



Characterization of Thin Films and Materials and Data Analysis

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Introduction to the Fourier-AI Innovations Software for Denoising Spectra

This article describes the Fourier-AI Innovations denoising software, which removes noise from data using Fourier analysis. The article first explains why the denoising of spectra is important. A brief overview of the use of Fourier analysis in denoising is then presented. Throughout the article, two innovative features of the software are emphasized: the binary residual map™ and algorithms for automatically positioning the transfer function. It is explained how to access and try out a demo version of the software. Finally, various features of the software are described in some detail. After reading this article, the user should be able to use the Fourier-AI Innovations software with some confidence. An upcoming article will describe some of the more advanced features of the software.

Introduction

Spectra are collected in science with many different types of instruments. Surface analysts collect X-ray photoelectron spectroscopy (XPS), low energy ion scattering (LEIS), time-of-flight secondary ion mass spectrometry (ToF-SIMS), and Auger electron spectroscopy (AES) spectra. Chemists collect mass spectra (of many types), nuclear magnetic resonance (NMR) spectra, ultraviolet-visible (UV-VIS) spectra, Fourier transform infrared (FTIR) spectra, and Raman spectra. De-

pending on acquisition conditions, the state of the instrument, and the sample, the various spectra that are collected may be noisy or they may have little noise on them. In general, we want as little noise as possible in our data. Higher levels of noise can make spectra uninterpretable. However, lower noise levels on spectra often come at a price of extra analysis time. For many instruments, one must scan more times (signal average) to obtain lower noise spectra. Of course, modest amounts of noise on spectra may not be a problem. For those with a trained eye, they can often still be relatively easy to interpret.

There is increasing interest in using spectra of all types to train artificial intelligence (AI) algorithms. However, computers are often less adept at dealing with noise than humans. Noise 'confuses' artificial intelligence (AI) algorithms. It can take many more noisy spectra to train an AI algorithm than spectra with less noise on them. Even data that may not appear to be very noisy to a human can pose problems for an AI algorithm because it has to figure out whether fluctuations (noise) in the data have real meaning.

Unfortunately, there are situations in XPS where noisy data are the norm. In high energy XPS (HAXPES), peaks are often noisy because photoelectron cross sections decrease with increasing photon energy. Sometimes analytes are present at

low levels at surfaces. In imaging studies, large numbers of spectra often need to be taken in relatively short amounts of time, which limits their quality. Furthermore, the analytical instruments used in surface science and chemistry can be expensive to purchase and maintain. Thus, time on these instruments can be expensive. It can easily cost US\$1000 for a basic XPS analysis of a surface from a commercial vendor. In addition, some instruments, e.g., XPS instruments in industry, are basically used non-stop, which limits the amount of time people can get on them. Accordingly, it would be advantageous for some users of these instruments to collect somewhat less data than they otherwise might and then to remove the noise from it, if a reasonable way were available to remove this noise.

Conventional ways to remove noise from data include the boxcar and Savitzky-Golay¹ smooths. In a boxcar smooth, we replace the middle point of each group of adjacent data points with the average of the points around it. In effect, a Savitzky-Golay smooth consists of fitting adjacent groups of data points to a polynomial and replacing the middle data point with the value of the polynomial at that point. We previously wrote in Vacuum Technology & Coating about the Savitzky-Golay smooth.² However, there is another approach that is arguably better. It is based on Fourier analysis with the discrete Fourier transform (DFT).³⁻⁸ We have shown that the Savitzky-Golay and boxcar-type smooths are fundamentally problematic and less sophisticated approaches to data smoothing than Fourier analysis.⁹

The Fourier transform, which is applied to continuous functions, and the discrete Fourier transform (DFT), which is applied to discrete data, reveal the amounts of the cosines and sines that make up the original function or data, respectively. In the Fourier denoising of a spectrum, the underlying frequencies that make up a spectrum are first determined with the DFT. In general, and this is the key point, the DFT separates the information in a spectrum into lower frequencies (lower-index Fourier coefficients), which correspond to the actual underlying signal, and higher frequencies (higher-index Fourier coefficients), which correspond to noise. We say that this information is in reciprocal space. All the Fourier coefficients in reciprocal space are then multiplied by a function called a transfer function. This function generally has a value close to one where the lower-index Fourier coefficients are, and a value close to zero where the higher-index Fourier coefficients are. Thus, multiplication by a transfer function largely preserves the information-rich, lower-index Fourier coefficients while largely removing the noise-containing higher-index Fourier coefficients. These modified Fourier coefficients are then back-transformed into direct space. If the transfer function had been reasonably placed, this process should result in a denoised spectrum.

