



Perspective Article

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

Varun Jain^a, Mark C. Biesinger^b, Matthew R. Linford^{a,*}^a Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT 84602, USA^b Surface Science Western, The University of Western Ontario, London, Ontario N6G 8K3, Canada

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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

* Corresponding author.

E-mail address: marklinford@chem.bryu.edu (M.R. Linford).

Surface Science An Introduction

Gabor A. Somorjai, Yimin Li



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Surface Science K. Oura, V.G. Lifshits, A.A. Saranin, A.V. Zotov, M. Katayama, 2013-03-14 Designed as a textbook for advanced undergraduate and graduate students in engineering and physical sciences who are seeking a general overview of surface science this book also provides the necessary background for researchers just starting out in the field It covers all the most important aspects of modern surface science from the experimental background and crystallographic basics to modern analytical techniques and applications to thin films and nanostructures All topics are presented in a concise and clear form accessible to a beginner At the same time the coverage is comprehensive and at a high technical level with emphasis on the fundamental physical principles Numerous examples references practice exercises and problems complement this remarkably complete treatment which will also serve as an excellent reference for researchers and practitioners

Surface Science K. Oura, V. G. Lifshits, Alexander Saranin, 2014-01-15

Surface Science John Hudson, 2013-10-22 The whole field of surface science is covered in this work Starting with a description of the structure and thermodynamics of clean surfaces the book goes on to discuss kinetic theory of gases and molecular beam formation This is followed by a large section on gas surface interactions and another major section on energetic particle surface interactions The final chapter provides the background to crystal nucleation and growth The approach adopted is interdisciplinary and slanted towards the experimental side with practical analytical techniques being used to illustrate general principles

Surface and Interface Science, Volumes 1 and 2 Klaus Wandelt, 2012-04-16 Covering interface science from a novel surface science perspective this unique handbook offers a comprehensive overview of this burgeoning field Eight topical volumes cover basic concepts and methods elemental and composite surfaces solid gas solid liquid and inorganic biological interfaces as well as applications of surface science in nanotechnology materials science and molecular electronics With its broad scope and clear structure it is ideal as a reference for scientists in the field as well as an introduction for newcomers

Introduction to Surface Chemistry and Catalysis Gabor A. Somorjai, Yimin Li, 2010-06-08 Now updated the current state of development of modern surface science Since the publication of the first edition of this book molecular surface chemistry and catalysis science have developed rapidly and expanded into fields where atomic scale and molecular information were previously not available This revised edition of Introduction to Surface Chemistry and Catalysis reflects this increase of information in virtually every chapter It emphasizes the modern concepts of surface chemistry and catalysis uncovered by breakthroughs in molecular level studies of surfaces over the past three decades while serving as a reference source for data and concepts related to properties of surfaces and interfaces The book opens with a brief history of the evolution of surface chemistry and reviews the nature of various surfaces and interfaces encountered in everyday life New research in two crucial areas nanomaterials and polymer and biopolymer interfaces is emphasized while important applications in tribology and catalysis producing chemicals and fuels with high turnover and selectivity are addressed The basic concepts surrounding various properties of surfaces such as

structure thermodynamics dynamics electrical properties and surface chemical bonds are presented The techniques of atomic and molecular scale studies of surfaces are listed with references to up to date review papers For advanced readers this book covers recent developments in in situ surface analysis such as high pressure scanning tunneling microscopy ambient pressure X ray photoelectron spectroscopy and sum frequency generation vibrational spectroscopy SFG Tables listing surface structures and data summarizing the kinetics of catalytic reactions over metal surfaces are also included New to this edition A discussion of new physical and chemical properties of nanoparticles Ways to utilize new surface science techniques to study properties of polymers reaction intermediates and mobility of atoms and molecules at surfaces Molecular level studies on the origin of the selectivity for several catalytic reactions A microscopic understanding of mechanical properties of surfaces Updated tables of experimental data A new chapter on soft surfaces polymers and biointerfaces Introduction to Surface Chemistry and Catalysis serves as a textbook for undergraduate and graduate students taking advanced courses in physics chemistry engineering and materials science as well as researchers in surface science catalysis science and their applications

Surface Science of Adsorbents and Nanoadsorbents Tawfik Abdo Saleh, 2022-09-15 Surface Science of Adsorbents and Nanoadsorbents Volume TBD Properties and Applications in Environmental Remediation presents a unique collection of timely information on the surface science of adsorbents and nanoadsorbents The book offers a perfect source to document developments and innovations ranging from materials development and characterization of properties to applications that encompass the enhancement of sorption degradation processes and their usage for the removal of different pollutants including heavy metals dyes and pesticides etc It is written for post graduate students scientists in academia and industry chemical engineers and water quality monitoring agencies working in water treatment efficient materials nanomaterials development and quality control Provides the theoretical and scientific foundation for understanding synthesis and applications in nano adsorbent material Presents numerous examples to help users gain an understanding of each subject Includes a variety of illustrations that further enhance the content

Surface Science Techniques Gianangelo Bracco, Bodil Holst, 2013-01-11 The book describes the experimental techniques employed to study surfaces and interfaces The emphasis is on the experimental method Therefore all chapters start with an introduction of the scientific problem the theory necessary to understand how the technique works and how to understand the results Descriptions of real experimental setups experimental results at different systems are given to show both the strength and the limits of the technique In a final part the new developments and possible extensions of the techniques are presented The included techniques provide microscopic as well as macroscopic information They cover most of the techniques used in surface science

Advances in Surface Science , 2001-10-20 Surface science has a wide range of applications that include semiconductor processing catalysis vacuum technology microelectronics flat panel displays compact disks televisions computers environmental monitoring of pollutants biomaterials artificial joints soft tissues food safety pharmacy and many

more This volume is intended for upper level undergraduate and graduate students in universities individual research groups and researchers working on surfaces of materials It is of interest to chemists solid state physicists materials scientists surface chemists polymer scientists electrical engineers chemical engineers and everyone involved in materials science

Introduction to Surface Physics M. Prutton, 1994 *Recent Progress in Surface Science* J. F. Danielli, K. G. A. Pankhurst, A. C. Riddiford, 2013-10-22 *Recent Progress in Surface Science* Volume 2 is a 10 chapter text that covers the significant advances in some aspects of surface science including in catalysis genetic control of cell surface and cell membrane The opening chapter deals with the major factors affecting adsorption at the gas solid interface The subsequent chapters explore the advances in understanding of heterogeneous catalysis in terms of fundamental surface processes as well as the concept of dynamic contact angles These topics are followed by discussions on emulsions flotation and the extraordinary complexity of cell surface structures and their chemical components Other chapters consider the experimental studies on the physiology of pinocytosis and the principles of plastron respiration The final chapters are devoted to the isolation characterization and electronmicroscopic studies of cell membrane This book is of value to surface scientists cell biologists and researchers in the allied fields

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