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Fit and background parameters of the 4f core level of the sixth-row elements using the double Lorentzian line shape.

In this work we will show the fit of some of the transition metals of the sixth period, using the Double Lorentzian line shape, specifically the 4f orbitals with their two branches $7/2$ and $5/2$ and the background used will be the Shirley-type background (SVSC). The fits were performed with the AAnalyzer© software and shared on the web at the <https://xpssoasis.org/> platform. The use of the DL line shape has allowed us to perform high-quality fits in addition to reducing the number of peaks used for each fit, simplifying the analysis process. The DL line shape very accurately models the main peak in all fits, but it was observed that it is always necessary to supplement it with an additional component. The DL line shape is a great alternative for fitting asymmetric spectra compared to the Doniach-Šunjić and Mahan profile which usually do not capture the line shape as well when using an energy range higher than 3 eV, such as when fitting both spin-orbit splitting peaks for p, d and f orbitals, as well as not being integrable. The use of AAnalyzer© software in combination with the DL line shape allowed the resolving overlapping peaks that are not obvious to the naked eye as in the case of Os 4f where the satellites overlap with the 5p component. this phenomenon is also present in the spectra of W4f and Re 4f.

Keywords

Double Lorentzian line shape, XPS, AAnalyzer, SVSC, 4f core level

Reference

A. Herrera-Gomez et al., "Double Lorentzian lineshape for asymmetric peaks in photoelectron spectroscopy," *Journal of Vacuum Science & Technology A*, vol. 41, no. 4, pp. 1–9, 2023, doi: 10.1116/6.0002602.

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