





Characterization of Thin Films and Materials and Data Analysis

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More Advanced Features of the Fourier-AI Innovations Software for Denoising Spectra

We discuss various advanced features of the Fourier-AI Innovations denoising software. It is professional software that removes noise from spectra using Fourier methods. Advanced features in the software are accessed through a configuration ('Config') button. These features include the transfer function that is employed, i.e., the Gauss-Hermite or brick-wall transfer function, the cutoff selection algorithm used, how results from different transfer functions can be simultaneously considered, the cell value type for the binary residual map, the axis labels, and a safety factor for denoising. There is also a settings panel, which allows the user to access practice data sets and control the colors throughout the software, e.g., one may choose color-blind friendly colors. The data and plots from the software can be downloaded. Multiple figures in this article illustrate these various features.

Introduction

In our last article in ***Vacuum Technology & Coating***, we introduced the Fourier-AI Innovations denoising software. It is a professional software package that effectively removes noise from data. In this article, we discuss some of the more advanced features of this software.

Conventional methods for reducing the amount of noise in spectra include the boxcar and Savitzky-Golay[1] smooths. We had previously written about the Savitzky-Golay smooths in Vacuum Technology & Coating.[2] Fourier analysis with the discrete Fourier transform (DFT) is also an accepted way for removing noise from data.[3-8] Indeed, it is inherently more powerful than the boxcar and Savitzky-Golay methods.[9] The Fourier approach takes advantage of a powerful way of representing data as frequencies in a 'reciprocal space'. As discussed in our last ***Vacuum Technology & Coating*** article, our approach is based on the convolution theorem in Fourier analysis. Based on this theorem, we multiply the Fourier coefficients of the data in reciprocal space by an S-shaped (sigmoidal) transfer function (the Gauss-Hermite transfer function). This product is then back-transformed to produce the denoised spectrum.[10-12]

We now discuss some of the more advanced features of the Fourier-AI Innovations denoising software.

Advanced Features in the Fourier-AI Software

The Configurations Button and Panel

Most of the more advanced features of the Fourier-AI denoising software are accessed through the configurations ('Config') button in the upper right corner of the main page of the software (see **Figure 1**). **Figure 2** shows the panel that opens up on the right side of the main software page when this button is pressed. We now go through some of the features in this configurations panel.

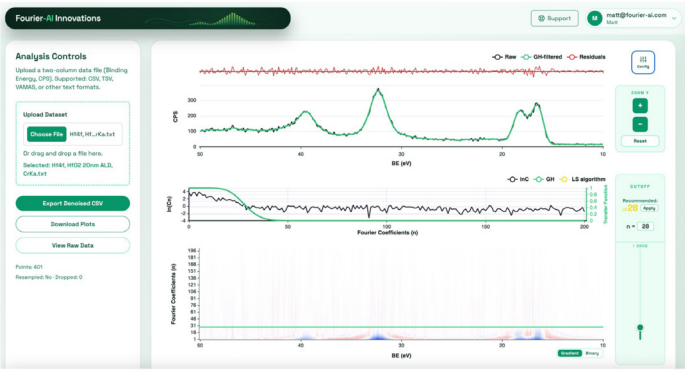


Figure 1. Main page of the Fourier-AI Innovations software with a dataset loaded into it. Note the 'Config' button in the upper right corner of the software, which provides access to many of the more advanced features of the software.

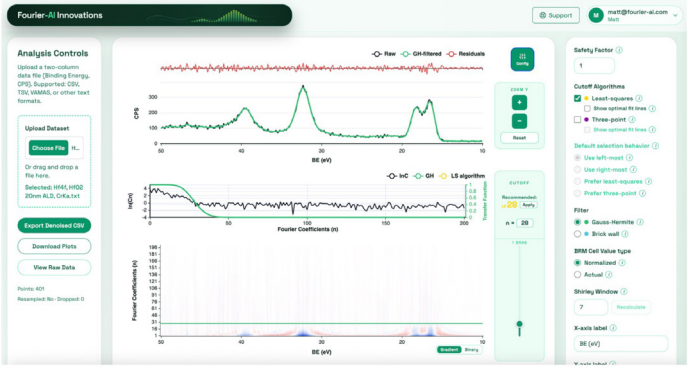


Figure 2. The main software page of the Fourier-AI Innovations software after the configurations button has been pressed.

