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

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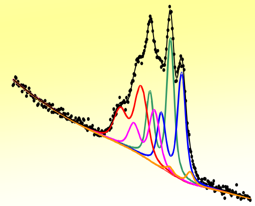


Abstract

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 spectral 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. Synthetically 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 (B_S), the Tougaard background for homogeneous samples (B_{TH}), and the newly developed advanced Tougaard background for laterally inhomogeneous samples (B_{TI}). 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 *Abbe* 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.

Basics

- The interactive background calculation is carried out using the model functions of the peak-fit components.
- 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 T_0 permits a better modelling of the loss structure of insulators [1].

Test Spectra

- The test spectra shall simulate realistic photoelectron spectra from a laterally inhomogeneous sample with two components and two different loss structures of the spectral component.
- Eighteen test spectra using IESCS-A and IESCS-B (Fig. 1) were generated.
- The test spectra are different in:
  1. Energy separation of the components (10, 20, 30 eV),
  2. Intensity ratio of the components (I_1/I_2: 5, 2, 1),
  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).

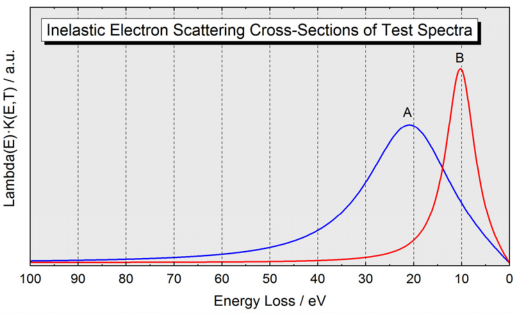


Fig 1: Comparison of IESCS-A and IESCS-B of test spectra

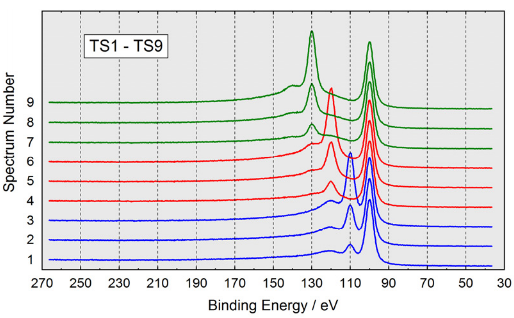


Fig 2: Test spectra with different intensity ratios of two peaks (5, 2 and 1) and IESCS functions (peak1 at 100 eV: IESCS-A, peak 2: IESCS-B), green: peak separation 30 eV, red: peak separation 20 eV, blue: peak separation 10 eV

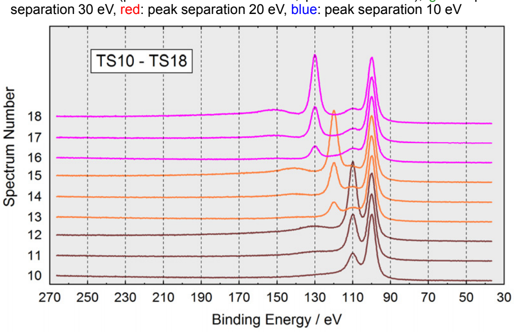
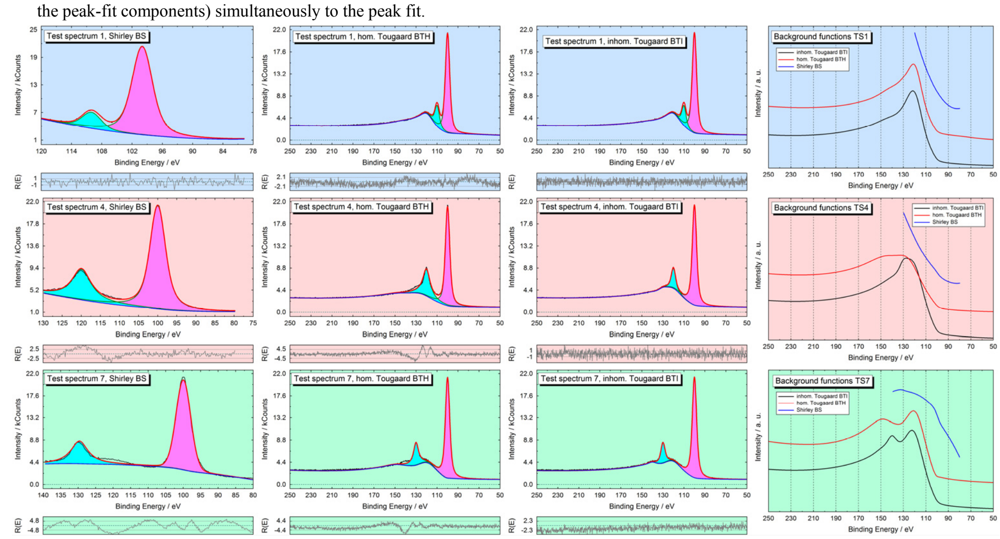


