided by these programs into a single data processing program, as well as attempts to support a wide variety of data file formats. While not an exhaustive review of the program features, many of the common features of the Toolkit are presented herein.

USER INTERFACE

The main graphical user interface (Figure 1(a)) displays a list of data channels in the file and opens a display window (Figure 1(b)) that shows the selected data channel with options such as scale bars, edge scales, points of interest, and other features. Common processing options are displayed as easy-to-access buttons, whereas other detailed processing and analysis routines are accessed from the menu bar. Directions for many of the keyboard shortcuts can be accessed from the "Help" menu. These include mouse-over display options for zooming, creating and fitting of arbitrary line profiles, and choosing regions of interest for examining the raw fluorescence spectrum.

In the correlation plotting interface (Figure 1(c)), any two columns can be plotted against each other. Display color can be toggled between light and dark so that it can be easily read on the screen or will minimize print in hardcopy. A particular correlation can be selected on the display by circling the region of interest. The region can

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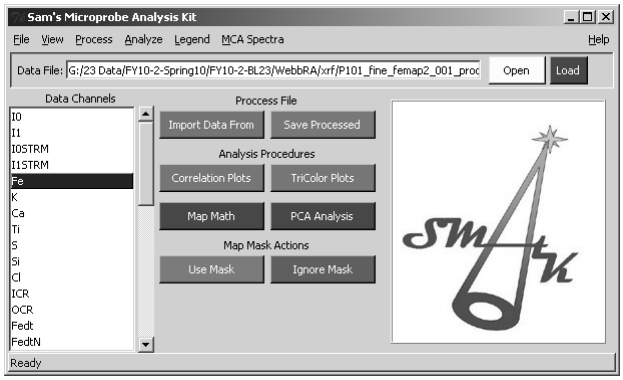
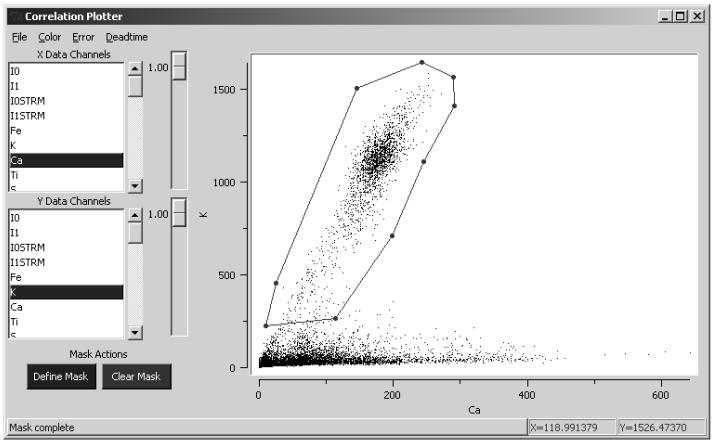
then be masked on the image display to only show the areas of the map where the selected correlation exists. One particular use of the correlation plotter is to calculate the detector dead time. By plotting incoming vs outgoing fluorescence counts, the detector dead time can be fitted in the correlation plotter and corrected for the rest of the analysis. Tri-color mapping plots can also be created for visualization of co-localization of different elements. A simple interface allows the user to select the elements of interest to plot. A legend of the color distribution can also be created. All of the plotting interfaces (the main display, tricolor display, and correlation display) have linked areas, so that if the image on the main display is zoomed, then the correlations and tricolor displays will automatically update to only show the zoomed region.

(a)



(b)



(c)

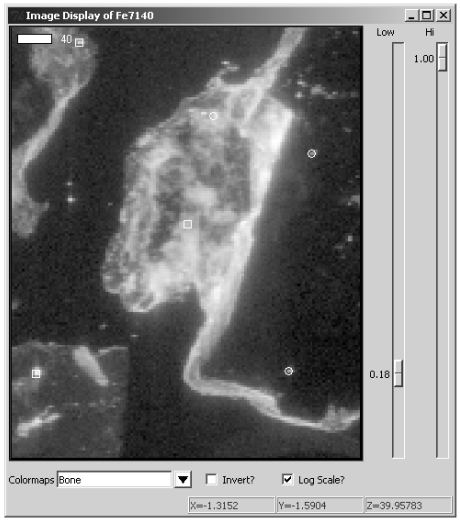


FIGURE 1. (a) Main graphical user interface window for the MicroAnalysis Toolkit. (b) The main display panel for data images. (c) Interface for the data correlation plotter.

