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Advanced Spectrum Analysis with Open Source Software

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The Cornell Spectrum Imager (CSI) [1] was developed to make it easier to analyze large spectral datasets in a short manner of time. While commercial software solutions exist, they are often incomplete and locked to a single computer, making it difficult for multiple users to process data. In response to the need for an all-in-one, user-friendly package, CSI is manifested as a plugin for ImageJ, a widely-accepted, open source image-processing tool. Our spectrum analysis suite includes hyperspectral visualization and analysis techniques (Fig.1). In addition, we have developed readers for multidimensional spectral datasets in Gatan `*.dm3` and FEI `*.ser` file formats.

Beyond standard spectrum visualization and analysis techniques [2] we implement several advanced algorithms to significantly improve the processing with a simple click of a button. In particular, by taking advantage of spatial oversampling, we can drastically improve background estimation where traditional fitting methods would fail (Fig. 2). With local background averaging (LBA), by smoothing out the more noise sensitive components of our background fit, we take advantage of the slowly varying nature of backgrounds to counteract their low counts. Secondly, by implementing a linear combination of power laws (LCPL) form for our background we eliminate the possibility of unphysical, divergent backgrounds [3]. Finally with the addition of principal component analysis (PCA), we make it easy to quickly ascertain what parts of the data are varying.

It is our goal with CSI to not only match the current commercial post-acquisition spectrum analysis options but to surpass them. With an open source community constantly advancing the capabilities, it provides an evolving toolset for visualizing and analyzing spectra of all types. The latest and future updates continue to increase its usability and efficiency [4,5].

References

[1] http://code.google.com/p/cornell-spectrum-imager/, Released under Mozilla Public License Version 1.1
[2] R.F. Egerton, *Rep. Prog. Phys.*, **72** (2009) 016502
[3] P. Cueva, et al., *Microsc. and Microanal.*, **18(4)**, (2012), 667
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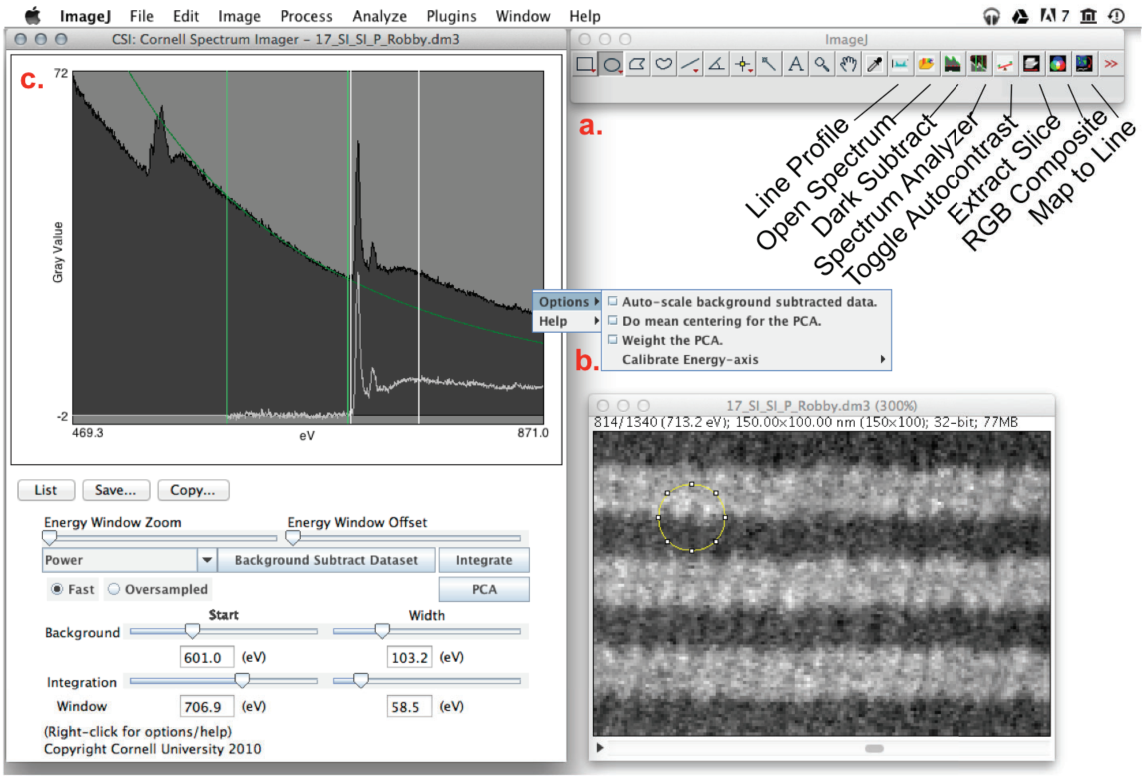

814/1340 (713.2 eV); 150.00x100.00 nm (150x100); 32-bit; 77MB

Background Start 601.0 (eV) Width 103.2 (eV)

Integration Window 706.9 (eV) 58.5 (eV)

(Right-click for options/help)
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Figure 1. Screenshot of the Cornell Spectrum Imager (CSI) software (v1.4) being used to analyze an EELS spectral map. Shortcut icons for manipulating the dataset (a), Spectrum image to be analyzed (b), Spectrum analyzer showing background subtraction (c).

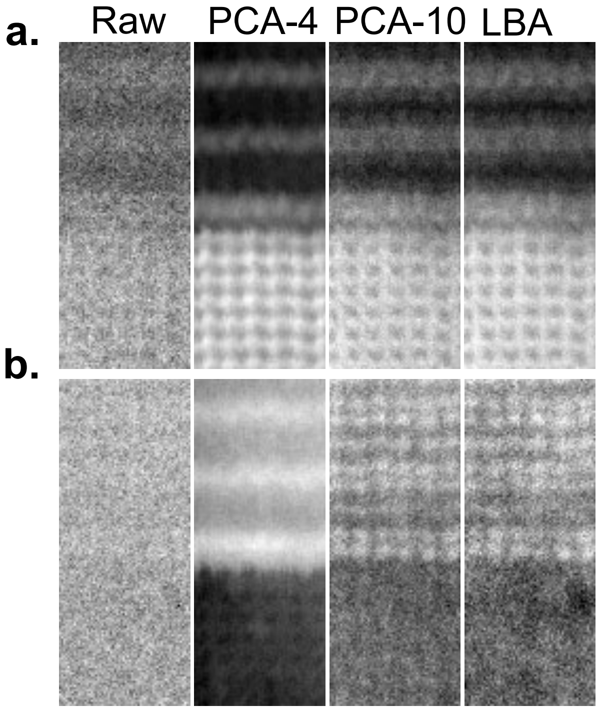

Figure 2. Comparison of noise reduction methods that exploit redundancy in the measured dataset for (a) the power-law-subtracted O-K and (b) Cu-L edges from the YBCO/Manganite interface (Raw) and again simple power law fits after weighted PCA filtering with 4 (PCA4) and 10 (PCA10) components, and finally the raw data after LBA and LCPL is applied instead (LBA). With 4 principal components, the maps do not reflect the physical positions of the atoms, while with 10 components (4 more than suggested by it scree plot), the PCA results comes closer to resembling the more plausible LBA/LCPL result.