

What is new in UNIFIT 2020?

Main focus of the advancement to the **version 2020** was in the optimization of a dynamical memory management for the reduction of the necessary main memory using the software UNIFIT as well as the reduction of the loading time of UNIFIT projects with a large number of spectra. Additionally, the size of the UNIFIT-project files could be reduced strongly. The functionality of the right mouse button was completely new defined.

- i) The used vectors and fields into the programme code were optimized. The memory size of the UNIFIT-project files was reduced strongly. The main memory used by UNIFIT and the loading time of UNIFIT projects were reduced (see Tab. 1).

Tab. 1. Comparison of the used main memory and loading time of UNIFIT projects of UNIFIT 2019 and UNIFIT 2020, folder of the tested projects: Unifit_2019_User_Files\examples and Unifit_2020_User_Files\examples, SW = standard window, DSW = displayed standard windows, 3DW = 3D window, PW = parameter window

Loaded UNIFIT project	Generated spectra windows	File size (KByte)		Used main memory (Mbyte)		Loading time of the project (min)	
		UNIFIT 2019	UNIFIT 2020	UNIFIT 2019	UNIFIT 2020	UNIFIT 2019	UNIFIT 2020
Stability-Measurement-Cu2p-1100-Spectra-Mono-Source.ufp	1,100 SW 4 DSW 1 PW	5,8	2,5	50	31	0.35	0.25
RAMAN-Si-Scratch.ufp	4,140 SW 16 DSW 1 3DW	62	55	144	75	3.30	2.55
RAMAN-Si-Mapping-101x101,ufp	10,201 SW 20 DSW 2 3DW	149	133	316	150	13.20	11.50
SAM-O-Ti-Si-64x64-PHI700.ufp	4.096 SW 8 DSW 6 3DW	15.7	9.1	134	65	0.55	0.39
SAM-Mapping-256x256-PHI700.ufp	65,536 SW 8 DSW 1 3DW	275	174	1,941	1,606	18.25	17.40

- ii) The processing speed can be increased strongly by an optimized setting of the used anti-virus software (see Tab. 2). The setting steps of the Windows defender (Win 10) are:

1. Open 'Windows Defender'.
2. Open 'Virus & Threat Protection'.
3. Open 'Virus & Threat Protection Settings'.
4. Open 'Exclusions'.

5. Activate 'Add or Remove Exclusions'.
6. Activate 'Add an Exclusion' and 'Process'.
7. Add 'Unifit2020.exe'.

Tab. 2. Comparison of loading time of different UNIFIT projects without and with the definition of Unifit2020.exe as exclusion process in the anti-virus software, operating software: Win 7, hard disk: normal HD (no SSD), anti-virus software: Microsoft security essentials, SW = standard window, DSW = displayed standard windows, 3DW = 3D window, PW = parameter window

UNIFIT 2020 Project	Generated Spectra Windows	Operation	Time without Exclusion UNIFIT 2020	Time with Exclusion UNIFIT 2020
Stability-Measurement-Cu2p-1100-Spectra-Mono-Source.ufp	1,100 SW 4 DSW 1 PW	Loading of the Project	25 sec	9 sec
RAMAN-Si-Scratch.ufp	4,140 SW 16 DSW 1 3DW	Loading of the Project	4.17 min	1.13 min
RAMAN-Si-Mapping-101x101.ufp	10,201 SW 20 DSW 2 3DW	Loading of the Project	11.50 min	6.35 min
SAM-O-Ti-Si-64x64-PHI700.ufp	4,096 SW 8 DSW 6 3DW	Loading of the Project	39 sec	13 sec
SAM-Mapping-256x256-PHI700.ufp	65,536 SW 8 DSW 1 3DW	Loading of the Project	17.40 min	1.48 min

iii) A batch-image export of all displayed windows was implemented. Now, three different image export options are available:

1. Export of the active window,
2. Export of all windows,
3. Export of the selected windows.

The names of the exported images using the batch export are: name + “_” + windows number (five digits, e.g. GaAs_00001.gif, GaAs_00002.gif,...).

iv) Now, the Unifit-software package offers the generation of animated gif-files. The windows used for the internal video sequence can be exported using the batch-image export function (see iii). After the export an animated gif-file can be created with the software gifanimator.exe. The animated gif-files can be implemented and shown in a PowerPoint presentation.

v) For a better navigation different back colours of the edit fields in the menu 'Select Windows' were implemented. The back colour will be changed (grey and blue, see Fig. 1).

