Improved Tougaard Background Calculation with Predetermined Inelastic Electron Scattering Cross Section Functions $\lambda \cdot K(T)$ Using the Software UNIFIT 2011

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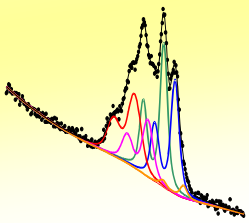

Aim

The new UNIFIT 2011 version allows an improved Tougaard background [1] calculation:
1. Introduction of the **F**our **P**arameter **I**nelastic **E**lectron **S**cattering **C**ross **S**ection (FPIESCS),
2. FPIESCS parameters were defined as fittable parameters,
3. Integration of the FPIESCS parameters in the fittable background function [2],
4. Estimation of the FPIESCS parameters parallel to the fit of the peaks and background function,
5. Determination and saving of FPIESCS of clean surfaces of elements and compounds.

Theory

1. Peak shape analysis by minimization of χ^2:

The determination of the parameter set $\vec{p}$ to describe the peak shape and the background function of photoelectron spectra can be made by minimization of χ^2

$$\chi^2(\vec{p}) = \frac{1}{N-P}\sum_{j=1}^{N}\frac{[S(i,\vec{p})-M(i)]^2}{M(i)}$$

with the measured spectrum $M(i)$ recorded at N energy values corresponding to channels i, the synthesized model curve $S(i,\vec{p})$ and the number of fit parameters P.

2. Definition of the model curve S:

In case of a calculation of the spectral background parallel to the peak fit the model curve can be described by

$$S(i,\vec{p}) = \sum_{j=1}^{k} SC_j(i,\vec{p}_j) + B(i,\vec{p}_B)$$

with k different species (components) $SC_j(i,\vec{p})$, the spectral background $B(i,\vec{p}_B)$ and the fittable background parameters $\vec{p}_B$ (the parameters $a, b, c, d, e, B, C, C', D$). The peak shape of the components $SC_j(i,\vec{p})$ are typically determined by a Lorentzian contribution L and a Gaussian broadening G [3] (product, sum or convolution of L and G).

3. Definition of the background function B:

The most universal description of the spectral background [2] includes a polynomial of low order to model the secondary electrons, the Shirley-type step function $S_B(E)$ and the more advanced Tougaard background model $T_B(E,B,C,C',D)$.

$$B(E,\vec{p}_B) = a + bE + cE^2 + dE^3 + eS_B(E) + T_B(E,B,C,C',D)$$

The background-fit parameters a – d define the polynomial and the parameter e gives the part of the Shirley-type background.

4. Definition of the Tougaard background T_B:

The Tougaard background $T_B(E)$ is defined by

$$T_B(E) = \lambda(E)\int_E^{\infty} K(E,T)M(E')dE'$$

with the energy loss $T = E - E'$ and the inelastic-electron scattering cross section $\lambda \cdot K$. The shape of the Tougaard background is strongly affected with the definition of $\lambda \cdot K$. The Two- and Three-parameter inelastic electron scattering cross section recommended by Tougaard is improved to the Four-parameter inelastic electron scattering cross section (FPIESCS) by implementation of the additional parameter C'. Now the IESCS fit parameters are B, C, C', D:

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

Input/Output Dialogs

The new UNIFIT 2011 allows the manual definition (see Fig. 1) of the Tougaard background parameters. All parameters may be increased or decreased stepwise using scrollbars or can be putted in directly in the edit fields. The B-parameter may be adjusted optionally.
Basically, the Tougaard-background parameters can be fitted parallel with the peak fit (see Fig 2). Optionally, the parameters may be fixed at certain values. The FPIESCS parameters can be saved and loaded separately.
The functions of calculated inelastic electron scattering cross sections may be plotted. The fitted background parameters are saved in the UNIFIT projects, too.

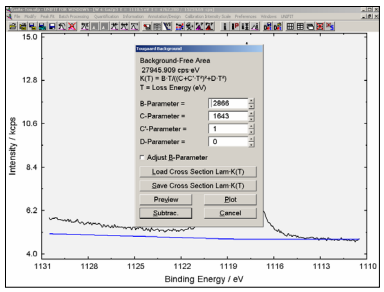

Fig 1: Tougaard-background input dialog for a approximation, saving and loading of the FPIESCS parameters

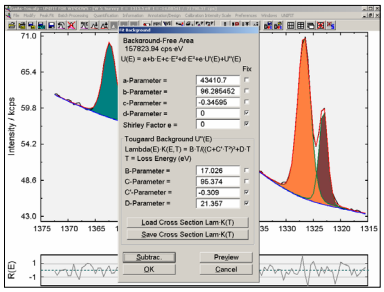

Fig 2: Fittable-background input dialog for the determination of the background-fit parameters parallel to the peak fit

Example: Oxidized GaAs

The Ga 2p and As 2p peaks of the XPS survey spectrum of GaAs oxidized by Ozone were corrected by the transmission function and fitted with:
1. Four components, model function: Sum of Lorentzian and Gaussian functions
2. Determination of the background consisting of a 2rd order polynomial and a Tougaard background (background-fit parameters: a, b, c, B, C, C', D) parallel to the peak fit.