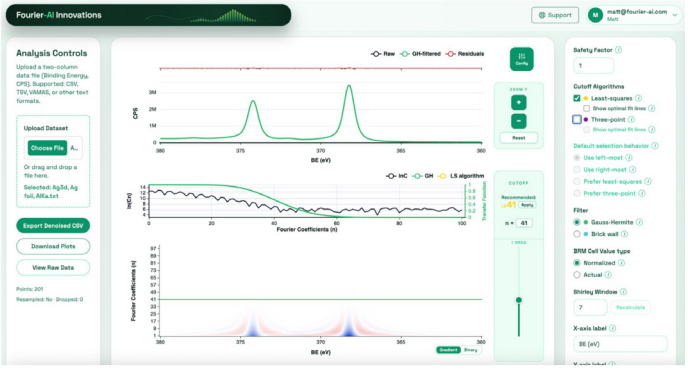


Figure 3. Denoising of an Ag 3d spectrum with the Gauss-Hermite transfer function.

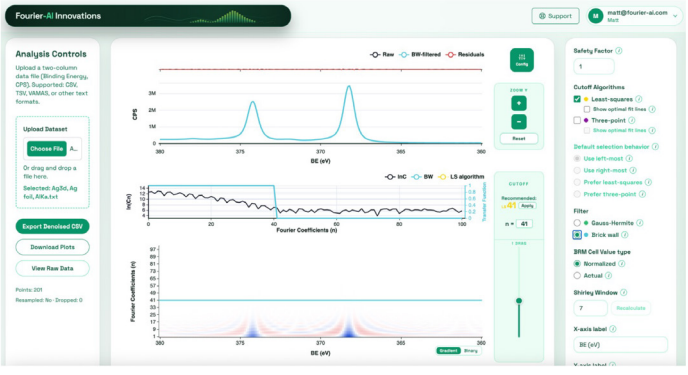


Figure 4. Denoising of an Ag 3d spectrum with the brick-wall transfer function.

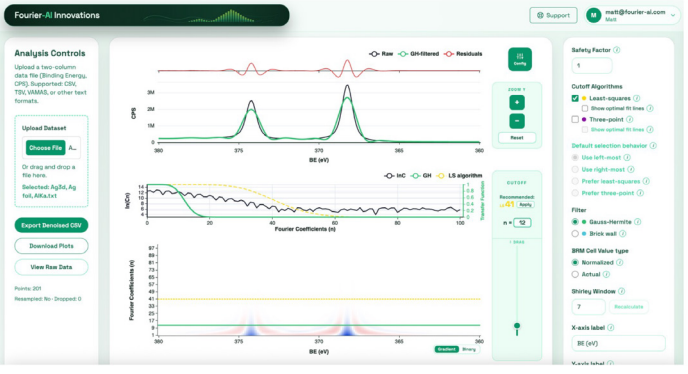


Figure 5. Denoising of an Ag 3d spectrum with the cutoff of the Gauss-Hermite transfer function placed too far to the left.

Filter (Transfer function)

The transfer function is a key part of Fourier denoising. The Fourier coefficients generated from a discrete Fourier transform of a dataset are multiplied by a transfer function, and this product is then back transformed to produce the denoised data.

The Fourier-AI Innovations software allows the user to elect either the Gauss-Hermite or brick-wall transfer function. The Gauss-Hermite transfer function is curved, and the brick-wall transfer function is abrupt. In general, the Gauss-Hermite transfer function is the better choice, although in the denoising of moderately broad spectra, little difference may be noted in their performance. However, the brick-wall transfer function especially may introduce artifacts into spectra when sharp features are present in them and its cutoff is positioned too far to the left. This is ultimately because of the convolution theorem from Fourier analysis and the fact that the Fourier transform of the brick-wall filter function is a sinc function, which has side lobes that decay slowly (as 1/n). In general, we recommend that the user stick with the Gauss-Hermite filter function, which performs very well and consistently across many different spectra. Expert users may find occasional uses for the brick-wall filter. **Figure 3** shows the denoising of an Ag 3d spectrum, which has some relatively narrow peaks, with the Gauss-Hermite transfer function. **Figure 4** shows the same denoising performed with the brick-wall transfer function. Nearly identical results are obtained. However, **Figures 5** and **6** show the results obtained when the transfer functions are placed too far to the left. The results are noticeably problematic, where the results are more distorted with the brick-wall transfer function.

