UNIFIT 2017 – the New Spectrum Processing, Analysis and Presentation Software for XPS, AES and XAS

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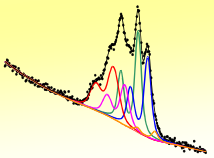

Abstract

Auger electron spectroscopy (AES) can provide information which is either complementary to such obtained by x-ray photoelectron spectroscopy (XPS) or opens additional experimental options. Therefore, possibilities for analysing AES data are implemented. Now measurements of photoelectron spectra (XPS), Auger electron spectra (AES) and X-ray absorption spectra (XAS) can be analysed. The identification of the Auger lines is supported by new implemented data bases. A special calculation tool allows for the estimation of AES sensitivity factors. The quantification can be carried out using integral or differential Auger spectra. Additionally, empirical sensitivity factors of different spectrometer types were implemented.
The calculation of the transmission function *T(E)* was improved, now allowing *T(E)* determination using variable kinetic energies, intensity ratios and atomic ratios of the used peaks. The total full width at half maximum (*FWHM*) of original and processed spectra can be estimated separately using a new developed routine. The total *FWHM* is displayed additionally in the fit-parameter table using the convolution routine at the peak fit. In order to load and analyse scanning Auger microscopy (SAM) measurements or XPS mappings of more than 65536 spectra (265x256), the main-memory management was optimized. As the result of the software optimisation the number of simultaneously processable spectra was increased to 75600. The generation and display of windows video sequences enhances the presentation of sputter depth profile multipoint measurements.

XPS, AES and XAS Spectra

- 330 different data formats of XPS, AES and XAS measurements can be loaded:
  1. multi region measurements
  2. parameter dependent measurements (e.g. ARXPS, sputter depth profile)
  3. multipoint measurements (e.g. Multipoint XPS, SAM)
  4. Multipoint sputter depth profile measurements.
- Ten different data presentations are offered: spectra, parameter plots, six different 3D plots, Wagnerplot and video sequences.
- Maximal 75600 spectra are simultaneously processable .
- Qualitative analysis is supported by a data base with more than 1500 XPS lines and AES transitions.
- Quantitative analysis may be carried out using different data bases of sensitivity factors for XPS and AES.
- In UNIFIT the chemical shifts of 325 XPS lines and AES transitions are saved for the chemical analysis.
- Peak fit using different model functions for the peak shape and spectral backgrounds available.
- Export of calculated data and designed presentable graphics are offered.

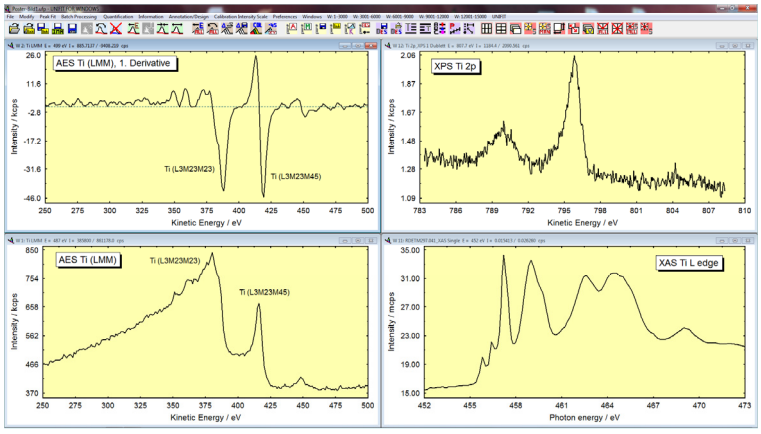

Fig. 1. Presentation of corresponding XPS, AES, and XAS lines in four windows, top left: 1. derivative of Ti (LMM), bottom left: Ti (LMM), top right: Ti 2p, bottom right: Ti L edge

Improved Method for the Estimation of Transmission Functions

The UNIFIT software offers two different methods for the estimation of the transmission functions *T(E)* (IERF – Intensity-Energy Response Function) of different recording settings of electron spectrometers [1]:
1. Survey spectra approach (SSA),
2. Quantification of reference-peak areas (QPA).

Typically, both methods use the reference materials Au, Cu and Ag. The second method QPA was improved for the use of reference compounds and variable excitation energies. The model function for the estimation of *T(E)* is given by

$$T(E) = a + b\varepsilon + c\varepsilon^2 + d\varepsilon^3 + e\varepsilon^4 + fE^g$$

with the fit parameters $a - g$ and $\varepsilon = (E - 1000\ \text{eV})/1000\ \text{eV}$. With the well known values of the inelastic mean free path $\lambda(E)$, the ionization cross section $\sigma(E, h\nu)$ and the peak area A_G the reference areas are given by

$$A(El) = \frac{A_G(El)}{\lambda(E)\sigma(E)}$$

The *T(E)* function can be estimated by fitting of the parameters $a - g$ in order to find the minimum of *FQS*

$$FQS = \sum_{n=1}^{k}\left(\frac{T(E_{2n})\cdot X_{2n-1}\cdot A_{2n-1}(El_{2n-1})}{T(E_{2n-1})\cdot X_{2n}\cdot A_{2n}(El_{2n})} - 1\right)^2$$

(*k* = number of pairs (max. 10), *El* = element, *X* = number of atoms of an element in the compound)

