What is new in UNIFIT 2023?

Main focus of the advancement to the **version 2023** was the optimization of the saving and loading procedure of Unifit projects and the batch processing sub-routine. The definition of the general programme parameters was improved. Additional design elements of 3D-plots were implemented. For a better and faster operation of the software the common Windows shortcuts were integrated. The undo function was completely reworked. Some sub-routines were optimized and the functionality was extended.

i) The setting of the general programme parameters was extended. The definition of the maximal numbers of presentable processing steps inside the parameter plot was implemented. The call 'Typical Values' is a new option (see Fig. 1).

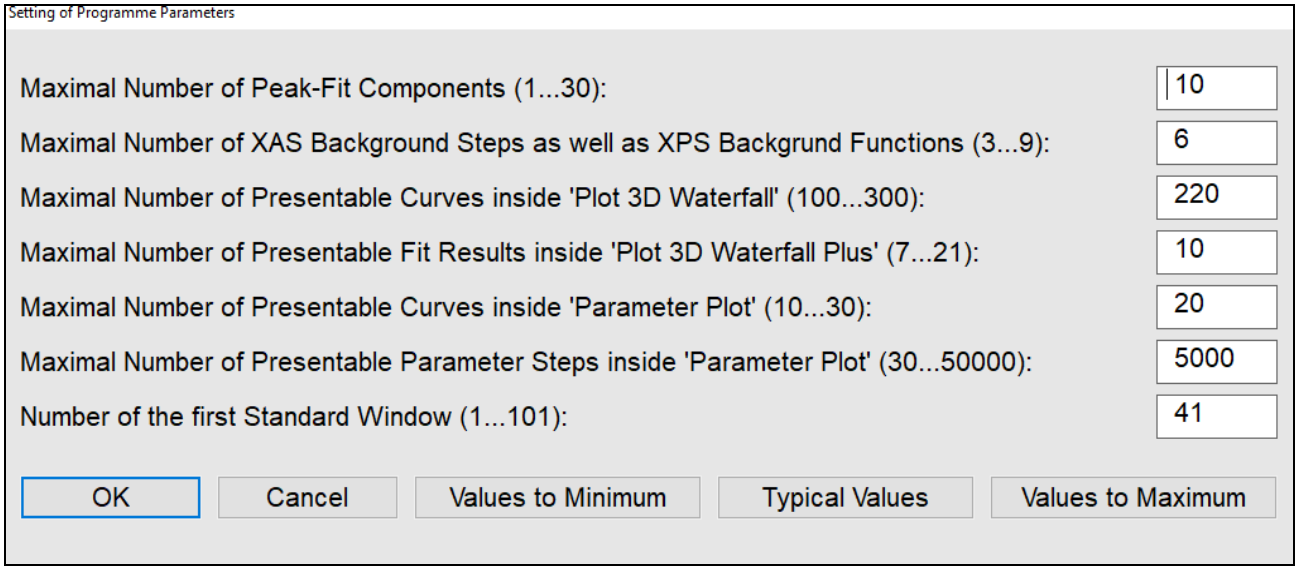

Fig. 1 Input dialogue for the setting of the general programme parameters

ii) 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 up to five with respect to the version UNIFIT 2022 (see Tab. 1). Now, the saving and loading of Unifit projects with more than 50,000 spectra are well possible and practicable.

iii) Because a file-copy operation of the measurement data files is now integrated into the saving procedure of Unifit projects, the generation and saving of backup-files can take a lot of processing time. Therefore, the generation of backup files of the Unifit projects can now activated or deactivated optionally. The Pull-Down Call is: [Preferences – Create and Save Unifit-Project Backup Files]. If the generation and saving of backup files is activated

and the number of standard windows is larger than 1000, an additional message box will be opened.