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The display interface also can load summary data files from other SSRL data collectors, such as x-ray absorption spectroscopy (XAS) and x-ray diffraction data (XRD) queues. The information from these files (i.e., the position of a series of independent XAS and XRD data points) can be loaded directly into the MicroAnalysis Toolkit and their locations overlaid onto the image map as circles, squares, other shapes, or text. Markers are displayed at their positions at any zoom level. Positions for data markers can also be directly selected from the image map or by manual input. Data labels can be turned on/off for easy selection. The labels and label formatting are stored separately from the data file

PROCESSING

Image processing is an important part of XRF data analysis. Basic thresholding operations can be done on the image pane directly or through menu items. The MicroAnalysis Toolkit supports pixel shifting (for offset rows), image shifting (image registration), stitching (assembling multiple datasets together), and applying I_0 normalization and detector dead-time corrections. All processing operations save the processed data in a separate channel so that the original data set need not be altered. Math manipulation on channels of data can be easily performed through the "Map math" option. Operations can be previewed or saved as a new data channel in the file. Math operations include: addition, subtraction, multiplication, division, dead-time correction, logarithms and exponentials, smoothing and sharpening, derivatives, square roots, and horizontal and vertical pixel shifts.

One of the most important aspects of post processing image information is the examination of the raw fluorescence spectrum of a particular pixel or region of pixels. This is particularly useful when data are collected as a series of regions of interest (ROIs) and confirmation of supporting lines (Kβ, etc.) is needed. Re-examination of the raw data (collected in a separate file to minimize the size of the smallest data file) is easily selected directly from the map image. The user can also step through the entire fluorescence spectrum, integrating small sequential energy regions and displaying the resulting image, to determine if a particular spectral region is important in the sample. A new channel of data can be re-integrated from the raw data if a particular channel/element was forgotten, or not believed to be important at the time of data collection. The raw fluorescence data can also be used to perform principal component analysis (PCA).

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ANALYSIS

Data analysis is at the heart of any measurement, and imaging data contains an extremely large amount of information content. Basic features, some of which are mentioned above in the interface section, include visualizing elemental distributions with false color and multi-channel tricolor maps; examining elemental correlations with the correlation plotter; masking regions of interest; plotting radial, horizontal, vertical, or arbitrary line profiles; creating histograms of data channel count distributions; and moment analysis (spatial and concentration correlations). The MicroAnalysis Toolkit also includes a semi-quantitative elemental analysis calculation. This assists the user in taking data from a standard measurement (i.e., a thin film elemental standard measured at the beamline under the experimental conditions of the sample) and converts the calibration data to form an appropriate conversion scale to concentration units (typically $\mu g\ cm^{-2}$). Future versions of the semi-quantitative analysis calculator will include theoretical conversion factors for different incident x-ray energies, variable path lengths between the sample and the detector, and simple sample matrix effects.

Chemical Speciation Mapping

One core aspect of synchrotron-based x-ray imaging is chemical speciation mapping, also known as XANES (x-ray absorption near edge spectroscopy) imaging. This is accomplished by collecting images of the element of interest at several different incident excitation x-ray energies through its absorption edge. This creates, in essence, a mini-XANES spectrum at every map pixel. This concept has been used extensively in scanning transmission x-ray microscopy with soft x-rays, where image stacks are collected over several excitation x-ray energies. Due to relatively large sample sizes and longer scan times of hard x-ray fluorescence scanning microprobes, the set of excitation x-ray energies is typically smaller, and are chosen to best delineate the expected species of the element of interest. Fitting of these image stacks can be performed by doing a linear-least squares fit of the data to a collection of standard spectra in the image XANES fitting routine.

In this routine, the normalized intensity of the absorption spectra is determined for each of the standards at each of the map energies. The process of obtaining the fitting values will be automated in future versions of the Toolkit. The fit is then performed with the standard compounds matrix and, as a result, the composition of each standard is given at each point in the map. As a data collection strategy, one can perform principal component analysis with the MicroAnalysis Toolkit on the image stack to identify regions within the image area where there are major changes in the speciation. This analysis and strategy are performed at the beamline and help avoid a common issue of over collecting spectroscopy at just the most intense areas of the map. Further confirmation of the speciation is typically done experimentally by collecting full XANES spectra at various areas of interest. Typically, with wise data collection strategies, the chemical speciation mapping and fit results from full XANES spectroscopy will agree within 5 percent.

CONCLUSIONS

The MicroAnalysis Toolkit is a useful tool for processing and analysis of x-ray fluorescence microprobe data. The program is continuously under development, and suggestions and comments are welcomed. The MicroAnalysis Toolkit is freely available as open source software on the web at microtoolkit.sams-xrays.com. Web-based documentation will also be coming soon.

ACKNOWLEDGMENTS

Many of the ideas for data visualization, processing, and analysis used by the MicroAnalysis Toolkit were provided by numerous users and members of the imaging community. Without the constant feedback and support of the imaging user community, the progress of the MicroAnalysis Toolkit would never have been realized.

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