

UNIFIT 2023/UNIFIT 2024 – the Improved Spectrum Processing, Analysis and Presentation Software for XPS, AES, XAS and RAMAN Spectroscopy

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Abstract

Main focus of the advancement of **UNIFIT 2023/UNIFIT 2024** were the optimization of the saving and loading procedure of Unifit projects and the batch processing sub-routine. For a better and faster operation of the software the common Windows shortcuts were integrated. The definition and display of the preferences were reworked and newly designed. The dialogue 'Programme Parameters' was redesigned and expanded. The definition of the excitation satellites was reworked completely. The pop-up and pull-down commands were improved. The setting options of the X-axis and Y-axis dialogues were refreshed. New export functions were implemented. In order to increase the processing speed of the software, the programme code was reworked and optimized.

Improved Setting of Preferences

The input management for the definition of the **preferences** (see Fig. 1) was completely reworked and

Excitation Satellites

The number of the **excitation sources** (see Fig. 2) was reduced to four. The dialogue for the definition of the satellites was redesigned and the parameters were clearly labelled. The files 'satellite.set' and 'satellite1.set' were removed. The parameters of the excitation satellites were integrated into the presetting files (*.set).

redesigned. A new preference dialogue was implemented. Former pull-down commands of the preferences were removed. Nine groups were defined: i) General, ii) Display, iii) Printer iv) Export, v) Import, vi) Peak Fit vii) Load/Define Transmission Function T(E), viii) Sources, ix) Batch Processing.

The operations will be carried out simultaneously. Therefore, the button 'Close' and not 'OK' leaves the dialogue. The transfer of reloaded preferences to open spectra windows can be carried out optionally using different ways. The preference 'Save Projects Automatically' was removed. The currently loaded preferences can be displayed optionally after the execution of the software Unifit 2024. The file name is displayed in the title bar.

rences: C:\Users\RHesse\Documents\Unifit_2024_User_Files\presetting\presetting.set						
Seneral Programme Parameters Number of the First Standard Window: 11		Language o German		● Point Character Display/Printer ○ Comma		
Points to Average: 5 Maximal Number of Peak-Fit Components: 30 Maximal Number of XAS Background Steps and XPS Backgrund Fu	Inctions: 9	Unifit Projects Save Backup Files Open with Quantification and Film Thickness Table 				
Maximal Number of Presentable Curves inside 'Plot 3D Waterfall': 300 Maximal Number of Presentable Fit Results inside 'Plot 3D Waterfall Plus': 21 Maximal Number of Presentable Curves inside 'Parameter Plot': 30 Maximal Number of Presentable Parameter Steps inside 'Parameter Plot': 30			 X-Axis ● XPS: Binding Energy ○ XPS: Kinetic Energy XAS: Photon Energy; AES/T(E): Kinetic Energy; Raman: Wave Number 			
Threshold Spike Correction: 20 Max. Spike Number/%: 5	Modify	Y-Axis ⊚ Counts	○ Counts per Second	Toolbar ☑ Activate Toolbar Modify		
Text Dialogs Arial, 17, Standard, Standard	Change	Background ○ Constant	XPS-Quantification Right Mo ○ Linear ● Shirley	ouse Button ○ Tougaard ○ Polynom+Shirley		
)isplay		Printer				
Graphs Standard Window/Wagner Plot Axes/Li	ines/Text	Graphs Sta	andard Window/Wagner Plot	Axes/Lines/Text		
3D Plot Waterfall/XY 3D Plot/Colour Profile 3D Plot Wat	e 3D Plot Waterfall 0° Plus		3D Plot Waterfall/XY 3D Plot/Colour Profile 3D Plot Waterfall 0° Plus			
Parameter Plot		Parameter Plot Print Options Display Setting ===> Printer Setting				
oad/Define Transmission Function T(E)	Export			Import		
oaded T(E): ESCALAB220_TWIN_SAE150_50EP.trm Load T(E) Define Parameters T(E)	⊂ Resolution Ima ○ Monitor Res	ages solution	 Decimal Character Data Point Comma 	VAMAS (*.VMS;*.NPL) ScientaSES-Spectra (*.TXT		
Peak Fit	⊙ 600 dpi	○ 800 dpi	Delimitation Data	SPECS Prodigy (*.XY)		

efinition Excita	ation Satellites				
C	N				
Source	Name:	AIKa	Mg Ka	Hel	Hell
Excitatio	on Energy	1486.6	1253.6	21.2	40.8
Peak	Peak height	100	100	100	100
	Displacement/eV	0	0	0	0
Sat. 1	rel. Peak Height	6.4	8	2	0
	Displacement/eV	9.8	9.4	1.9	0
Sat. 2	rel. Peak Height	3.2	4.1	0.5	0
	Displacement/eV	11.8	10.2	2.5	0
Sat. 3	rel. Peak Height	0.4	0.55	0	0
	Displacement/eV	20.1	17.5	0	0
Sat. 4	rel. Peak Height	0.3	0.45	0	0
	Displacement/eV	23.4	20	0	0
Sat. 5	rel. Peak Height	0.55	0.5	0	0
	Displacement/eV	69.7	48.5	0	0
OK Cancel					