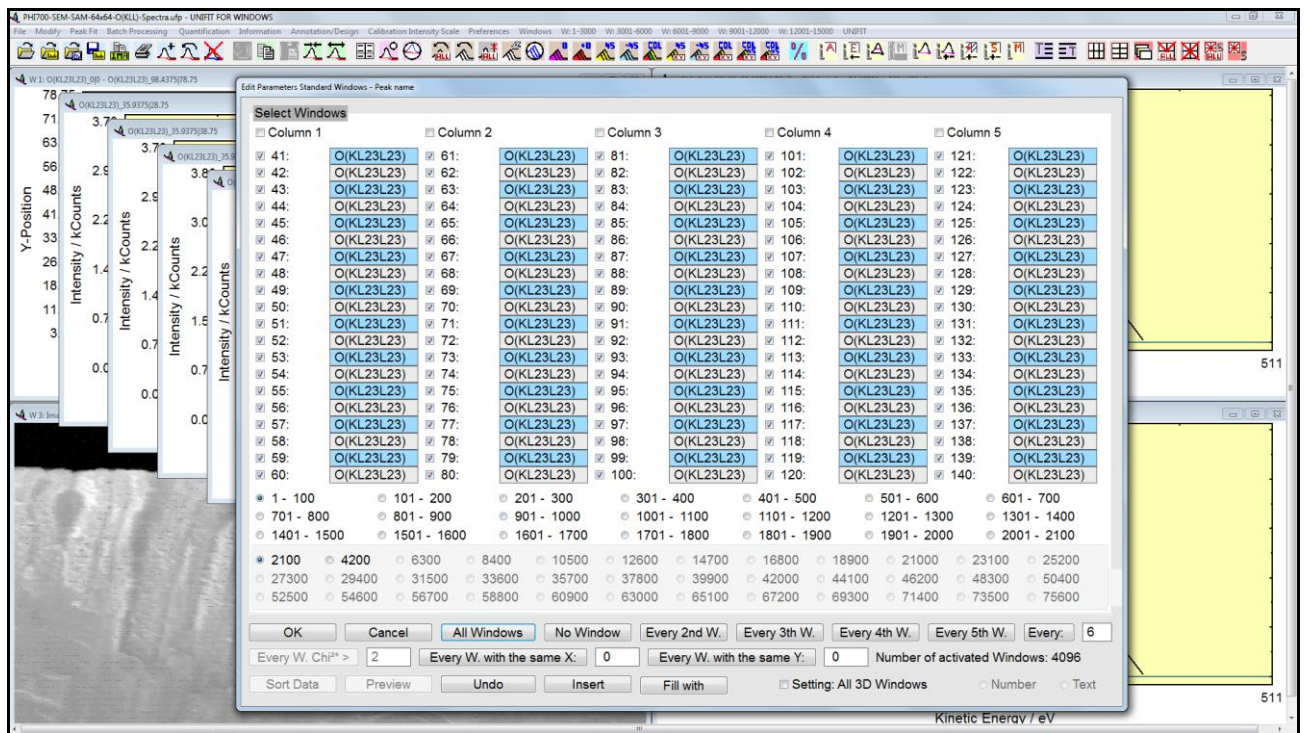


Fig. 1. Different back colours of the edit or text fields of the menu ‘Select Windows’

vi) A new windows arrangement option was introduced. For the windows arrangement functions:

- a) Cascade
- b) Side by Side
- c) On Top of Each Other

the automatic changing of the window sizes can be deactivated.

vii) A automatic rearrangement of the peak labelling was integrated. After ten operations ‘Reduction’ or ‘Changing Energy Axis’ the labelling positions are shifted to the correct energies.

viii) A new functionality of the right-mouse button for all different Unifit-window types was created. By pressing the right mouse button at the middle of the window a popup menu is opened. The following functions can be activated:

1. Standard Windows:

Without reduction-marker lines: (see Fig. 2)

Design:

- a) Graphs Standard Windows/Wagner Plot Display...
- b) Axes/Lines/Text Display...
- c) Plot Energy/Wavenumber Axis...
- d) Pot Intensity Axis...

Modify:

- e) Original/Accept Preferences

f) Undo

g) Program-Internal Coping + Program-Internal Insertion

h) Expansion

Edit:

i) Edit Spectra Names...

Peak ID:

j) Automatic Peak ID

- with check of the main lines (not appropriated for narrow spectra)
- Defined ΔE and ΔI are used from the Menu 'Information – Identify Lines'

Quantification:

k) Use Peak for XPS Quantification (Mono) + Background
without satellite subtraction

l) Use Peak for XPS Quantification (Twin) + Background
with satellite subtraction

- Background can be defined using background-subtraction routines.
- If no annotation of the activated spectrum is available, an Automatic Peak ID is carried out.

