

What is new in UNIFIT 2017?

In order to load and analyse multipoint measurements or mappings of more than 65536 spectra (265x256) using UNIFIT, the main aim of the improvement of the **UNIFIT 2017 software** was the optimization of main-memory management by UNIFIT. As the result of the software optimisation the number of simultaneously processable spectra was increased from 14400 to 75600. A third method was implemented in the new software. Now measurements of photoelectron spectra (XPS), Auger electron spectra (AES) and X-ray absorption spectra can be analysed.

- i)** The definition of the general programme parameters of the UNIFIT software was optimized. Now, the number of the fit components can be settled from 1 to 30.
- ii)** The highest number of the first standard window was increased from 41 to 101. This allows the generation of 100 3D or parameter plot windows.
- iii)** The maximum number of simultaneously processable spectra windows was increased to 75600. The standard-window selection dialogue was adjusted to the large number of processable spectra.
- iv)** The generation and showing of windows video sequences of standard, 3D and parameter plot windows was implemented.
- v)** A batch processing routine for the generation of a large number of 3D windows was created. This procedure allows a fast preparing of windows video sequences of sputter depth profile multipoint measurements.
- vi)** The parameter plot can be created with respect to the x axis or y axis position of the recording point.
- vii)** Now the UNIFIT logo (*.wmf) is available in the folder Unifit_2017_User_Files and can be replaced easily by the own company logo.
- viii)** The manual setting of the maximum intensity of '3D Colour Profiles' was added into the programme code.
- ix)** The energy range of the plot of transmission functions T(E) was increased. The plot is displayed from 200 to 5100 eV (see Fig. 1).
- x)** The calculation of the transmission function T(E) was improved. A separate new routine allows the T(E) calculation using variable kinetic energies, intensity ratios and atomic ratios of the used peaks (see Fig. 2). Ten peak pairs can be used.
- xi)** The export of data was improved. Now the export of data of standard windows is possible from the active window, from the windows selected before and from all windows. Every exported data set is saved in a separate file (*.dat).

- xii) The FWHM can be estimated separately using a new developed routine. The FWHM can be displayed of original spectra and modified spectra. The FWHM is displayed additionally in the fit-parameter table using the convolution routine at the peak fit.

