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MULTILAYER MODEL SOFTWARE FOR CHEMICAL COMPOSITION ANALYSIS FROM XPS DATA

X-ray Photoelectron Spectroscopy (XPS) is renowned for its acute sensitivity to surface characteristics, which enables detailed quantitative analysis of the elemental and chemical state of surface layers up to approximately 10 nanometers deep. XPS is extensively employed across various industrial and academic settings due to the widespread availability of commercial systems that facilitate comprehensive quantitative studies.
The precision of quantitative XPS analyses hinges on the meticulous fitting of emission peaks and the accurate extraction of their intensities from spectral data, which are critical for correctly determining the sample's chemical makeup. However, this process is complicated by the lack of a unified method within the XPS community for calculating surface compositions, with prevalent studies often misestimating the areas under the emission peaks. The misinterpretations of the data are exacerbated by the extended use of flawed modeling approaches and merely qualitative quantification methods like sensitivity factors and maximum entropy models.
In this study, we present a computational tool that implements the multilayer method (MLM). It is based on databases containing key physical parameters, including photoelectron cross sections, effective electron attenuation lengths, and take-off angles. The analysis is tailored to each elemental species, which significantly refines the precision of structural parameter uncertainties.
We demonstrate the effectiveness of this method by accurately replicating the chemical compositions of several first-row transition metal oxides, such as ferric oxide 〖Fe〗 *(2.00±0.05) O_3 [1], cobalt in cobalt spinel* 〖*Co*〗 *_3 O*(4.0±0.25) [2] and zinc oxide 〖ZnO〗 _(1.00±0.10) [3]. These examples highlight the usefulness of the software and its potential to advance research in materials science.

[1] Bravo Sanchez, M., Huerta-Ruelas J.A., Cabrera-German D., Herrera-Gomez A. Composition assessment of ferric oxide by accurate peak fitting of the Fe 2p photoemission spectrum. Surf Interface Anal. 2016;49:253-260. https://doi.org/10.1002/sia.6124

Keywords

Photoemission spectra, Chemical Quantification, MultiLayer Model

Reference

Cabrera-German, D., Gomez-Sosa, G., Herrera-Gomez, A. Accurate peak fitting and subsequent quantitative composition analysis of the spectrum of Co 2p obtained with Al Kα radiation: I: cobalt spinel. Surf. Interface Anal. 2016, 48, 252–256. https://doi.org/10.1002/sia.5933

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Author approval

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