Fig 3: Test spectra with different intensity ratios of two peaks (5, 2 and 1) and IESCS functions (peak1 at 100 eV: IESCS-B, peak 2: IESCS-A), magenta: peak separation 30 eV, orange: peak separation 20 eV, brown: peak separation 10 eV

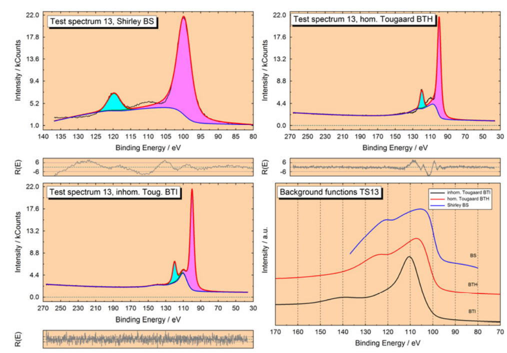
Fit of Test Spectra

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 B_S, a common homogeneous Tougaard background B_{TH} (seven background-fit parameters) and an inhomogeneous Tougaard background B_{TI} (four plus i·5 background-fit parameters, i = number of the peak-fit components) simultaneously to the peak fit.



Figs 4 - 15: Fit of test spectra using Shirley BS, homogeneous Tougaard BTH and inhomogeneous Tougaard background BTI, fit procedure: convolution of Lorentzian and Gaussian functions, blue: peak 2 below the loss maximum, red: peak 2 on the loss maximum, green: peak 2 above the loss maximum



Figs. 16 - 19: Fit of test spectra using BS, BTH and BTI, fit procedure: convolution, inverted IESCS with respect to test spectrum TS4 (Figs. 8 – 11, red)

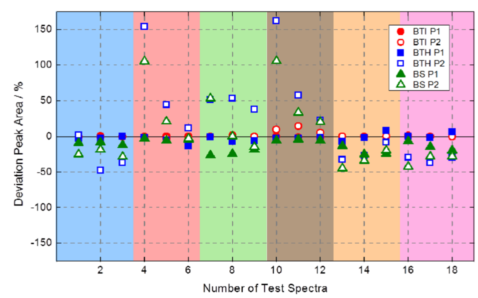


Fig. 20: Deviations (in %) of the fitted peak areas from the true values, blue: 2. Peak below loss maximum, red: 2. Peak on the loss maximum, green: 2. Peak above the loss maximum, brown: inverted IESCS with respect to blue, orange: inverted IESCS with respect to red, magenta: inverted IESCS with respect to green

Fit of Inhomogeneous Real Wide Range Spectra

The wide range spectra of Al_2O_3/SiO_2 and Al_2O_3/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.

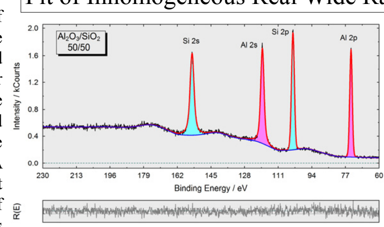


Fig. 21: Peak fit of the Al_2O_3/SiO_2 wide range spectrum using the inhomogeneous Tougaard background

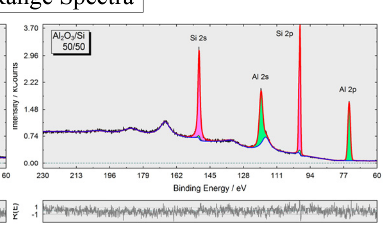


Fig. 22: Peak fit of the Al_2O_3/Si wide range spectrum using the inhomogeneous Tougaard background

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 T_0 of the 5-PIESCS permits a more reliable modelling of XPS spectra of insulators.

Lit: [1] R. Hesse, M. Weiß, R. Szargan, P. Streubel, R. Denecke, Improved Peak Fit Procedure of XPS Measurements of Inhomogeneous Samples – Development of the Advanced Tougaard Background Method, accepted, J. Electron Spectrosc. Relat. Phenom.