

What is new in UNIFIT 2007

The latest upgrade of the spectra processing, analysis and presentation software UNIFIT 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) UNIFIT 2007 offers now all three commonly applied models for fitting photoelectron spectra: product, sum and convolution of Gaussian and Lorentzian functions. For all three models relative or absolute parameters can be used. The background can be estimated simultaneously to the peak fitting routine.

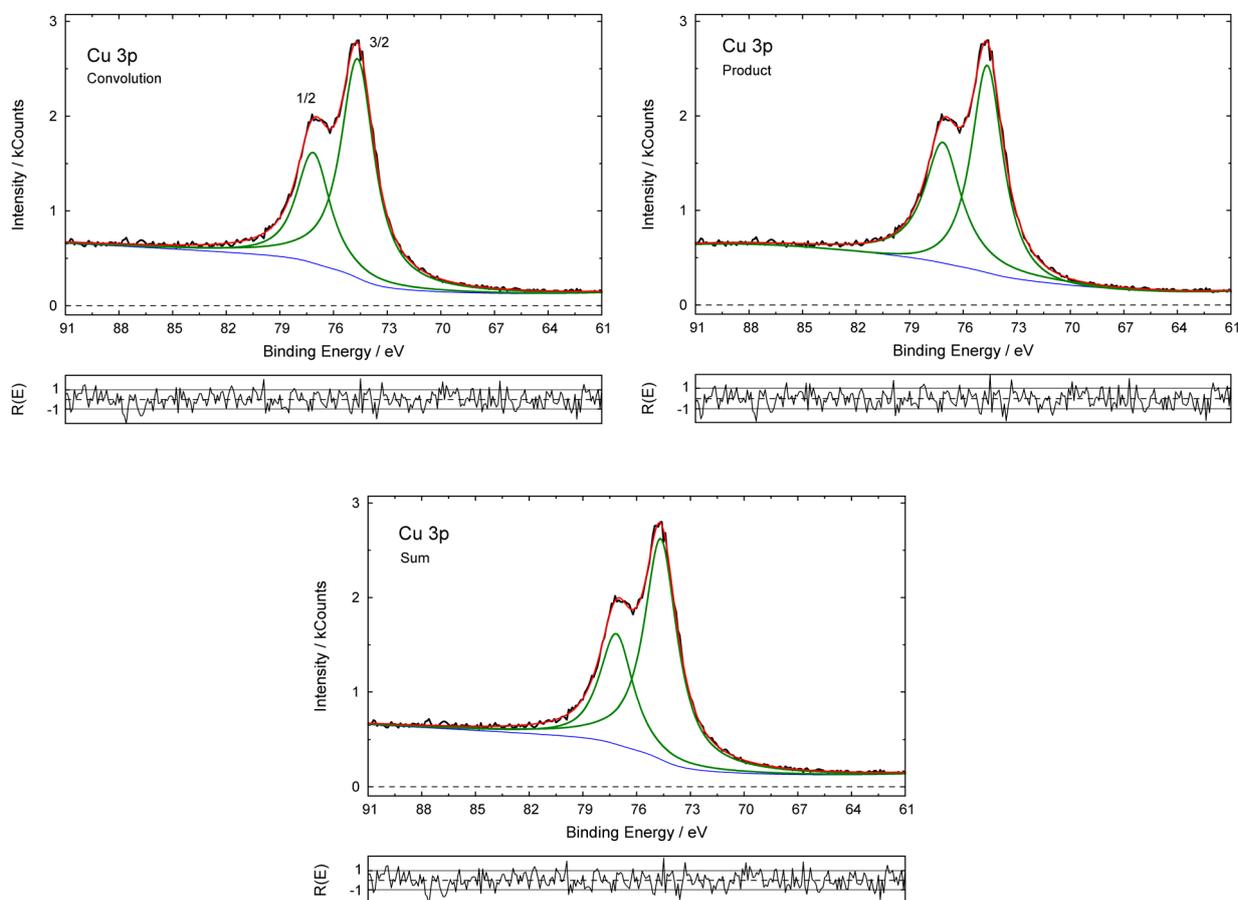


Fig. 1. Fit of a Cu 3p spectrum using different model functions, convolution, product and sum of Gaussian and Lorentzian functions, area ratios Cu 3p_{3/2}/Cu 3p_{1/2}: convolution: 2.04, product: 1.23, sum: 2.06

The fit parameter errors for all three models can be calculated. In order to demonstrate the performance of this new part of the program three different fits of a Cu 3p spectrum and the area ratio of the both peaks are presented (see Fig. 1). The theoretically expected intensity

ratio $\text{Cu } 2p_{3/2}/\text{Cu } 2p_{1/2} = 2$ is well reproduced applying the sum or convolution approaches only (see publications).