Cutoff Selection Algorithms

The Fourier-AI Innovations software uses one or two possible cutoff selection algorithms to estimate the cutoff (half-height) for the transfer function, which are referred to as the 'three-point' (3P) and 'least-squares' (LS) algorithms. In practice, these algorithms give fairly similar results. However, the interested user has the option to select whether one or both of the algorithms is employed. When both algorithms are selected, both corresponding transfer functions are displayed on the Fourier coefficients. Furthermore, if both algorithms are selected, the user can have the software always use the

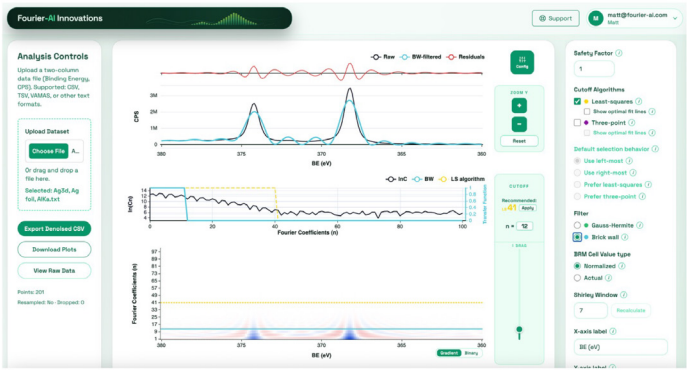


Figure 6. Denoising of an Ag 3d spectrum with a brick-wall transfer function where its cutoff has been placed too far to the left (the same position as the Gauss-Hermite transfer function in Figure 5) showing even greater distortion in the reconstructed spectrum (top) due to the side lobes of the sinc function.



Figure 7. The main software page of the Fourier-AI Innovations software after both cutoff selection algorithms (the least-squares and three-point algorithms) have been activated.

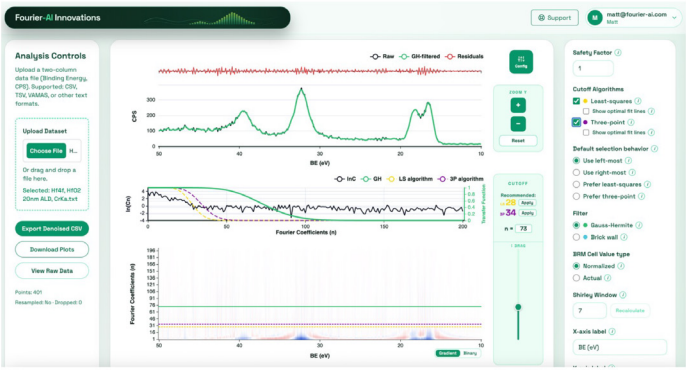


Figure 8. The main software page of the Fourier-AI Innovations software after both cutoff selection algorithms have been activated, but the position of the transfer function has been changed by the user to a higher value than is recommended by either algorithm.

left-most cutoff prediction of the algorithms, which will, in general, produce the greatest amount of smoothing, the right-most cutoff prediction of the algorithms, which, in general, will lead to less smoothing, or the result from a selected algorithm whether its cutoff is further to the left or to the right. **Figure 7** shows an example of where both algorithms and also the 'Use left-most' algorithm features are selected. Notice that when both of the resulting Gauss-Hermite transfer functions are shown on the Fourier coefficients, both cutoffs for the transfer functions are listed above the slider that controls the position of the transfer function. Also, as shown in **Figure 8**, even when both transfer functions are selected, the user still has the ability to use the slider to move the transfer function to a different position.

Finally, with regards to the Cutoff Algorithms in the Config panel, note the boxes that can be checked to 'Show optimal fit lines' for both the 'Least-squares' and 'Three-point' algorithms. The least-squares and three-point algorithms predict a cutoff for the transfer function by optimizing the positions of two fit lines. Also note the 'LS algorithm' and '3P algorithm' buttons above the Fourier coefficients in the main software page. These show or hide the transfer function determined by the corresponding algorithm.

BRM Cell Value Type and Axis Labels

When the mouse is run over the binary residual map, the residuals at each point are displayed. The default in the software is to display the normalized residuals, where this normalization is with respect to the magnitude of the largest residual value (positive or negative). However, if a setting is changed, the actual (not normalized) residual value is displayed.

The x- and y-axis labels on the figures can be changed. Their defaults are 'BE (eV)' and 'CPS', which are appropriate for most X-ray photoelectron spectroscopy (XPS) data.

Safety Factor

In general, the Fourier coefficients of the discrete Fourier transform (DFT) of a spectrum nicely divide the information (the lower-index Fourier coefficients) from the noise (the higher-index Fourier coefficients). In Fourier denoising, one positions the cutoff of a transfer function at the transition between the information- and noise-containing Fourier coefficients to preserve as much of the real information in the spectrum as possible while removing as much noise as possible. The Fourier-AI Innovations software uses algorithms to find a reasonable cutoff for the transfer function on the Fourier coefficients. In general, these algorithms work very well. However, there may be some datasets where this is not the case. There may also be times when one wishes to only partially denoise a spectrum. The 'Safety Factor' can be used in these situations. For a Safety Factor value of 1, the software positions the transfer function at the position recommended/found by one of the algorithms. For a Safety Factor value of 2 or 3, the software positions the transfer function at a position that is twice or three times that found by one of the algorithms, respectively, and denoises the spectrum using this shifted transfer function. **Figure 2** and most of the other figures in this document show spectra with the safety factor set at one. However, **Figure 9** shows the same data as in **Figure 2**, but with a safety factor of 2. For most work, it is best to leave the safety factor at its default position of 1.

