What is new in UNIFIT 2016?

The aim of the improvement of the **UNIFIT 2016 software** was the development of a calculation method for the modelling of spectral background functions for XPS measurements of inhomogeneous samples. Additionally, the Five-Parameter Inelastic Electron Scattering Cross Section was introduced. The additional gap-energy parameter allows a better simulation of the loss structure of insulators. The efficient usage of the main memory by the software UNIFIT was improved, too. As the result of the software optimization the number of simultaneously processable spectra was increased from 9000 to 14400.

- i) A two times more efficient usage of the main memory of the used computer system by UNIFIT is realized.
- ii) The window number of the first standard window can be selected (1 41) and the 3D and parameter-plot windows may be displayed in the windows with low numbers (1 40). Thereby the used main memory by UNIFIT is reduced considerably.
- iii) The maximum number of simultaneously processable spectra windows was increased to 14400.
- iv) The standard-window selection dialogue was adjusted to the large number of processable spectra (see Fig. 1). The number of the selection functions has been enhanced.

elect Wind	ows								
Column 1		🗆 Column 2	2	🗆 Column 3	3	🗏 Column 4	4	Column 5	;
W 11:	-1	🔳 W 31:	20	🔳 W 51:	40	🔳 W 71:	60	🔲 W 91:	80
W 12:	1	🔳 W 32:	21	🔳 W 52:	41	🔲 W 72:	61	🔳 W 92:	81
W 13:	2	🔳 W 33:	22	🔳 W 53:	42	🖻 W 73:	62	🔲 W 93:	82
W 14:	3	🗏 W 34:	23	🗆 W 54:	43	🖻 W 74:	63	🗏 W 94:	83
W 15:	4	🔲 W 35:	24	🔲 W 55:	44	🔲 W 75:	64	💷 W 95:	84
W 16:	5	🔲 W 36:	25	🔲 W 56:	45	🔲 W 76:	65	🔲 W 96:	85
W 17:	6	🔳 W 37:	26	🔲 W 57:	46	🔲 W 77:	66	🔲 W 97:	86
W 18:	7	🔲 W 38:	27	🔲 W 58:	47	🔲 W 78:	67	🔲 W 98:	87
W 19:	8	🔲 W 39:	28	🔲 W 59:	48	🔲 W 79:	68	🔲 W 99:	88
W 20:	9	🔳 W 40:	29	🔲 W 60:	49	🔲 W 80:	69	🔲 W 100:	89
W 21:	10	🔳 W 41:	30	🔳 W 61:	50	🔳 W 81:	70	🔳 W 101:	90
W 22:	11	🔳 W 42:	31	🔳 W 62:	51	🔳 W 82:	71	🔳 W 102:	91
W 23:	12	🔳 W 43:	32	🔳 W 63:	52	📼 W 83:	72	🔳 W 103:	92
W 24:	13	🔳 W 44:	33	🔲 W 64:	53	🔲 W 84:	73	🔲 W 104:	93
W 25:	14	🗆 W 45:	34	🔲 W 65:	54	🔲 W 85:	74	🗏 W 105:	94
W 26:	15	🗆 W 46:	35	🔲 W 66:	55	🗆 W 86:	75	🗏 W 106:	95
W 27:	16	🔲 W 47:	36	🔲 W 67:	56	🔲 W 87:	76	🔲 W 107:	96
W 28:	17	🔲 W 48:	37	🔲 W 68:	57	🔲 W 88:	77	🔲 W 108:	97
W 29:	18	🔲 W 49:	38	🔲 W 69:	58	🔲 W 89:	78	🔲 W 109:	98
W 30:	19	■ W 50:	39	🔲 W 70:	59	🔲 W 90:	79	🔲 W 110:	99
1 - 100		◎ 101 - 200	© 201	- 300	301 - 400	0	401 - 500	© 501 -	600
601 - 700		◎ 701 - 800	© 801	- 900	◎ 901 - 1000	0	1001 - 1100	◎ 1101	- 1200
1 - 1200		◎ 1201 - 2400	◎ 240	1 - 3600	© 3601 - 4800	0 0	4801 - 6000	◎ 6001	- 7200
7201 - 84	00	◎ 8401 - 9600	◎ 960	1 - 10800	◎ 10801 - 120	000 💿	12001 - 13200	◎ 1320	1 - 14400
OK	Can	cel All Wir	ndows	Window	very 2nd W. E	very 3th W.	Every 4th W.	Every 5th V	V. Every: 6
Sort Data	Prev	iew Un		Insert	Fill with		a: All 3D Window		

Fig. 1. The new designed selection dialogue for maximum14400 standard windows

- v) The dialogue 'Hide Standard Spectra' was improved. Five new options are offered (see Fig. 2, right side).
- vi) The saving of the UNIFIT projects was optimized. The storage space was halved.