(ii) In contrast to the traditional procedure defining the valence-band edge by a linear approximation a more realistic approach convoluting square root and Gaussian functions is used. During the iteration procedure the line width of the Gaussian function may be varied or fixed at a certain value. The adaptation of a synthetic test spectrum (FWHM-Gaussian peak: 2.5 eV, valence-band edge: 1.5 eV, normal distributed noise) is demonstrated (see Fig. 2).

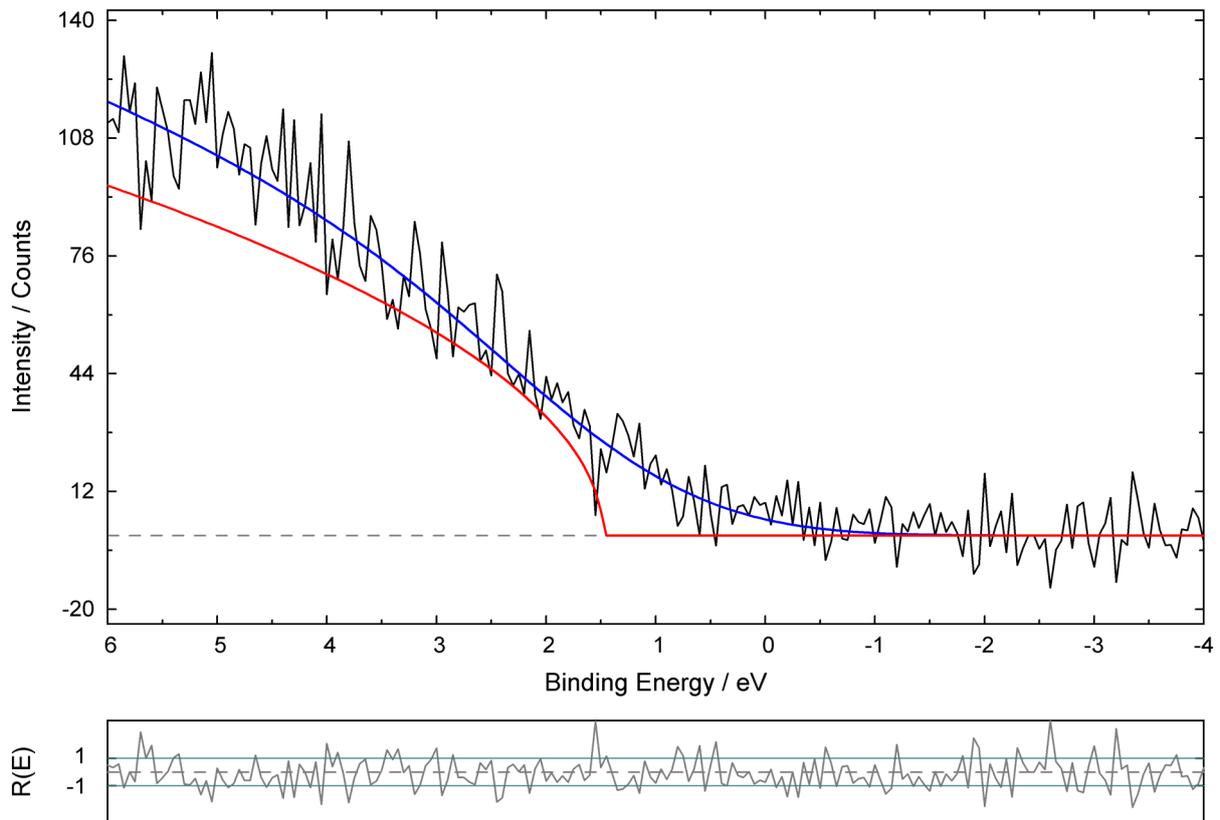


Fig. 2. Valence-band edge estimation of a test spectrum using the fit procedure of UNIFIT 2007, calculated valence-band edge: 1.47 eV, red: square root function (rescaled), blue: convolution of square root and Gaussian functions

(iii) In addition to the 3D-plot presentations of parameter dependent measurements in the former version the UNIFIT 2007 presents the possibility for an additional 3D-plot of the fitted spectra. Extensive tools and a high resolution export routine permit the graphical design and a quick export and implementation of the figures into Word- or Power Point documents with an excellent quality (see Fig. 3).

