Comparative Study of Improved Tougaard Background and Shirley Background Calculations using Test Functions and Real Photoemission Spectra

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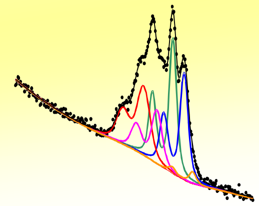

Aim

The shape of the background in x-ray photoemission spectra is affected by secondary electrons and inelastic energy loss processes. A polynomial of low order has very often turned out to model the secondary electron background. The Tougaard background model [1] has been successfully used to characterise the inelastic loss processes. However, the correct usage of the Tougaard background needs a well defined $\lambda(E)\cdot K(E,T)$ function (T = energy loss). The introduction of a four parameter **I**nelastic **E**lectron **S**cattering **C**ross-**S**ection (4-IESCS)

$$\lambda(E)\cdot K(E,T) = \frac{BT}{(C + C'T^2)^2 + DT^2}$$

with the fitting parameters B, C, C' and D implemented in the fittable background function [2, 3] permits the generation of an improved Tougaard background. The fitting results of test spectra and a real photoemission measurement using the improved Tougaard background and the traditional Shirley background will be compared and the advantage of the new method will be shown.

Generation of Test Spectra

- Nine test spectra were generated using a new developed iteration procedure
- The test spectra shall simulate realistic photoelectron spectra with a typical loss structure (e.g. SiO_2). Steps:

1. Generation of the primary spectrum with 2 peaks (Voigt profile):
   a) energy range: 36.6 eV – 266.3 eV,
   b) peak separation: 10 eV, 20 eV, 30 eV,
   c) intensity ratio: 0.5, 2.0, 5.0
2. Generation of the background with a
   a) polynomial function and a
   b) Tougaard background including a loss structure defined by the IESCStest (B = 300 (eV)^2, C = 550 (eV)^2, C' = 1, D = 500 (eV)^2)
3. Iterative generation of the test spectra using 20 cycles.
4. Test spectra were affected with statistical noise.

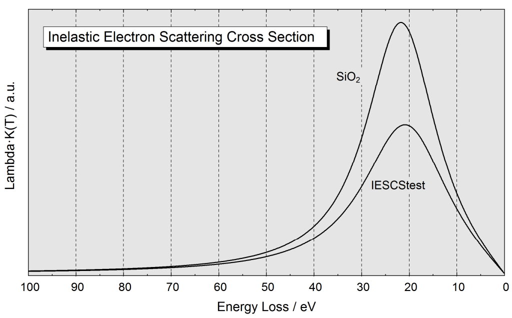

Fig 1: Comparison of a real IESCS of SiO_2 and the IESCStest used for the generation of the test spectra

Intensity/counts Intensity ratio	Separation/eV and Peak position/eV		
	Separation: 10 Peak 1: 100 Peak 2: 110	Separation: 20 Peak 1: 100 Peak 2: 120	Separation: 30 Peak 1: 100 Peak 2: 130
P1: 10000 **P2:** 20000 Intensity ratio: 0.5	Test spectrum **1**	Test spectrum **4**	Test spectrum **7**
P1: 20000 **P2:** 10000 Intensity ratio: 2	Test spectrum **2**	Test spectrum **5**	Test spectrum **8**
P1: 20000 **P2:** 4000 Intensity ratio: 5	Test spectrum **3**	Test spectrum **6**	Test spectrum **9**

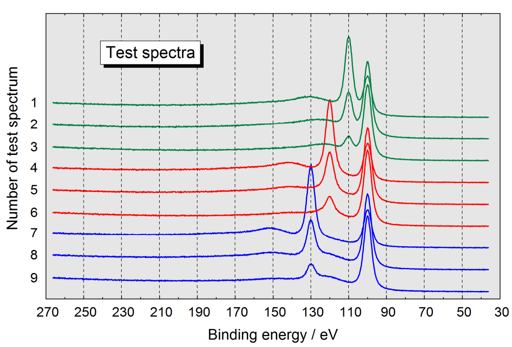

Fig 2: Test spectra with different intensity ratios of two peaks (0.5, 2.0 and 5.0), green: peak separation 10 eV, red: peak separation 20 eV, blue: peak separation 30 eV

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 or Tougaard background (background-fit parameters: a, b, c, B, C, C', D) simultaneously to the peak fit.