We now describe the Fourier-AI Innovations denoising software. One of the innovations in this software is the algorithms it uses to automatically position the half-height of the transfer

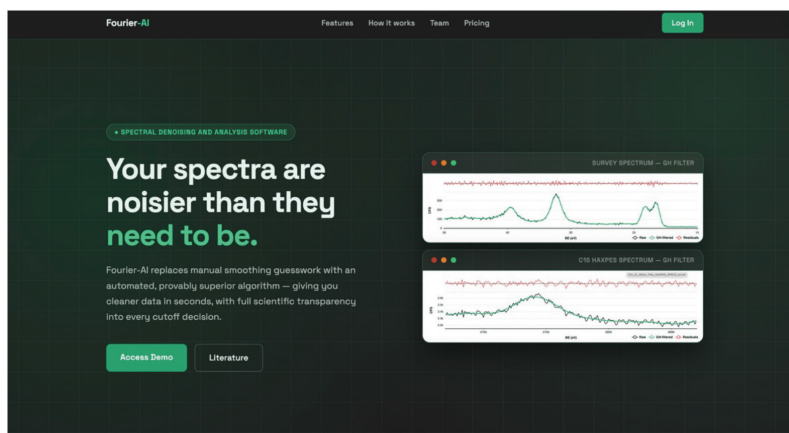


Figure 1. The Fourier-AI Innovations web page.

function. Another key innovation is called the binary residual map. Both of these capabilities are described below with the software.

How to use the Fourier-AI Innovations software

1. Getting access to a demo version of the software. You can try a demo version of the Fourier-AI Innovations software at fourier-ai.com. When you go to the fourier-ai.com website you will see what is in **Figure 1**. Press the green button in the upper right corner of this webpage that says 'Log In'. You will then see the sign-in page that is shown in **Figure 2**. If you are new to the software, click 'Create account' at the bottom of this page. You will then be taken to the page shown in **Figure 3**. Create a username and password. That is, fill out this form, and press the big 'Create Account' button. Shortly thereafter you will be sent an email to verify that your email address is real. Confirm that it is, and you will be able to log into the software. Now log in.

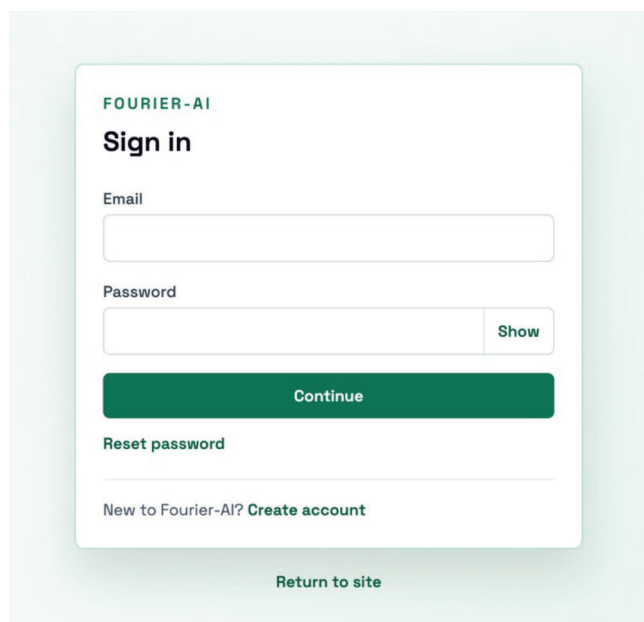


Figure 2. Sign-in page at the fourier-ai.com web site. To access a demo version of the software, press 'Create account' at the bottom of this page.

Figure 3. Screen/page for creating an account at fourier-ai.com to access the demo version of the software.

2. What you see when you log in – exploring the software

a. The original and denoised spectra in the top panel.

When you first log in, you should see something like what is in **Figure 4**. This is the demo mode of the software, so you cannot enter your own spectra and denoise them. Rather, there are some spectra provided for you to try out the software. In the long top panel, you see a spectrum, which was read in by the software and automatically denoised. As noted above, a key feature of the software is its use of algorithms to predict the position (of the half-height) of the transfer function. Both the original spectrum and denoised version of it are shown in the top panel, along with the residuals above the spectra that compare the original spectrum to the denoised version of it. Note the buttons just above and on the right side of this panel that read 'Raw', 'GH-filtered', and 'Residuals'. With these buttons, you can turn on and off the original spectrum, the denoised spectrum, and the residuals. Try this. Of course, the spectrum shown in **Figure 4** has almost no noise in it, so there is very little difference between the spectrum and the denoised version of it.

b. The Fourier coefficients in the middle panel.

