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The case for denoising/smoothing X-ray photoelectron spectroscopy data by Fourier analysis

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ABSTRACT

Traditionally, the smoothing of X-ray photoelectron spectroscopy (XPS) data has been avoided. Data smoothing should not be viewed as a means of "fixing" poorly collected or extremely noisy XPS data. However, it is not always possible or desirable to acquire high-quality data. Here, we suggest that, under appropriate circumstances, and with good algorithms, it may be appropriate to denoise XPS spectra. In particular, we propose the Fourier denoising of XPS data. Fourier analysis is commonly used in science and engineering. Fourier analysis of spectra is advantageous because it naturally divides the data into signal- and noise-dominated coefficients in reciprocal space. Accordingly, Fourier analysis has long been used to reduce or remove the high frequencies (noise) from data, leaving the lower frequencies (signal and baseline trends). We provide an overview of the Fourier transform. The Gauss-Hermite Fourier filter employed in this study shows improvements over the commonly used boxcar and Savitzky-Golay smooths, and also over other apodization approaches used in Fourier analysis, e.g., boxcar apodization. The Gauss-Hermite filter avoids sharp cutoffs that can introduce significant artifacts into data. The Fourier denoising/reconstruction of two XPS narrow scans, an Auger signal, and a valence band signal is demonstrated. Filtered spectra are compared to corresponding "true" spectra, that are obtained by signal averaging. Spectra denoised through the Gauss-Hermite filter can be more accurate approximations to the "true" spectra than the original noisy spectra.

I. INTRODUCTION

From the perspective of crystallography with its ideal representation of crystals as infinite lattices, surfaces are crystal/material defects. Indeed, surfaces are inherently challenging to analyze because they are different from their corresponding bulks, and usually only contain very small amounts of material. This lack of material presents significant challenges to the analyst, where this situation is exacerbated by the fact that the little matter that is present is often distributed in different forms, e.g., as overlayers/thin films and substrate atoms, defects, surface contaminants, different oxidation/chemical states, and in various crystal structures and morphologies.

During the past two decades, X-ray photoelectron spectroscopy (XPS) has emerged as the most important method for chemically analyzing surfaces.[1–5] Nevertheless, there is a significant amount of inadequately analyzed XPS data in the current scientific literature, which suggests that XPS spectral analysis of many materials is challenging.[4,6–13] In addition, instrument parameters are often not well reported, and terminology is sometimes misused, e.g., XPS peak fitting is not "deconvolution."[14,15] Other fields also struggle with incorrect analysis and reporting.[16]

Unfortunately, surface analysis does not have a single tool that can fully reveal the structures of surfaces. In contrast, nuclear magnetic resonance (NMR) is used by organic chemists to fully