New features of the spectra processing, analysis and presentation software for XPS – UNIFIT 2007

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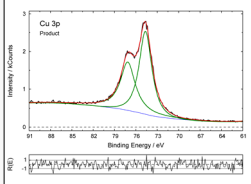
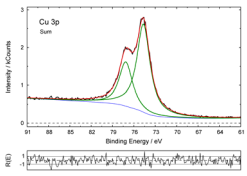
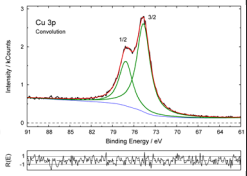
Abstract:

The new version of the spectra processing, analysis and presentation software UNIFIT will be presented. The latest upgrade includes four new features: (i) the implementation of the sum model for fitting photoelectron spectra, (ii) the estimation of valence-band edges, (iii) the 3D-presentation of fitted spectra and (iv) an improved quantification sub-routine.

(i) Implementation of the sum model for fitting photoelectron spectra

The latest upgrade offers now all three commonly applied models for fitting photoelectron spectra: **product**, **sum** and **convolution** of Gaussian and Lorentzian functions. The Cu 3p spectrum was fitted with two independent single lines and an adjustable background consisting of a 3rd degree polynomial and a Shirley background. The theoretically expected intensity ratio of the **$3p_{3/2}/3p_{1/2}$** of **2:1** is well reproduced applying the sum or convolution model function.
(G', G'', L', L'' with the mixing ratio modified Gaussian and Lorentzian functions)

Product	Sum	Convolution
$f(E) = G'(E) \cdot L'(E)$	$f(E) = G''(E) + L''(E)$	$f(E) = G(E) * L(E)$
		
Area ratio Cu $3p_{3/2}$/Cu $3p_{1/2}$: 1.23	**Area ratio Cu $3p_{3/2}$/Cu $3p_{1/2}$: 2.06**	**Area ratio Cu $3p_{3/2}$/Cu $3p_{1/2}$: 2.04**

(ii) Estimation of the valence-band edge using curve fit

In contrast to the traditional procedure defining the valence-band edge by a linear approximation a more realistic approach convoluting square root *W(E)* and Gaussian function *G(E)* is used. A synthetic test spectrum *f(E)* was generated with the following conditions:
*f(E) = W(E)*G(E)*
Valence-band edge (zero point of *W(E)*): 1.50 eV
FWHM Gaussian peak: 2.5 eV
normally distributed statistical noise
The presented examples show the approach with the traditional method (linear function, Fig. 1) and the more realistic approach (convolution function, Fig. 2).

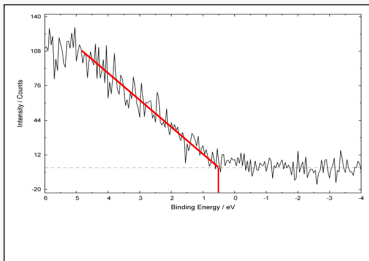


Fig. 1. Estimated valence-band edge: **0.5 eV** red: linear function

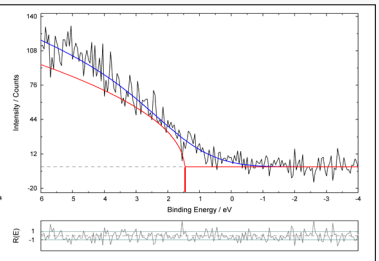


Fig. 2. Estimated valence-band edge: **1.47 eV**, FWHM Gaussian function: 2.72 eV, red: square root function, blue: convolution

(iii) 3D presentation of fitted spectra

In addition to the 3D plot of parameter dependent measurements in the former version the UNIFIT 2007 presents the possibility for an 3D plot of fitted spectra.

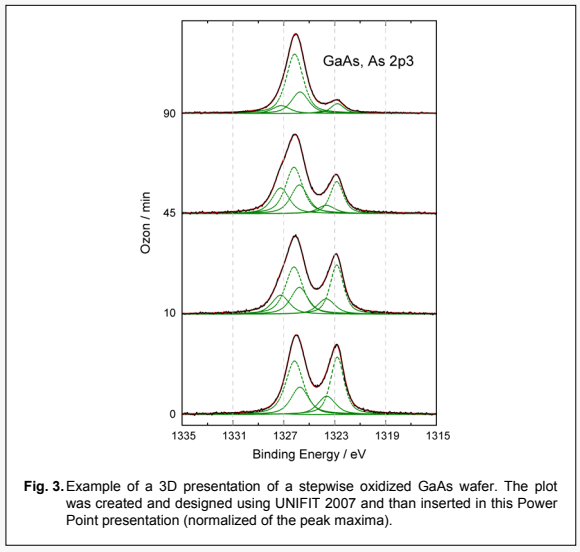


Fig. 3. Example of a 3D presentation of a stepwise oxidized GaAs wafer. The plot was created and designed using UNIFIT 2007 and than inserted in this Power Point presentation (normalized of the peak maxima).

(iv) Improved quantification sub-routine

Now the results of the peak fitting procedure are transferred directly to the quantification sub-routine (Fig. 4). A special feature is a quick export of the quantification table with an excellent resolution of 600 dpi (Fig. 5). The exported table can be integrated in other documents implementing suitable descriptions of the chemical components.

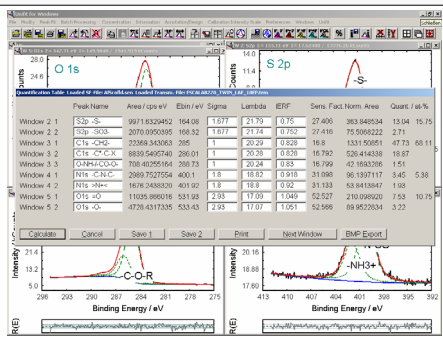


Fig. 4. Quantification sub-rotine of UNIFIT 2007

Fig. 5. Exported and in this Power Point paper inserted quantification table

Peak Name	EB / eV	Area / cps eV	Sens. Fact.	Norm. Area	Quant. / at-%	
S2p -S-	164.08	9971.6329	27.406	363.84853	13.04	15.75
S2p -SO3-	168.32	2070.0950	27.416	75.506822	2.71	
C1s -CH2-	285	22369.343	16.8	1331.5085	47.73	68.11
C1s -C*-C-X	286.01	8839.5495	16.792	526.41433	18.87	
C1s -CO-NH- / -CO-O-	288.73	708.40255	16.799	42.169328	1.51	
N1s -C-N-C-	400.1	2989.7527	31.098	96.139711	3.45	5.38
N1s -'N+'-	401.92	1676.2438	31.133	53.841384	1.93	
O1s =O	531.93	11035.866	52.527	210.09892	7.53	10.75
O1s -O-	533.43	4728.4317	52.566	89.952283	3.22	

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