The long middle panel shows the

Fourier coefficients of the original spectrum (in black). Again, this is the reciprocal space representation of the spectrum, where, technically speaking, these are the magnitudes of the Fourier coefficients, which are themselves actually complex. Note that these coefficients are on a log scale. Also shown is the transfer function (in green), where, again, we multiply the Fourier coefficients by this function. The S-shaped (sigmoidal) Gauss-Hermite transfer function, which is used here, is well shaped for Fourier denoising.¹⁰⁻¹² Importantly, the cutoff or inflection point of the transfer function is located close to the place where the Fourier coefficients transition from being meaningful to where they mostly represent noise. As shown on the scale on the right of this plot, the Gauss-Hermite transfer function is indeed unity at lower Fourier coefficient values and zero at higher Fourier coefficient values.

c. The binary residual map. The bottom panel shows the binary residual map. This is an exciting innovation in the software. In this case, the binary residual map contains information about ca. 100 different smooths of the spectrum in question. That is, each position along the y-axis of the binary residual map corresponds to a different cutoff position for the transfer function, and each row at that height in the map contains the color-coded residuals for that smooth. The inflection point of the transfer function in the top panel and the horizontal green line in the bottom panel represent the same position. The two main colors (red and blue in **Figure 4**) in a binary residual map correspond to positive or negative residuals. The shades of these two colors give the magnitudes of the residuals. This binary residual map shows that the smooths are poor when the transfer function is positioned far to the left (at low Fourier coefficient values). In a poor smooth, we usually see long consecutive runs of residuals of the same color. Both the residuals and also the longer runs of a single color become smaller as the transfer function is moved to the right. It is not a coincidence that the position of the transfer function in the top panel in **Figure 4** corresponds to a green line that is around the top of the larger residuals in the binary residual map.

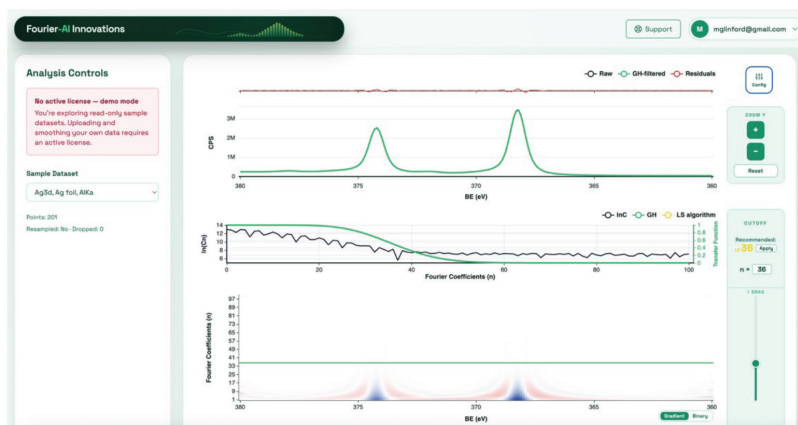


Figure 4. What you first see when you log into the Fourier-AI Innovations software.

d. The vertical slider on the right. As noted, an important feature of the Fourier-AI Innovations software is that it has algorithms that automatically predict a reasonable position for the transfer function. However, while we have found these algorithms to work quite well, it would be impossible to guarantee that they will be ideal for every data set. Accordingly, the software gives the user the ability to change the position of the transfer function with a slider, which is on the far right. Play around with this slider. Move it up and down and notice how the transfer function and corresponding horizontal green line in the binary residual map move when you do this. Move the transfer function far to the left. Notice how poor (and ridiculous) the 'smoothed' spectrum is in the top panel. When the transfer function is too far to the left, too many meaningful Fourier coefficients are significantly reduced in intensity for the spectrum to be reasonably reconstructed.