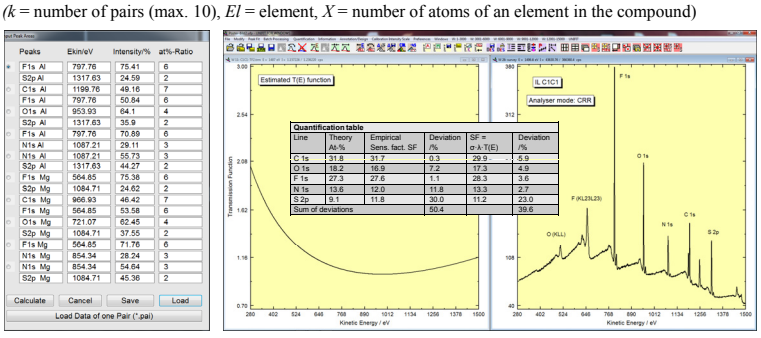

Fig. 2. Left: Table shows the reference areas of the IL C1C1 which consists of 22 atoms ($C_7O_4F_6N_3S_2$), chosen reference pairs: F1s/S2p, C1s/F1s, O1s/S2p, N1s/F1s, N1s/S2p, right: estimated transmission function and survey of C1C1, inset: table of quantification using different sensitivity factors .

AES Emission Yield Calculation Tool

A pseudo-first principle technique for Auger quantification is used to calculate relative Auger electron emission yield σ_{AES} of the element *i* and transition *u* as calculated by [2].

$$\sigma_{AES,i} = \gamma_i \cdot \sigma_{u,i} \cdot r$$

where $\sigma_{u,i}$ is the ionization cross section of the *u*th level (in cm²), *r* the backscatter correction factor and γ the Auger transition probability. For the relative quantification the Auger sensitivity factor *SF* of an element *i* with the transmission function of the spectrometer *T* and the mean free path λ is therefore given by

$$SF_i = \sigma_{AES,i} \cdot \lambda_i \cdot T(E)$$

The necessary input data are:
1. Atomic number Z ,
2. The value a for K-, L-, M- and N-electrons (available in UNIFIT and can be selected),
3. Number of electrons in the ionization sub shell (available in UNIFIT and can be selected) ,
4. Excitation energy E_P
5. Binding energy of the target atom sub shell (saved in a data base, can be changed and extended)

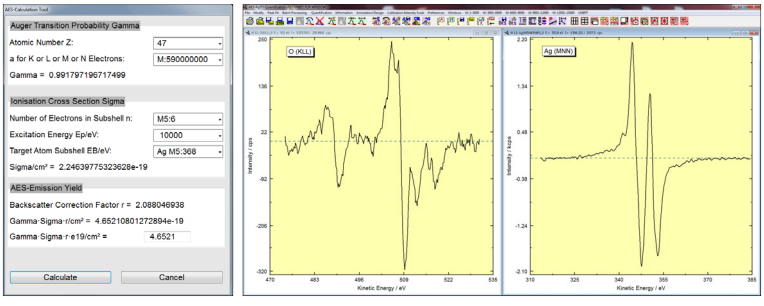

Fig. 3. Left: Dialogue for the calculation of the AES-emission yield (example shows the calculation for the transition Ag (M5N45N45) at the excitation energy 10000 eV), right:: 1. Derivative of O (KLL) and Ag (MNN) of the sample Ag_2O

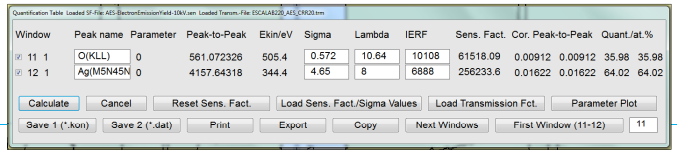

Fig. 4. Quantification table of sample Ag_2O, Sigma values of the AES lines are calculated using the AES-emission yield calculation tool.

Dynamical Presentations as Windows Video Sequences

A new dynamic presentation tool was implemented in the software UNIFIT. All available windows types (e.g. standard spectra, 3D presentations) can be presented as windows video sequence. The following settings are possible:
1. Normalization of the Min/Max values,
2. Frame-dwell time of presentation of each window,
3. Size and position of all windows presented using the video sequence.

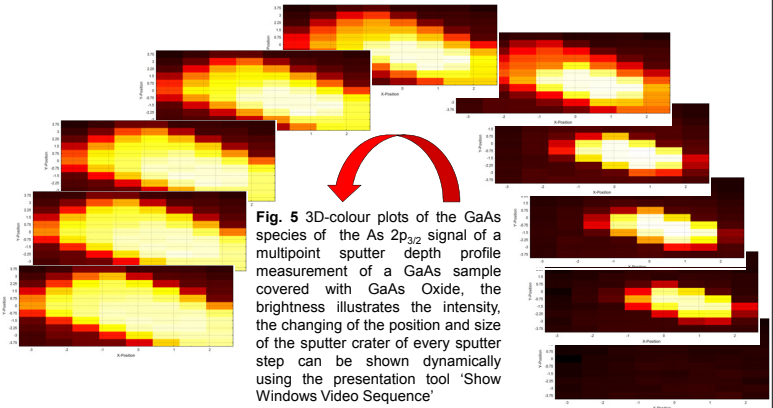

Fig. 5 3D-colour plots of the GaAs species of the As $2p_{3/2}$ signal of a multipoint sputter depth profile measurement of a GaAs sample covered with GaAs Oxide, the brightness illustrates the intensity, the changing of the position and size of the sputter crater of every sputter step can be shown dynamically using the presentation tool 'Show Windows Video Sequence'

References
[1] Improved accuracy of quantitative analysis using predetermined spectrometer transmission functions with UNIFIT 2004, R. Hesse, P. Streubel, R. Szargan, *Surf. Interface Anal., 37 (2005) 589 – 607* ,
[2] Quantitative AES of binary alloys: A comparison between handbook and pseudo-first principles correction, S. Mroczkowski, D. Lichtman, *Surf. Science, 127 (1983) 119*

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