Fit Background XPS			Hide Standard Windows			
Background-Free Area 24731.164 cps eV			Selection			
$U(E) = a+b\cdot E+c\cdot E^2+d\cdot E$	3+e·U'(E)+U''(E))				
-(-,	· · · · · ·	Fix	 Show all Standard Windows 			
a-Parameter =	137.277		Show Every 2nd Standard Window			
b-Parameter =	0.132198		Show Every 4th Standard Window			
c-Parameter =	0	V	Show Every 8th Standard Window			
d-Parameter =	0		Show Every 16th Standrad Window			
Shirley Factor e =	0		Show Every 32th Standard Window			
Tougaard Background	U''(E)		Show Every 64th Standard Window			
Lam(E)·K(E,T)=B·T/((0	C+C'·T²)²+D·T²)		 Show Every 128th Standard Window 			
T = Loss Energy (eV)			 Show Every 256th Standard Window 			
B-Parameter =			Show Every 512th Standard Window			
C-Parameter =			Show Every 1024th Standard Window			
C'-Parameter = -1.674			 Show Every 2048th Standard Window 			
D-Parameter =	D-Parameter = 1018.526		,			
Gap-Param. (T0) = 6.911 🗉			Show Every 4096th Standard Window			
			Show Every 8192th Standard Window			
Load Cross Sect			 Show Every 16384th Standard Window 			
Save Cross Sect	ion Lam·K(T)					
			Preview			
Subtract	Preview					
OK	Cancel		OK Cancel			

Fig. 2. Left: dialogue of the Tougaard background of homogeneous samples, right: dialogue for displaying and hiding of standard windows

Fit Background XPS											
Background-Free Area 297864.01 cps·eV Adjust e-Parameter											
$U(E) = a+b\cdot E+c\cdot E^2+d$	I·E³+e·U'(E)+U''(E)		Adjust B-Parameter								
		Fix									
a-Parameter =	1793		Subtract								
b-Parameter =	0.2857494		Preview								
c-Parameter =	0.0003686		Four end								
d-Parameter =	0	V	Export								
Shirley Factor e =	0	V	Сору								
Tougaard Background/Absolute											
Peak B-Param.	Fix C-Param. Fix	C'-Pa	iram, Fix	D-Param. Fix	Gap-Par.	Fix					
• 1 841.584	☑ 614.792 ☑	-1.90	03 🔍	1332.475 🛛	6.786	V					
© 2 428.864	☑ 365.634 ☑	-1.17	77 🔍	636.876	7.057	V					
o 3 841.584	Ø 614.792 Ø	-1.90	03 🗵	1332.475 🗷	6.786	V					
· 4 428.864	☑ 365.634 ☑	-1.17	77 🛛	636.876	7.057	V					
Load Cross Section Lam·K(T) Save Cross Section Lam·K(T)											
ОК	Cano	Undo									

- Fig. 3. Dialogue for the Advanced-Tougaard background, input and display of all background parameters, four background functions are used (imply four peak-fit components), parameters peak 1 and 3: Al_2O_3 , parameters peak 2 and 4: SiO_2 (see Fig. 4 and 5)
- vii) The Legend/Select Curves dialogue may be selected by clicking the right mouse button of a legend displayed in the active window.

- viii) The number of marker lines was increased to 15.
- ix) The Five-Parameter Inelastic Electron Scattering Cross Section is introduced. The additional gap-energy parameter allows a better simulation of the loss structure of insulators (Fig. 2, left).



- **Fig. 4.** Peak fit of the 2s and 2p lines of AI_2O_3 and SiO_2 using the Advanced-Tougaard Background method, parameters of the background functions are shown in Fig. 3, the corresponding $\lambda \cdot K(T)$ functions are plotted in Fig. 5
- x) The Advanced-Tougaard Background was developed for a better modelling of the spectral background function of XPS measurements of inhomogeneous samples. The spectral background of every peak-fit component is calculated separately (see Fig 3, 4 and 5).
- xi) After the loading of spectra all acquisition parameters can be modified. A special interpolation routine is started if the step width, the start or end energy are changed. Modified spectra are calculated.
- xii) A new input routine of measurement data files recorded at the Laussane Nanolab (XAS) was implemented.
- xiii) The input routine of measurement data files recorded using the Scienta SES spectrometer software was revised. The sum of the intensities of all slices per energy step (number of saved regions = number of loaded spectra) or the intensities of all saved slices (number of regions · number of slices = number of loaded spectra) may be loaded.



Fig. 5. Plot of the $\lambda \cdot K(T)$ functions of Al₂O₃,and SiO₂, corresponding parameters are shown in Fig. 3