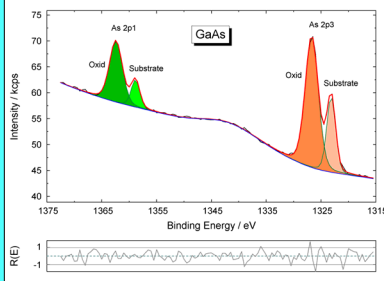

Fig 3: Spectrum fit of the As 2p peak form oxidized GaAs using 4 peaks and fittable background with polynomial and Tougaard background

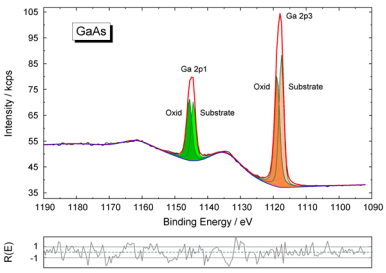

Fig 4: Spectrum fit of the Ga 2p from oxidized GaAs using 4 peaks and fittable background with polynomial and Tougaard background

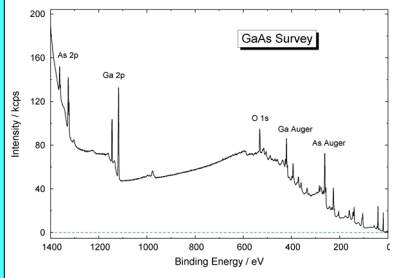

Fig 5: Survey of oxidized GaAs

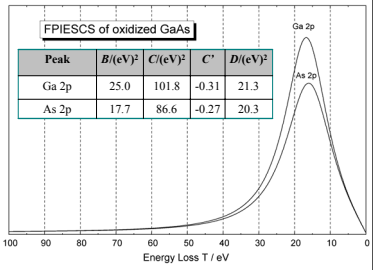

Fig 6: Calculated FPIESCS of oxidized GaAs deviated from the Ga 2p and As 2p peak, image created using UNIFIT 2011, exported and inserted in this paper

Comparison of the results of Tougaard and Hesse

The inelastic electron scattering cross sections recommended by Tougaard and calculated by Hesse are compared using three examples: PMMA (Fig. 7), Au (Fig. 8) and SiO_2 (Fig. 9).

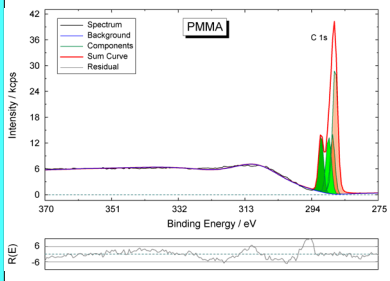

Fig 7: Spectrum fit of the C 1s peak form PMMA using 4 peaks and fittable background with polynomial and Tougaard background

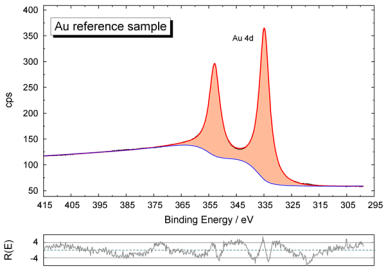

Fig 8: Spectrum fit of the Au 4d peak form the Au reference sample using 1 doublet and fittable background with polynomial and Tougaard background

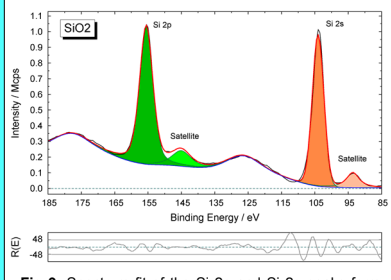

Fig 9: Spectrum fit of the Si 2p and Si 2s peaks form SiO_2 using 4 peaks and fittable background with polynomial and Tougaard background

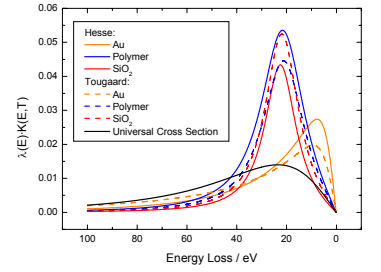

Fig 10: Comparison of the calculated inelastic electron scattering cross sections recommended by Tougaard [1] (dashed lines) and calculated by Hesse (solid lines)

Summary

1. The introduction of the FPIESCS with adjustable parameters permits the determination of the inelastic electron scattering cross section parallel to the peak fit using UNIFIT 2011.
2. The peak fit over a wide energy range with a fittable background consisting of polynomial and improved Tougaard background gives an excellent description of the energy loss structures.
3. The new determined IESCSs of Au, PMMA and SiO_2 are different from those recommended by Tougaard. But the general profiles and energy positions of the maximum are similar.
4. Tougaards Universal cross section is not suitable for the fit of all studied photoelectron lines.

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, P. Streubel, R. Szargan, Surf. Interface Anal. 39 (2007) 381

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