Tab. 1. Comparison of the storage space of Unifit 2023 projects and Unifit 2022 projects, SW – standard windows, 3DW - 3D windows, PW – parameter plot windows

UNIFIT project	Saved spectra windows	Storage space UNIFIT 2022 (MByte)	Storage space UNIFIT 2023 (MByte)
SAM-Mapping-256x256-PHI700.ufp	65536 SW, 1 3DW	275	149
SAM-O-Ti-Si-64x64-PHI700.ufp	4096 SW, 6 3DW	15	8
RAMAN-Si-Mapping-101x101,ufp	10201 SW, 2 3DW	133	26
RAMAN-After-Spike-Correction.ufp	86 SW	1.2	0.2
Cu2p-14300-Spectra-with-BackgroundSubtraction.ufp	14300 SW, 1 PW	73	32
Si2p_AreaScan_26x26_ AfterSputtering.ufp	676 SW, 9 3DW, 1 PW	2.6	1.9

iv) The procedure ‘Marker Lines’ was reworked. Now, the position and length of marker lines are correct displayed and plotted after a resize operation of the windows.

v) 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 (see Fig. 2 and Fig. 3).

vi) The common Windows shortcuts were implemented into the software Unifit. Five ways to send a call are available (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 Programme-Internal Copying
- Ctrl-b Fit Background
- Ctrl-c Charge Correction
- Ctrl-d Differentiation
- Ctrl-e Expansion
- Ctrl-f Fit-Parameter Table
- Ctrl-g Calculate Background
- Ctrl-h Subtract Background
- Ctrl-i Iteration
- Ctrl-j Edit Acquisition Parameters
- Ctrl-k Subtract Satellite
- Ctrl-l Fit-Parameter Limits Table
- Ctrl-m Spectrum Manipulation
- Ctrl-n Normalization

- Ctrl-o Spectrum Operation
- 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 Programme-Internal Insertion
- Ctrl-w z-Axis
- Ctrl-x x-Axis
- Ctrl-y y-Axis
- Ctrl-z Undo

vi) 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 is deactivated at the following two processes:

- Operations at Wagner-Plot Windows
- Batch processing operations
- Windows operations

vii) In order to increase the processing speed 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 2 illustrates a comparison of the processing time of different processing operations using all standard spectra with Unifit 2022 and Unifit 2023.