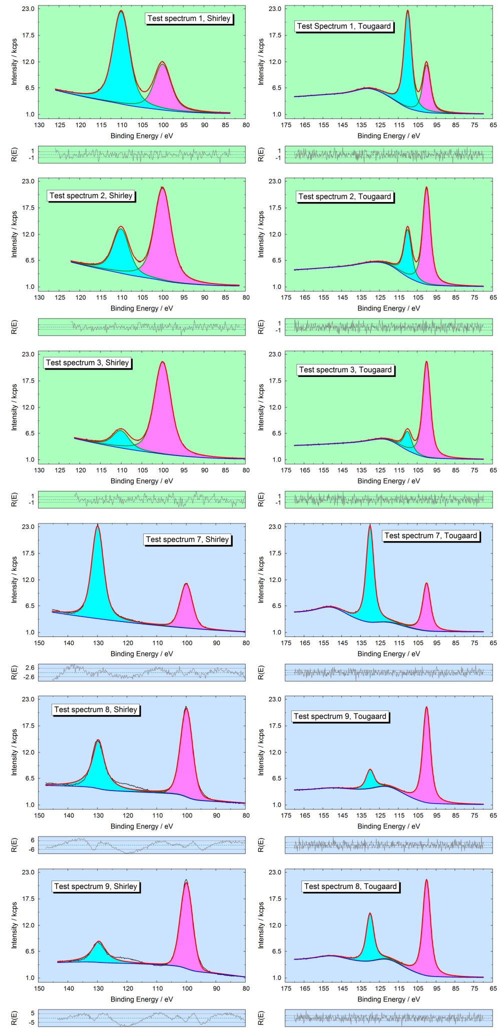

Fig 3 - 20: Fit of test spectra using Shirley and Tougaard background, fit procedure: convolution of Lorentzian and Gaussian functions, green: peak 2 below the loss maximum, red: peak 2 on the loss maximum, blue: peak 2 above the loss maximum

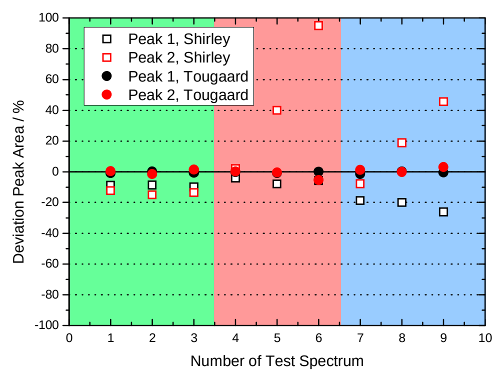

Fig. 21: Deviations (in %) of the fitted peak areas from the true values, green: 2. Peak below loss maximum, red: 2. Peak on the loss maximum, blue: 2. Peak above the loss maximum

Fit of Au Survey Spectrum

The Au survey spectrum was fitted with five peaks and two different background models:
1. Polynomial plus Shirley background
2. Polynomial plus Tougaard background and fittable parameters of the Inelastic Electron Scattering Cross Section (no direct interference of loss maximum with peak separation)

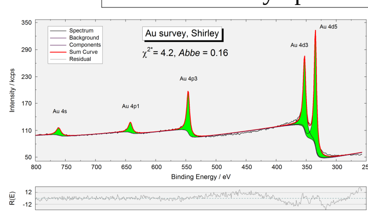

Fig. 22: Peak fit of the Au survey using polynomial and Shirley background

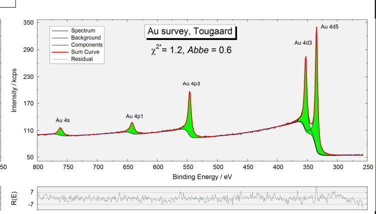

Fig. 23: Peak fit of the Au survey using polynomial and improved Tougaard background

Summary

1. The improved Tougaard background (integrated fit of IESCS parameters) permits a perfect simulation of the spectral background.
2. The commonly used Shirley method is not qualified to model a photoelectron background with strong loss structures.
3. The peak-area errors can exceed 100% in case of specific intensity ratios and peak separations and using the Shirley background.
4. The Au survey spectrum can be fitted satisfactorily using the improved Tougaard background only (however, relative peak areas similar).

Lit: [1] S. Tougaard, Surf. Interface Anal. 25 (1997) 137, [2] R. Hesse, T. Chassé, R. Szargan, Fresenius J. Anal. Chem., 365 (1999) 48, [3] R. Hesse, R. Denecke, Surf. Interface Anal. (accepted, early view)