Output:

m) Save project

n) Copy Image Active Window

o) Print...

With reduction-marker lines:

a) Reduction

b) Reduction + Program-Internal Coping + Program-Internal Insertion

c) Remove Reduction Lines

d) Extract Peak for XPS Quantification (Mono), Background

e) Extract Peak for XPS Quantification (Twin), Background

- Background can be defined using background-subtraction routines.
- If no annotation of the activated spectrum is available, an Automatic Peak ID is carried

2. Wagner Plot Windows

Design:

a) Graphs Standard Windows/Wagner Plot Display...

b) Axes/Lines/Text Display

Output:

- c) Save project
- d) Copy Image Active Window
- e) Print...

3. Parameter Plot Windows

- a) Parameter Plot Display...
- b) Axes/Lines/Text Display
- c) Plot Parameter Axis
- d) Plot Intensity Display

Output:

- f) Save project
- g) Copy Image Active Window
- h) Print...

4. Plot 3D Waterfall 0° Plus

Design:

- a) 3D-Plot Waterfall 0° Plus Display
- b) Axes/Lines/Text Display
- c) Plot Energy/Wavenumber Axis or Plot x-Axis
- d) Plot Intensity Axis
- e) Parameter Plot Display or Plot y-Axis

Output:

- f) Save project
- g) Copy Image Active Window
- h) Print...

5. Plot 3D Waterfall 0°, Plot 3D Waterfall 45°, Plot 3D; Waterfall -45°

Plot 3D Color Profile, XY 3D Plot 45°, XY 3D Plot -45°, XY 3D Color Profile, XY 3D 45° Color Profile, XY 3D -45° Color Profile Windows

Design:

- a) 3D-Plot Waterfall/XY-3D Plot Waterfall/Color Profile Display
- b) Axes/Lines/Text Display
- c) Plot Energy/Wavenumber Axis or Plot x-Axis
- d) Plot Intensity Axis
- e) Parameter Plot Display or Plot y-Axis

Output:

- f) Save project

g) Copy Image Active Window

h) Print...

6. Image Windows

Output:

a) Save project

b) Copy Image Active Window

c) Print...