(iv) The quantification sub-routine was improved. Now the results of the peak fitting procedure are transferred directly to the quantification sub-routine. A special feature is the quick export of the calculated quantification table with an excellent resolution of 600 dpi (see

Fig. 4). The exported table can be integrated easily in other documents implementing freely selectable characters.

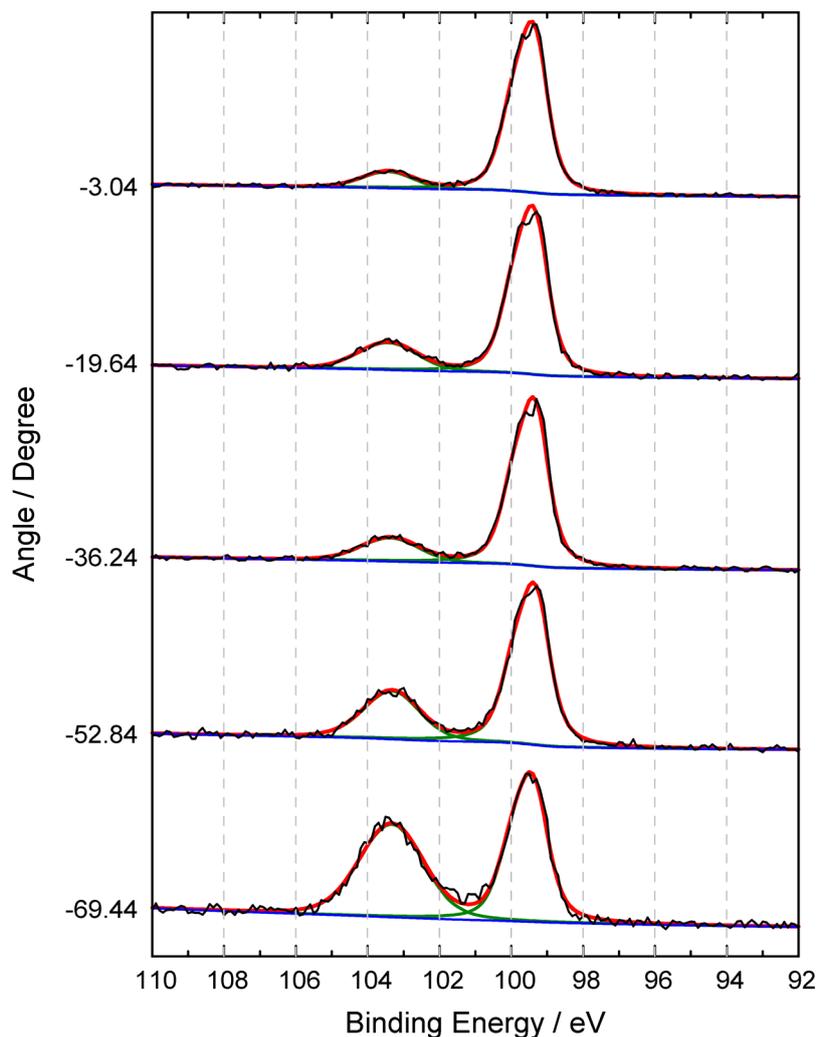


Fig. 3. Example of a 3D presentation of fitted spectra from an ARXPS measurement of SiO₂ with UNIFIT 2007. The plot was created using UNIFIT 2007 than exported as BMP-file and inserted as graphic in this Word document. The angle-dependent height of the SiO₂ signal can be observed. Spectra are normalized.

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	

Fig. 4. BMP plot of the quantification table generated and exported with UNIFIT 2007 and inserted in this Word document. The quantification includes four elements (O 1s, S 2p, C 1s, N 1s). (example: *Unifit 2007\examples\projects\sulphur_study.ufp)

Additionally the number of the readable measurement formats was increased by three (PHI-545/590, PHI-1600/1600C, Avantage-AVG format). The input sub-routine of the VGX-900 data format and the printing outs of the results were improved. Now the start parameters of the peak fit can be selected using the data banks of UNIFIT 2007.