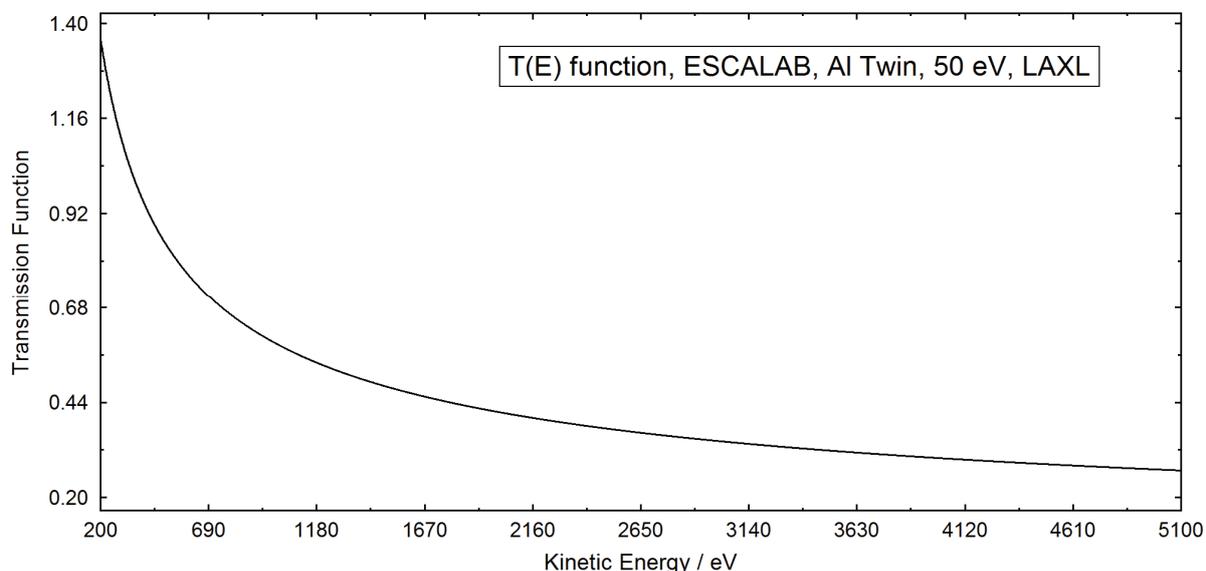


Fig. 1. Plot of the transmission function $T(E)$ of the spectrometer ESCALAB 220 iXL, recording condition: source: Al Twin, pass energy: 50 eV, lens mode: LAXL

Peaks	Ekin/eV	Intensity/%	at%-Ratio
<input checked="" type="radio"/> F1s Al	797.76	75.41	6
<input type="radio"/> S2p Al	1317.63	24.59	2
<input type="radio"/> C1s Al	1199.76	49.16	7
<input type="radio"/> F1s Al	797.76	50.84	6
<input type="radio"/> O1s Al	953.93	64.1	4
<input type="radio"/> S2p Al	1317.63	35.9	2
<input type="radio"/> F1s Al	797.76	70.89	6
<input type="radio"/> N1s Al	1087.21	29.11	3
<input type="radio"/> N1s Al	1087.21	55.73	3
<input type="radio"/> S2p Al	1317.63	44.27	2
<input type="radio"/> F1s Mg	564.85	75.38	6
<input type="radio"/> S2p Mg	1084.71	24.62	2
<input type="radio"/> C1s Mg	966.93	46.42	7
<input type="radio"/> F1s Mg	564.85	53.58	6
<input type="radio"/> O1s Mg	721.07	62.45	4
<input type="radio"/> S2p Mg	1084.71	37.55	2
<input type="radio"/> F1s Mg	564.85	71.76	6
<input type="radio"/> N1s Mg	854.34	28.24	3
<input type="radio"/> N1s Mg	854.34	54.64	3
<input type="radio"/> S2p Mg	1084.71	45.36	2

Buttons: Calculate, Cancel, Save, Load

Load data of one Pair (*.pai)

Fig. 2. Dialogue for the input of the Reference-peak names, kinetic energies, intensity ratios and atomic concentration of the used peaks, ten peak pairs can be used for the calculation of the $T(E)$ function

- xiii) A third method was implemented in the new software. Now measurements of photoelectron spectra (XPS), Auger electron spectra (AES) and X-ray absorption spectra can be analysed.
- xiv) A special calculation tool allows the estimation of AES sensitivity factors. The quantification can be carried out using integral or differential AES spectra.

Additionally, empirical sensitivity factors of different spectrometer types were implemented (see Fig. 3).

AES-Calculation Tool

Auger Transition Probability Gamma

Atomic Number Z: 47

a for K or L or M or N Electrons: M:590000000

Gamma = 0.991797196717499

Ionisation Cross Section Sigma

Number of Electrons in Subshell n: M5:6

Excitation Energy Ep/eV: 10000

Target Atom Subshell EB/eV: Ag M5:368

Sigma/cm² = 2.24639775323628e-19

AES-Emission Yield

Backscatter Correction Factor r = 2.088046938

Gamma · Sigma · r/cm² = 4.65210801272894e-19

Gamma · Sigma · r · e19/cm² = 4.6521

Calculate Cancel

Fig. 3. Dialogue for the calculation of the AES sensitivity factors (examples shows the calculation for the transition Ag M5N45N45 at the excitation energy 10000 eV)

- xv) Two new measurement data formats were implemented in the input routine. Now the sputter depth profile multipoint format of Thermo spectrometers (*.avg) and the mapping format of PHI instruments (*.map) are readable by UNIFIT. The input routine was extended for the loading of AES spectra saved in different data formats (e.g. PHI formats: *.spe, *.map, *.pro, *.lin).