Improved Peak Fit Procedure of XPS Measurements of Inhomogeneous Samples – Development of the Advanced Tougaard Background Method

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Abstract

A new method for the fitting of x-ray photoelectron spectra using an advanced Tougaard background model for laterally inhomogeneous samples is presented. New is the use of a separate loss function for each peak component. Additionally, a new Five parameter inelastic electron scattering cross section (5-PIESCS) including a variable parameter to treat the electronic band gap energy is introduced for a better modelling of the loss structures of insulators. Synthetic generated test spectra using two peaks with strongly different loss structures and measured spectra from different samples are fitted with the traditionally used Shirley background (BSh), the Tougaard background for homogeneous samples (BTH), and the newly developed advanced Tougaard background for laterally inhomogeneous samples (BTI). It was found that the fit results for the peak areas and peak positions of the three methods are strongly different. In many cases the use of the Shirley background and the Tougaard background for homogeneous samples resulted in completely wrong component areas in spite of sometimes rather satisfying residual functions and chi² criteria. In contrast, the advanced Tougaard background for inhomogeneous samples gave excellent results for all wide range spectra including pronounced loss structures. The new source code of the UNIFIT software (Version 2016 or higher) to calculate the advanced Tougaard-background parameters for inhomogeneous samples was verified.

Test Spectra

• The test spectra shall simulate realistic photoelectron spectra from a composition.
• The background calculation based on the Tougaard-background model.
• The number of the separate Tougaard backgrounds with different IESCSs has to be the same as the number of peak-fit components.
• The background calculation is a series calculation.
• The newly introduced 5-PIESCS with the additional band-gap energy parameter (g) permits a better modelling of the loss structure of insulators [1].

Basics

1. Energy separation of the components (10, 20, 30 eV),
2. Intensity ratio of the components (1, 2, 3),
3. Combination with the IESCS-A or IESCS-B (Fig. 1),
   first component with A, second component with B (Fig. 2),
   first component with B, second component with A (Fig. 3).

Fit of Test Spectra

The generated test spectra were fitted with:
1. Model function of photoelectron peaks: Convolution of Lorentzian and Gaussian functions, two components
2. Fit parameters: peak height, Lorentzian and Gaussian FWHM and peak position variable, asymmetry set to zero and fixed
3. Model of background: 2nd order polynomial and a Shirley BSh, a common homogeneous Tougaard background BTg (seven background-fit parameters) and an inhomogeneous Tougaard background BTI (four plus i·5 background-fit parameters, i = number of the peak-fit components) simultaneously to the peak fit.

Summary

1. The advanced Tougaard background (separate Tougaard background function and IESCS parameters for every peak-fit component) permits a perfect simulation of the spectral background of XPS measurements of laterally inhomogeneous samples.
2. The commonly used Shirley or Tougaard method is not qualified to model photoelectron spectra of laterally inhomogeneous samples.
3. The new introduced gap-energy parameter (g) of the 5-PIESCS permits a more reliable modelling of XPS spectra of insulators.

Fit of Inhomogeneous Real Wide Range Spectra

The wide range spectra of Al₂O₃/SiO₂ and Al₂O₃/Si were fitted with the new advanced Tougaard background model for inhomogeneous samples. The peaks as well as the complicated background function were simulated exactly. A quantification after the peak fit gives the correct composition of the laterally inhomogeneous samples.