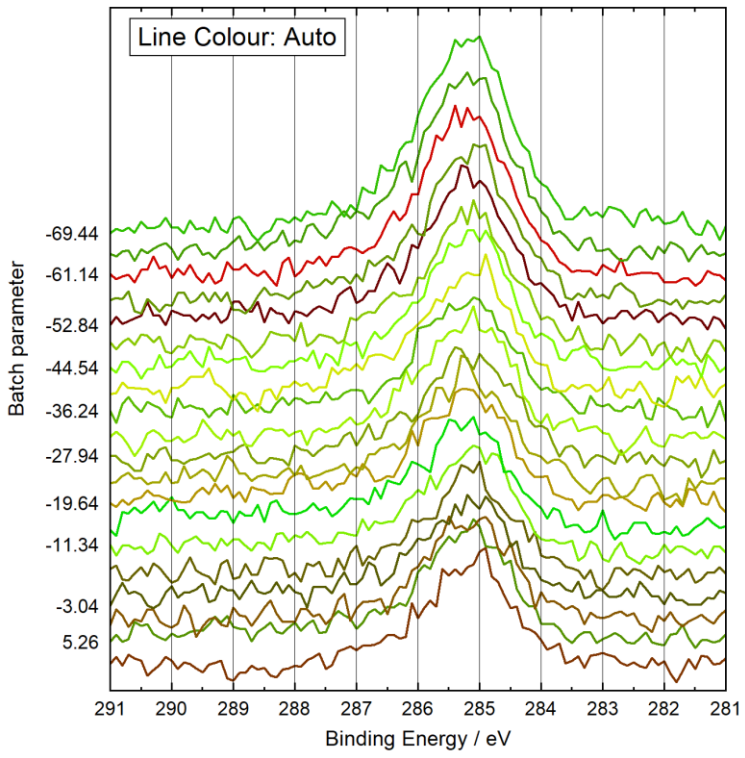

Fig. 2.‘Plot 3D Waterfall 0°’, line colour: automatic

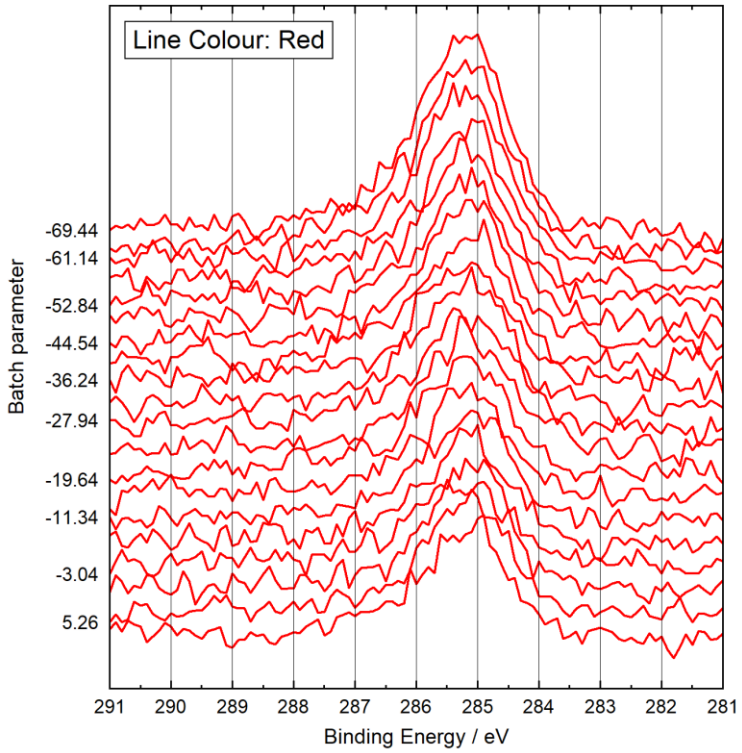

Fig. 3.'Plot 3D Waterfall 0°', line colour: red

Tab. 2. Comparison of the processing time of different batch-processing operations using all standard spectra with Unifit 2022 and Unifit 2023
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

viii) Now, the calculation of the normalization factor can have carried out using a defined numbers of average points (without the option 'Norm. to a Fixed Value'). The sub-menu 'Points to Average' can be opened directly form that menu point (see Fig 4).

