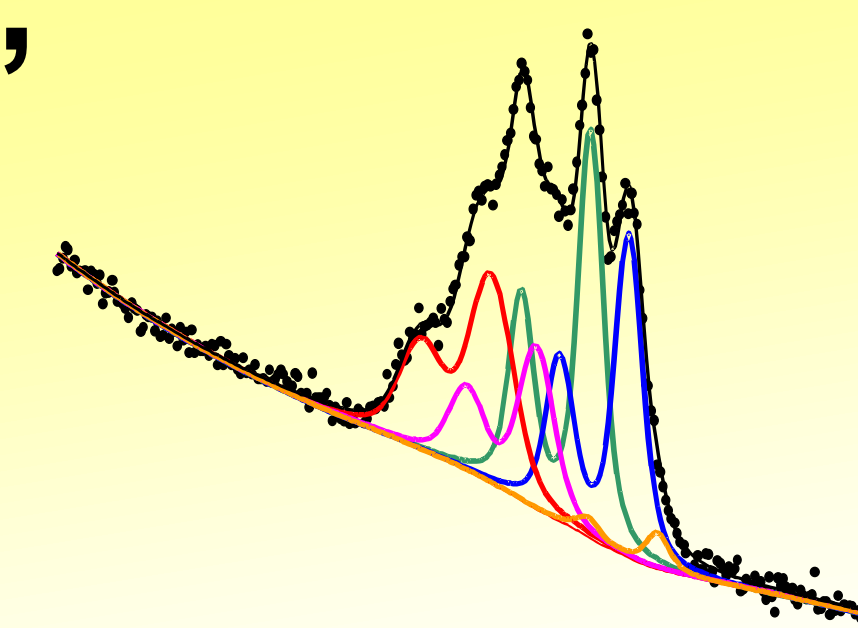




UNIFIT 2023/UNIFIT 2024 – the Improved Spectrum Processing, Analysis and Presentation Software for XPS, AES, XAS and RAMAN Spectroscopy



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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 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.

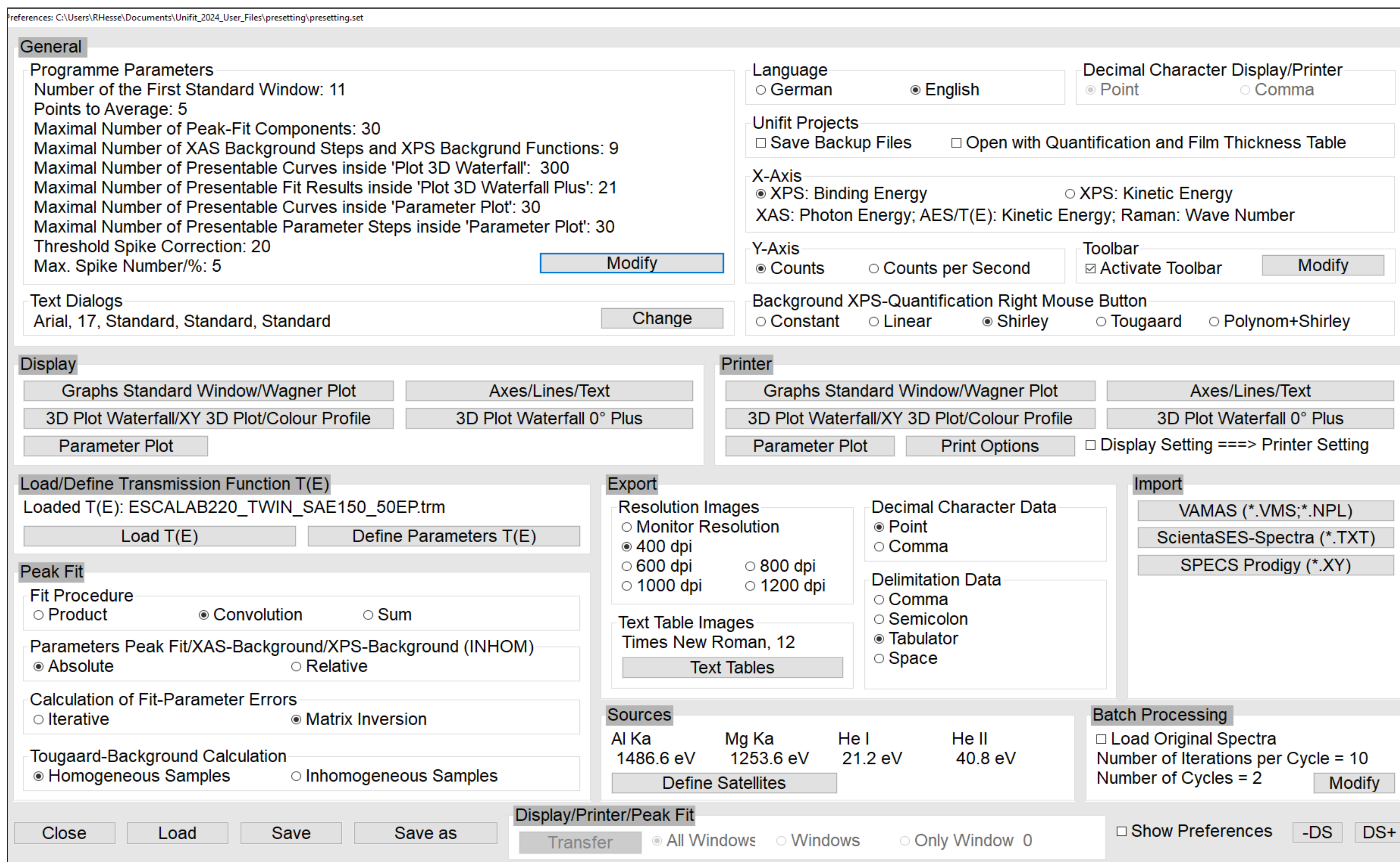


Fig. 1 Screen shot: Dialogue for definition of the preferences of the programme handling

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
2. Shortcut with ‘Alt-Character’
3. Pop-Up Commands
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-i Iteration	Ctrl-j Edit Acquis. Para.	Ctrl-k Subtract Satellite	Ctrl-l Fit-Parameter Limits Table
Ctrl-m Spectr. Manipul.	Ctrl-n Normalization	Ctrl-o Spectrum Oper.	Ctrl-p Print-Out
Ctrl-q Quantification	Ctrl-r Reduction	Ctrl-s Save Project	Ctrl-t Correction with $T(E)$
Ctrl-u Copy Image	Ctrl-v Internal Insertion	Ctrl-w Z-Axis	Ctrl-x X-Axis
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.
3. 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:
 1. Operation at Wagner-Plot Windows,
 2. Batch-processing operations,
 3. Windows operations.
4. 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.

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).

Source Name:	Al Ka	Mg Ka	He I	He II
Excitation Energy	1486.6	1253.6	21.2	40.8
Peak	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

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

Programme Parameters

The number of the general **programme parameters** (see Fig. 3) was extended to ten.

Setting of Programme Parameters	Value
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 Background 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
Maximal Number of Presentable Parameter Steps inside 'Parameter Plot' (30...50000):	50
Threshold Multiplier of Spike Correction (5...100):	20
Maximal Number of Spikes/% (5...33):	20
<input type="checkbox"/> Show Spectra of Spike Correction after Laplace operation	

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.

Tab. 1 Comparison of the processing time of different batch-processing operations using all standard spectra using Unifit 2022 and Unifit 2023/UNIFIT 2024

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