JVST A
Journal of Vacuum Science & Technology A

TUTORIAL

avs.scitation.org/journal/jva

Practical guide for curve fitting in x-ray photoelectron spectroscopy

Cite as: J. Vac. Sci. Technol. A 38, 061203 (2020); doi: 10.1116/6.0000377
Submitted: 5 June 2020 · Accepted: 18 September 2020 ·
Published Online: 6 October 2020

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Note: This paper is part of the Special Topic Collection on Reproducibility Challenges and Solutions.
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ABSTRACT

The use of peak fitting to extract information from x-ray photoelectron spectroscopy (XPS) data is of growing use and importance. Due to increased instrument accessibility and reliability, the use of XPS instrumentation has significantly increased around the world. However, the increased use has not been matched by the expertise of the new users, and the erroneous application of curve fitting has contributed to ambiguity and confusion in parts of the literature. This guide discusses the physics and chemistry involved in generating XPS spectra, describes good practices for peak fitting, and provides examples of appropriate use along with tools for avoiding mistakes.

I. INTRODUCTION

Over the past 30 years, x-ray photoelectron spectroscopy (XPS) has become the most widely used surface analysis tool and has been an essential component of many research studies.[1] Curve fitting has been widely used for more than 50 years for extracting chemical information from the overlapping features in high-resolution XPS spectra.[2] Despite computational advances and higher accessibility of software resources, it has been challenging to develop a chemically and physically meaningful approach to curve fitting. The absence of a distinct theoretical description of XPS fitting has led to the publication of erroneous conclusions about surface chemistry.[2,3] In an ongoing study of XPS data in three high profile journals,[3] it was observed that roughly 70% of the papers using XPS analyzed the data using some type of curve fitting. Furthermore, errors, misconceptions, and bad curve-fitting practices accounted for most of the serious problems in both the measured XPS data and the spectral analysis that were identified in more than 30% of the papers analyzed. This guide is intended to help address this important problem.

Curve fitting, also known as peak fitting,[4] is the process used to extract information from the spectral data for a number of techniques. Although the details of curve fitting depend on the technique in question, the curve fitted spectra generally contain overlapping peaks. Each of these peaks is represented by a function that reflects the physical process involved in generating the original signal. XPS data interpretation and representation range from a rudimentary understanding/extraction of the elements present in a material to advanced peak fitting and background analysis that reveal chemical states and sample morphologies.

In XPS, it is convenient to identify two spectral regions, namely, the core region (electrons with binding energies, BEs, greater than 30 eV) and the valence band region (BE < 30 eV). In the core region, the spectral features arise from photoelectrons generated from core energy levels (atomic orbitals), which are characteristic of the individual atoms in the sample.[5] In contrast, the features in the valence band region arise from photoelectrons generated from energy levels that typically involve the chemical