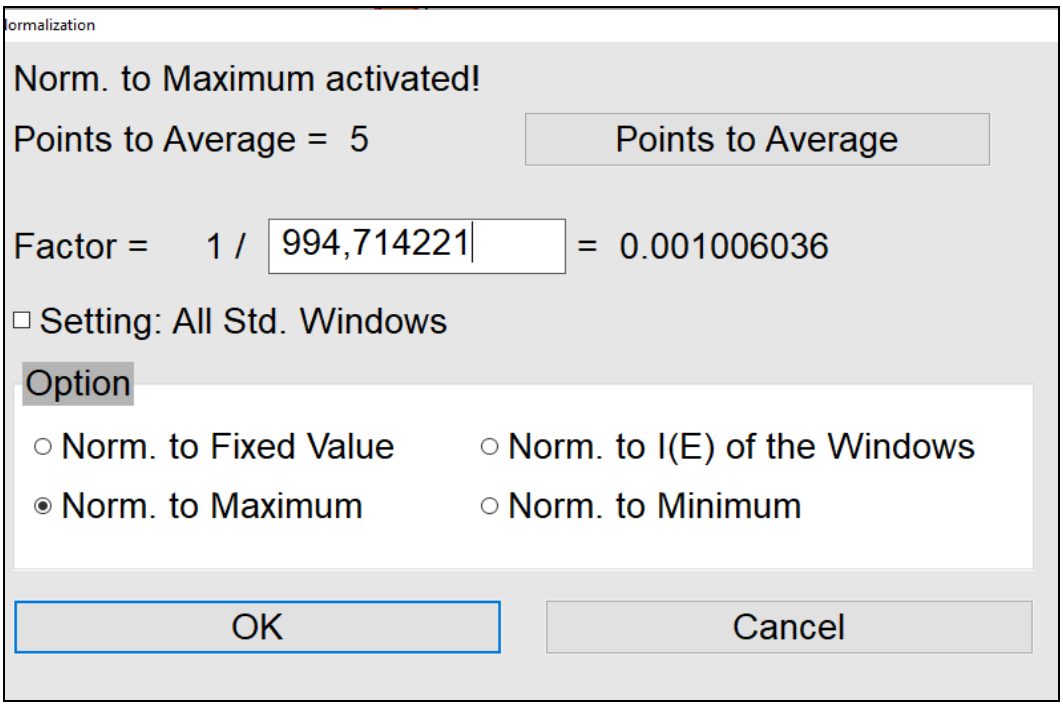

Fig. 4. Dialogue 'Modify - Normalization'

ix) The sub-routines 'Calculate Background' were reworked. The background calculation can be applied to all standard windows directly activated from the menus 'Constant', 'Linear', 'Shirley', 'Tougaard' and 'Polynom+Shirley'. The additional call 'Batch Processing' is not necessary. The sub-menu 'Points to Average' can be opened directly form that menu point (see Fig. 5, Shirley background).

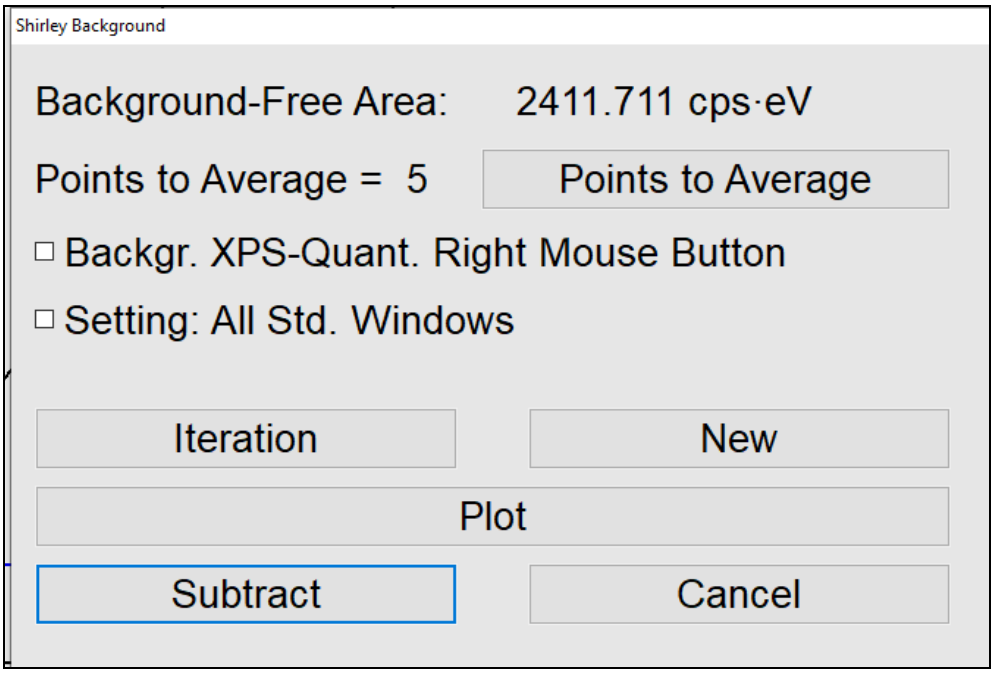

Fig. 6. Dialogue 'Modify – Calculate Background - Sjirley'