Fig. 2 Screen shot: Dialogue for definition of the excitation satellites

Programme Parameters

The number of the general **programme parameters**

Fit Procedure	 ○ 1000 dpi ○ 1200 dpi ○ Comma 	
• Product • Convolution • Sum	Text Table Images	
Parameters Peak Fit/XAS-Background/XPS-Background (INHOM)	Times New Roman, 12 Space	
	Text Tables	
 Calculation of Fit-Parameter Errors Iterative Matrix Inversion 	Sources	Batch Processing
Tougaard-Background Calculation ● Homogeneous Samples	Al Ka Mg Ka He I He II 1486.6 eV 1253.6 eV 21.2 eV 40.8 eV Define Satellites	 Load Original Spectra Number of Iterations per Cycle = 10 Number of Cycles = 2 Modify
Close Load Save Save as Tran	Printer/Peak Fit ● All Windows ○ Windows ○ Only Window 0	□ Show Preferences -DS DS+

Fig. 1 Screen shot: Dialogue for definition of the preferences of the programme handling

Implementation of Common Windows Shortcuts

The common **Windows shortcuts** were implemented into the software UNIFIT. Currently five ways are available to send a call to the software (not for all sub-routines):

1. Pull-Down Commands

3. Pop-Up Commands

2. Shortcut with 'Alt-Character'4. Shortcut with 'Ctrl-Character'

5. Icons (Icons can be selected by the user.)

Ctrl-a Internal Copying **Ctrl-b** Fit Background Ctrl-c Charge Correction Ctrl-d Differentiation **Ctrl-e** Expansion **Ctrl-f** Fit-Parameter Table **Ctrl-g** Calculate Backgr. Ctrl-h Subtract Background **Ctrl-l** Fit-Parameter Limits Table Ctrl-i Iteration Ctrl-k Subtract Satellite **Ctrl-j** Edit Acquis. Para. Ctrl-n Normalization Ctrl-o Spectrum Oper. **Ctrl-p** Print-Out Ctrl-m Spectr. Manipul. **Ctrl-q** Quantification **Ctrl-r** Reduction **Ctrl-s** Save Project **Ctrl-t** Correction with T(E) **Ctrl-v** Internal Insertion **Ctrl-w** Z-Axis Ctrl-x X-Axis Ctrl-u Copy Image

Setting of Programme Parameters

Number of the First Standard Window (1...101): 41 Points to Average (1...19; odd): 3 Maximal Number of Peak-Fit Components (1...30): 10 Maximal Number of XAS Background Steps and XPS Backgrund Functions (3...9): 6 Maximal Number of Presentable Curves inside 'Plot 3D Waterfall' (100...300): 200 Maximal Number of Presentable Fit Results inside 'Plot 3D Waterfall Plus' (7...21): 10 Maximal Number of Presentable Curves inside 'Parameter Plot' (10...30): 20 50 Maximal Number of Presentable Parameter Steps inside 'Parameter Plot' (30...50000): 20 Threshold Multiplier of Spike Correction (5...100): 20 Maximal Number of Spikes/% (5...33): Show Spectra of Spike Correction after Laplace operation Values to Minimum **Typical Values** Cancel OK Values to Maximum

Fig. 3 Screen shot: Dialogue for definition of the programme parameters

Increasing the Processing Speed

In order to increase the **processing speed** of the software, the programme code was reworked and optimized. Now, batch-processing operations using more than 50,000 spectra are well possible and practicable. Table 1 illustrates a comparison of the processing time of different processing operations using all standard spectra with Unifit 2022 and Unifit 2023/UNIFIT 2024.

Ctrl-y Y-Axis

Ctrl-z Undo

Additional New Features

- 1. The procedure **'Marker Lines'** was reworked. Now, the position and length of marker lines are correctly displayed and plotted after a resize operation of the windows.
- 2. Now, the **fill colours** and **colours** of the lines of **3D plots** can be generated automatically. The calculation is carried out using a randomize operation.
- The 'Undo' function was reworked and improved. Up to 100 processing steps are saved for the 'Undo Operation'. All processing and design operations are supported. In former Unifit versions one processing step was supported only. The 'Undo' function does not support the following three processes:

 Operation at Wagner-Plot Windows, 2. Batch-processing operations, 3. Windows operations.

 In order to reduce the storage space of Unifit projects the sub-routines 'Save Projects', 'Save Projects as' and
- 'Load Projects' were completely reworked and optimized. The storage space was reduced to as much as 20 % with respect to the version UNIFIT 2022. Now, the saving and loading of Unifit projects with more than 50,000 spectra are well possible and practicable.

Tab. 1 Comparison of the processing time of different batchprocessing operations using all standard spectra using Unifit 2022 and Unifit 2023/UNIFIT 2024 SW – standard windows 3DW - 3D windows PW – parameter plot windows

UNIFIT project	Saved and reloaded spectra Operation	Processing time UNIFIT 2022	Processing time UNIFIT 2023
SAM-Mapping-256x256- PHI700.ufp	65536 SW, 1 3DW Background subtraction	2 min 19 sec	1 min 14 sec
SAM-Mapping-256x256- PHI700.ufp	65536 SW, 1 3DW Differentiation	1 min 51 sec	0 min 37 sec
SAM-Mapping-256x256- PHI700.ufp	65536 SW, 1 3DW Peak fit, 1 Comp., Sum, Fittable background	13 min 18 sec	12 min 36 sec
RAMAN- MicroAnalysis.ufp	2601 SW, 12 3DW, 1 PW Reduction, Peak fit, 1 Comp., Sum, Fittable backg.	2 min 12 sec	2 min 05 sec
Cu2p-14300-Spectra-with- BackgroundSubtraction.ufp	14300 SW, 1 PW Background subtraction	0 min 31 sec	0 min 13 sec