Settings

Finally, as shown in **Figure 10**, the user can access a settings button in the upper right corner of the main software page, which opens the panel shown in **Figure 11**. This panel controls two things. First, the 'Sample Datasets' button at the top allows the user to access a series of sample (practice) datasets. When this button is pressed, a 'Samples' button appears near the top of the left side of the page (see **Figure 12**). A series of practice data sets can then be accessed. Below the 'Sample



Figure 9. The same data as in **Figure 2**, but denoised with a transfer function placed based on a Safety Factor of 2, i.e., at a cutoff value of 56, which is twice the recommended value of 28.

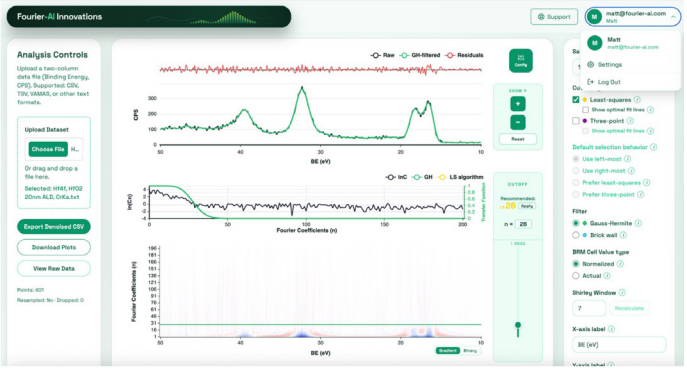


Figure 10. The main software page showing how to access the 'Settings' in its upper right corner

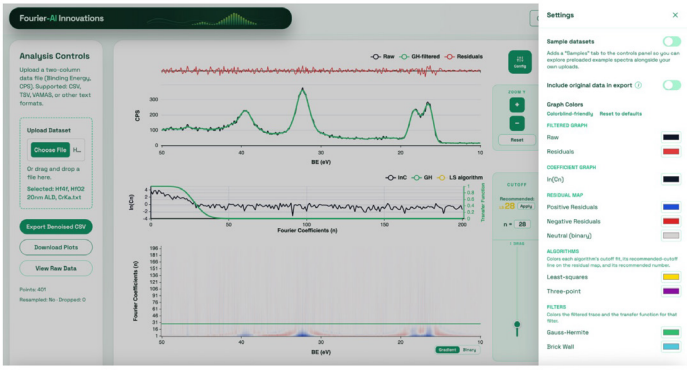


Figure 11. The 'Settings' tab on the right side of the main software page.

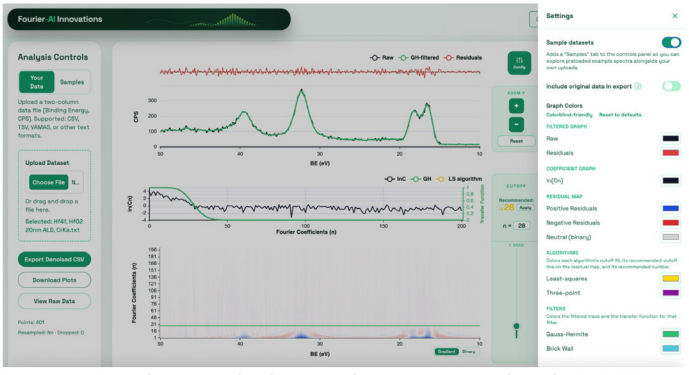


Figure 12. The 'Sample datasets' button activated in the 'Settings' tab, which opened up a 'Samples' button on the left of the software page. After the 'Samples' button is pressed, the user can access various practice datasets.

Datasets' button in the Settings are buttons that control the colors of the lines in the various plots. For example, one may choose colorblind friendly colors. One may also reset the colors to their default values.

Exporting Data

The denoised data and plots created by the software can be downloaded using the buttons in the left-most panel entitled: "Export Denoised CSV", "Download Plots", and "View Raw Data".

Conclusions

We have discussed various advanced features in the Fourier-AI Innovations denoising software. These include algorithms used to determine the cutoffs (half-heights) of the transfer functions, different transfer functions that can be employed, the cell value type for the binary residual map, the axis labels, and a safety factor for denoising. Through a settings panel, the user can also access practice data sets and control the colors in the software. Options exist to export filtered results in figure or CSV form. Finally, more, interesting features are in the works that will be added to the software.

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