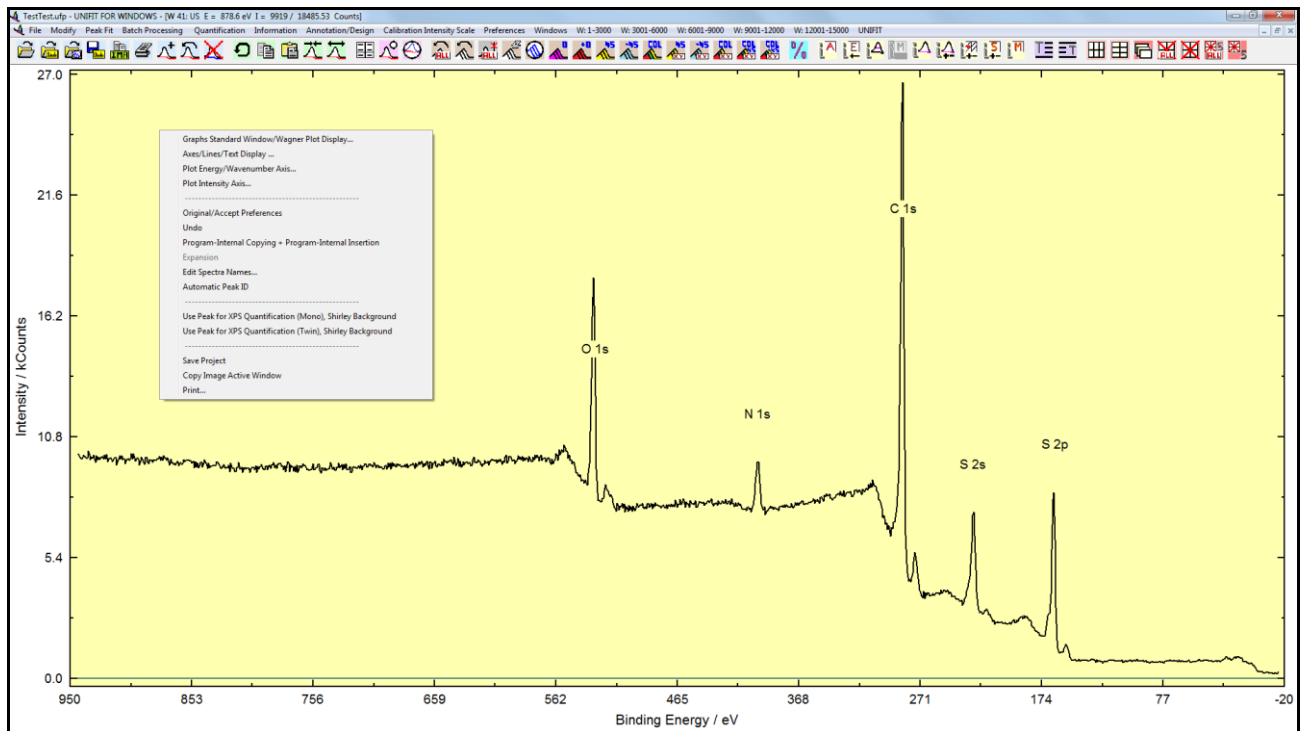


Fig. 2. Example of the activated popup menu (right mouse button) of a standard window without defined reduction-marker lines

ix) New functions of the menu 'Spectrum Title 1' were implemented for appropriate preparation of the windows layout for a later export of the windows to generate an animated-gif video.

The new functions for the title annotation are:

a) For selected windows only.

b) Title plus the windows number

c) Title plus batch parameter

d) Title plus numbering.

A progress bar was implemented, too (see Fig. 3).

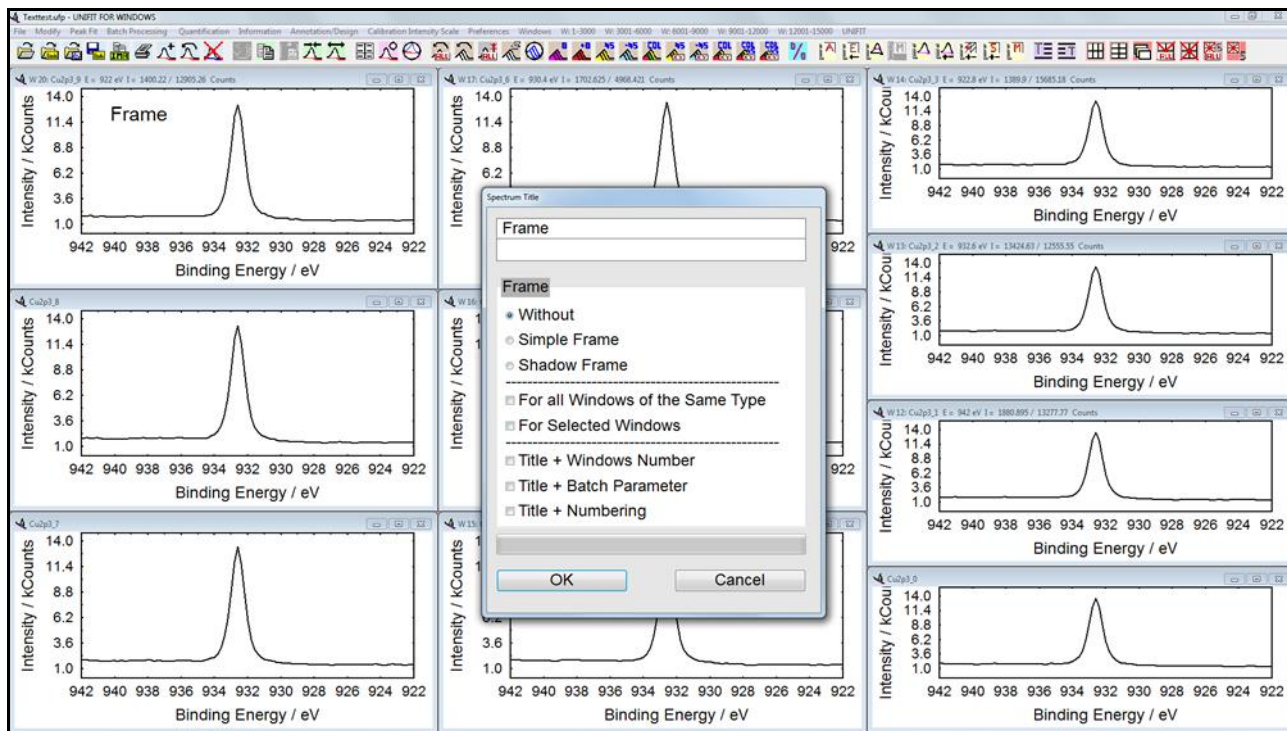


Fig. 3. New designed and improved menu 'Spectrum Title 1'