



Perspective Article

The Gaussian-Lorentzian Sum, Product, and Convolution (Voigt) functions in the context of peak fitting X-ray photoelectron spectroscopy (XPS) narrow scans



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ABSTRACT

X-ray photoelectron spectroscopy (XPS) is arguably the most important vacuum technique for surface chemical analysis, and peak fitting is an indispensable part of XPS data analysis. Functions that have been widely explored and used in XPS peak fitting include the Gaussian, Lorentzian, Gaussian-Lorentzian sum (GLS), Gaussian-Lorentzian product (GLP), and Voigt functions, where the Voigt function is a convolution of a Gaussian and a Lorentzian function. In this article we discuss these functions from a graphical perspective. Arguments based on convolution and the Central Limit Theorem are made to justify the use of functions that are intermediate between pure Gaussians and pure Lorentzians in XPS peak fitting. Mathematical forms for the GLS and GLP functions are presented with a mixing parameter m . Plots are shown for GLS and GLP functions with mixing parameters ranging from 0 to 1. There are fundamental differences between the GLS and GLP functions. The GLS function better follows the ‘wings’ of the Lorentzian, while these ‘wings’ are suppressed in the GLP. That is, these two functions are not interchangeable. The GLS and GLP functions are compared to the Voigt function, where the GLS is shown to be a decent approximation of it. Practically, both the GLS and the GLP functions can be useful for XPS peak fitting. Examples of the uses of these functions are provided herein.

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1. Introduction

X-ray photoelectron spectroscopy (XPS) is arguably the most popular and important high vacuum surface analytical tool [1]. It is unique in being highly surface sensitive, quantitative, and available in many laboratories and facilities, providing the elemental compositions of all the elements except helium and hydrogen, and yielding chemical/oxidation state information about the elements it detects [2]. Important decisions in the laboratory and in industry are made based on XPS results [3], where much of the key information derived from XPS is based on peak fitting narrow (high resolution) scans. Indeed, as explained by Sherwood, peak fitting is an indispensable part of XPS data analysis because the chemical shifts that provide the rich chemical information available through the technique and the widths of the fit components have comparable values [4]. For many years XPS practitioners have employed a variety of functions/peak shapes in their fitting. These have included pure Lorentzians, which model

the fundamental/theoretical line shape, pure Gaussians, which often model amorphous materials well, e.g., polymers and glasses, Gaussian-Lorentzian sum and product functions, which consist of either the sum [5] or product [4] of these two functions, Voigt functions, which are the convolutions of Gaussian and Lorentzian functions, and other more complex functions, including the Doniach-Sunjic line shape [6]. Asymmetry must often be added to fit components/peaks to model conducting materials [7].

In this paper we discuss five functions that have been widely explored and used in XPS peak fitting: the Gaussian function, the Lorentzian function, the Gaussian-Lorentzian sum function (GLS), the Gaussian-Lorentzian product (GLP) function, and the Voigt function, which is a convolution of Gaussian and Lorentzian functions. A primary goal of this work is to compare the GLS and GLP functions. Indeed, different software packages for XPS peak fitting have different mathematical functions available in them. Thus, it is important to understand these synthetic line shapes, i.e., to know where they are best used and how to apply them. Arguments based on convolution and the Central Limit Theorem are made to justify the use of functions that are intermediate between pure Gaussians and pure Lorentzians in XPS peak fitting. This is

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