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The equivalent width as a figure of merit for XPS narrow scans

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ABSTRACT

X-ray Photoelectron Spectroscopy (XPS) is a widely used surface analytical tool that provides information about the near surface regions of materials. And while indispensable for XPS data analysis, peak fitting of narrow scans is often a fairly subjective exercise. Herein we introduce the equivalent width (EW) as an additional and less subjective figure of merit for XPS narrow scans. We believe that this parameter will prove particularly useful for analyzing series of similar or nominally identical spectra, perhaps as a component of an expert software system for the machine interpretation of spectra. It also appears to be useful, shedding light on the chemical state of materials, when additional information about a sample is known. The EW_{XPS} is simply defined as the area of a narrow scan divided by the height of the maximum of its peak envelope. To limit any ambiguity in EW_{XPS} for a series of spectra, we may also list the peak position of the maximum of the envelope (PE_{max}). The potential usefulness and limitations of the EW_{XPS} and PE_{max} parameters are demonstrated by their application to the narrow scans of: (i) four sets of ozone-treated carbon nanotubes ($EW_{XPS} \sim 2.11$–2.16 eV for a Shirley background, and up to 2.88 eV for no background, $PE_{max} \sim 284.4$–284.5 eV), (ii) a series of silicon wafers with different oxide thicknesses ($EW_{XPS} \sim 1.5$–2.8 eV, $PE_{max} \sim 99$–103 eV), (iii) hydrogen-terminated silicon before and after derivatization with pentyl groups, and after annealing of the pentyl-modified material ($EW_{XPS} \sim 0.7$–1.0 eV, $PE_{max} \sim 25.9$–26.1 eV), and (iv) five nanodiamond samples, where three of the spectra showed charging ($EW_{XPS} \sim 2.6$–4.9 eV, $PE_{max} \sim 272.7$–293.9 eV). In this final example, EW_{XPS} was plotted against PE_{max} to identify the region corresponding to the materials that showed the least charging. EW_{XPS} and PE_{max} appear to correlate with the expected chemistries of all the systems studied. We calculate EW_{XPS} using a Shirley baseline and with no baseline at all. In setting the baseline limits for EW_{XPS}, we consider the derivative of C 1s narrow scans. We also show the application of EW_{XPS} to single, fitted components within a narrow scan.

1. Introduction

XPS is a quantitative, surface sensitive technique that is extremely important for understanding surface chemistries [1]. It is a core electron spectroscopy that functions by illuminating a sample with X-rays and then measuring the kinetic energies of the ejected photoelectrons. These kinetic energies are then converted into binding energies that are plotted as survey (lower resolution) or narrow (higher resolution) scans. Peak fitting of XPS narrow scans often plays a central role in revealing chemical information about a surface or material. However, peak fitting almost always involves at least some degree of user bias/subjectivity. Fortunately, this is not a significant issue in a number of cases. Well-understood and/or relatively simple materials often yield narrow scans that can be well fit and interpreted, especially by experienced practitioners and when additional information, such as process knowledge, is available. However, narrow scans of more complex materials can be difficult to fit, and these problems become particularly severe when inexperienced users apply too many fit parameters to their data without having a solid rationale for their choices. But even competent practitioners appear to struggle with challenging peak fitting problems. As Sherwood emphasized in his paper on peak fitting XPS narrow scans: "there is never a unique solution to fitting the data" [2]. As an additional example, Wepasnick and co-workers fitted the same C 1s narrow scan of oxidized carbon nanotubes using peak parameters from two previously published fits [3–5]. They showed that the *overall* fits to the signals were good in both cases. However, in one fit the signal due to carboxyl groups was 5.9% and in the other 11.0%. Clearly this is a substantial discrepancy that significantly changes one's understanding of this material.

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