e. **Entering new data.** It is important to be able to switch datasets and thereby enter new data into the software. To enter different sample datasets, go to the far left panel. In the dropdown menu under 'Sample Dataset' select: "Hf4f, HfO₂ 20nm ALD, CrKa". You should then see what is shown in **Figure 5**. As suggested in the name of this dataset, it shows the Hf 4f signals from a thin, 20 nm film of HfO₂ deposited by atomic layer deposition, where the data were collected with a Cr K α X-ray source using a SPECS EnviroMETROS instrument. Notice that the software has predicted the position of the transfer function in the middle panel to be close to the 'knee' in the Fourier coefficients and that, again, this position is close to the top of the larger (more colored) residuals in the binary residual map (in the bottom panel). The residuals in the top panel suggest that the reconstructed, smoothed spectrum follows the contour of the original spectrum quite well. For practice, turn off the 'Raw' data in the top panel, leaving just the filtered/smoothed data. Now move the transfer function to the right as far as it will go, watching the GH-filtered spectrum. Notice that as the transfer function moves to the right, more noise is incorporated into the 'smoothed' spectrum. Finally, notice that at the top of the slider it says "Recommended" and that right below this is the software's algorithmically-based recommendation for the position of the transfer function.

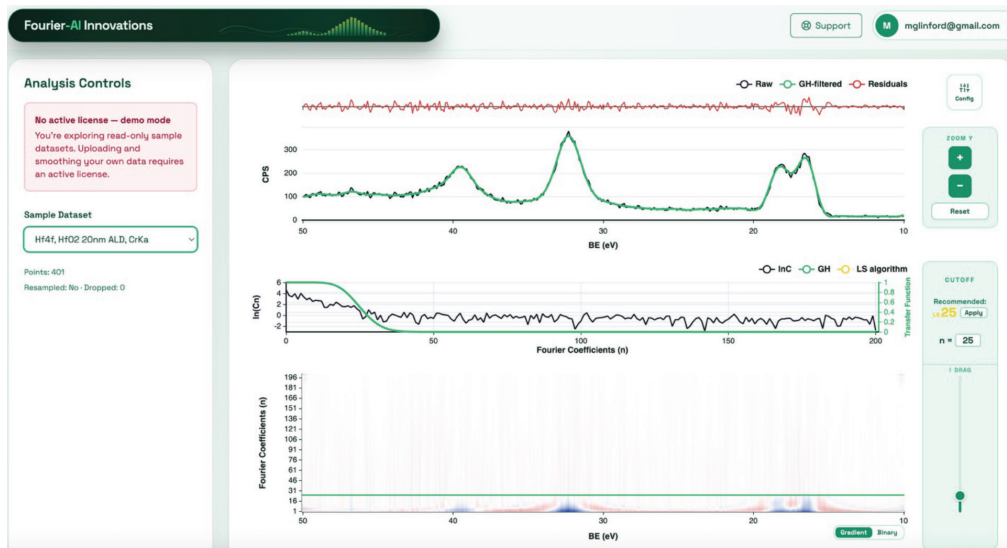


Figure 5. The Fourier-AI Innovations denoising software with the dataset "Hf4f, HfO₂ 20nm ALD, CrKa" uploaded into it.

After you have moved the transfer function back and forth, hit the 'Apply' button to return the transfer function to the software-recommended position for it.

f. **More advanced features.** As would be expected, the Fourier-AI Innovations software can download the results obtained after denoising data. However, this capability is not active in the demo mode. There are also other advanced features that have not been covered in this article. These can be accessed through the 'Config' button in the upper right corner of the page. Our next Vacuum Science and Technology article will discuss some of these more advanced capabilities.

3. Final comments

a. **Other data sets.** Please note that while the examples shown in this article are of XPS data sets, data from other techniques can also be denoised with the software.

b. **Patent pending.** Provisional patents have been filed on some of the capabilities shown here for the software, including for the binary residual map and the automated algorithms for predicting the transition point for the transfer function.

c. **Learning more about Fourier analysis.** If you wish to learn more about the theory of Fourier analysis, please download a copy of a tutorial article we just wrote about it.¹³ **Figure 1** shows how to do this. Press the 'Literature' button shown in this figure at the fourier-ai.com website to be given access to this tutorial.

d. **Support and questions.** If you have questions about using this software, please do not hesitate to reach out to us by email at support@fourier-ai.com.

e. **Purchasing the software.** Information about purchasing the software is shown at the bottom of the fourier-ai.com web page. There is both a basic package and a premium package with more advanced capabilities.

Conclusions

In this article, we have discussed the Fourier-AI Innovations software package for denoising spectra. Two examples were

shown of the software denoising spectra. The software has some unique features. It automatically recommends a position for the transfer function and also automatically creates binary residual maps. In our next article we will discuss some of the other advanced features of our software.

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