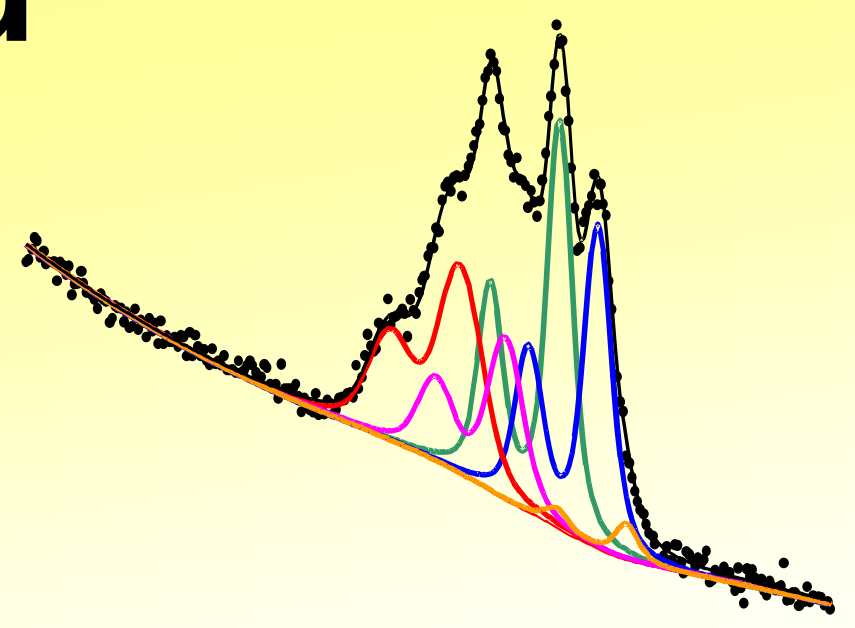




UNIFIT 2020 – the Improved Spectrum Processing, Analysis and Presentation Software for XPS, AES, XAS and RAMAN Spectroscopy

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Abstract

UNIFIT is a well-established specialized software for data analysis and presentation of photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), X-ray absorption spectroscopy (XAS) and RAMAN data. 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. A batch image export of all displayed windows was implemented. Now, three different image export options are available. The UNIFIT software package offers the generation of animated gif files. An animated GIF file (video sequence) can be generated using the internal Windows video sequence, the batch-image export function and a standalone converting software. The functionality of the right-mouse button for all fourteen different UNIFIT window types was improved according typical popup menus.

Optimized Memory Management

The aims of the **i)** optimization of the memory management and the **ii)** optimized setting of the used anti-virus software at the installation of the UNIFIT software (definition as exclusion process) were:

1. Increasing of the processing speed of the UNIFIT software.
2. Reduction of the memory size of the UNIFIT-project files.
3. Reduction of the necessary main memory using the UNIFIT software.
4. Reduction of the loading time using a large number of spectra.

The two tables below show the test results of different Windows defender settings (Win 10, with and without exclusion from anti-virus check) and the using of UNIFIT 2019 and UNIFIT 2020. The used computer was a i5-8400 2.8 GHz with SSD and 16 GB main

UNIFIT 2020 Project	Saved Spectra	Operation	Time without Exclusion (min)	Time with Exclusion (min)
Si-SiO ₂ -14390-Spectra-PeakFit.ufp	14390	Loading	2.58	2.06
Si-SiO ₂ -14390-Spectra-PeakFit.ufp	14390	Peak Fit, 2 Components, Convolution	39.20	38.40
RAMAN-Si-Mapping-101x101.ufp	10201	Loading	4.24	1.30
SAM-Mapping- 256x256-PHI700.ufp	65536	Loading	7.49	1.30
Si-SiO ₂ -14390-Spectra-PeakFit.ufp	14390	Shirley-Background Subtraction	1.08	0.24

UNIFIT Project SW: Standard Window DSW: Displayed SW PW: Parameter Window 3DW: 3D Window	Generated Spectra Windows	File Size (MB)		Used Main Memory (MB)		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	1100 SW 4 DSW, 1 PW, 1 3DW	6	4	42	26	0.06	0.05
Si-SiO ₂ -14390-Spectra-PeakFit.ufp	14390 SW 28 DSW	91	68	446	206	2.12	2.06
RAMAN-Si-Mapping-101x101.ufp	10201 SW 20 DSW 2 3DW	146	129	309	143	1.35	1.30
SAM-Mapping-256x256-PHI700.ufp	65536 SW 8 DSW 1 3DW	268	170	1930	1350	1.38	1.30
RAMAN-Si-Scratch.ufp	4140 SW 20 DSW 2 3DW	60	54	140	73	0.38	0.24

Popup Menus

The aims of the development of the improved functionality of the right mouse button were:

1. The implementation of a typical Window popup menu.
2. The optimization of the quantification using XPS survey spectra.
3. The optimization of the handling by combination of different processing functions (e.g. 'Reduction' + 'Satellite Subtraction' + 'Background Calculation' + 'Programme Internal Copying' + 'Programme Internal Insertion').
4. A quick start of typical design menus.
5. A direct call of the 'Save', 'Copy' and 'Print' commands.

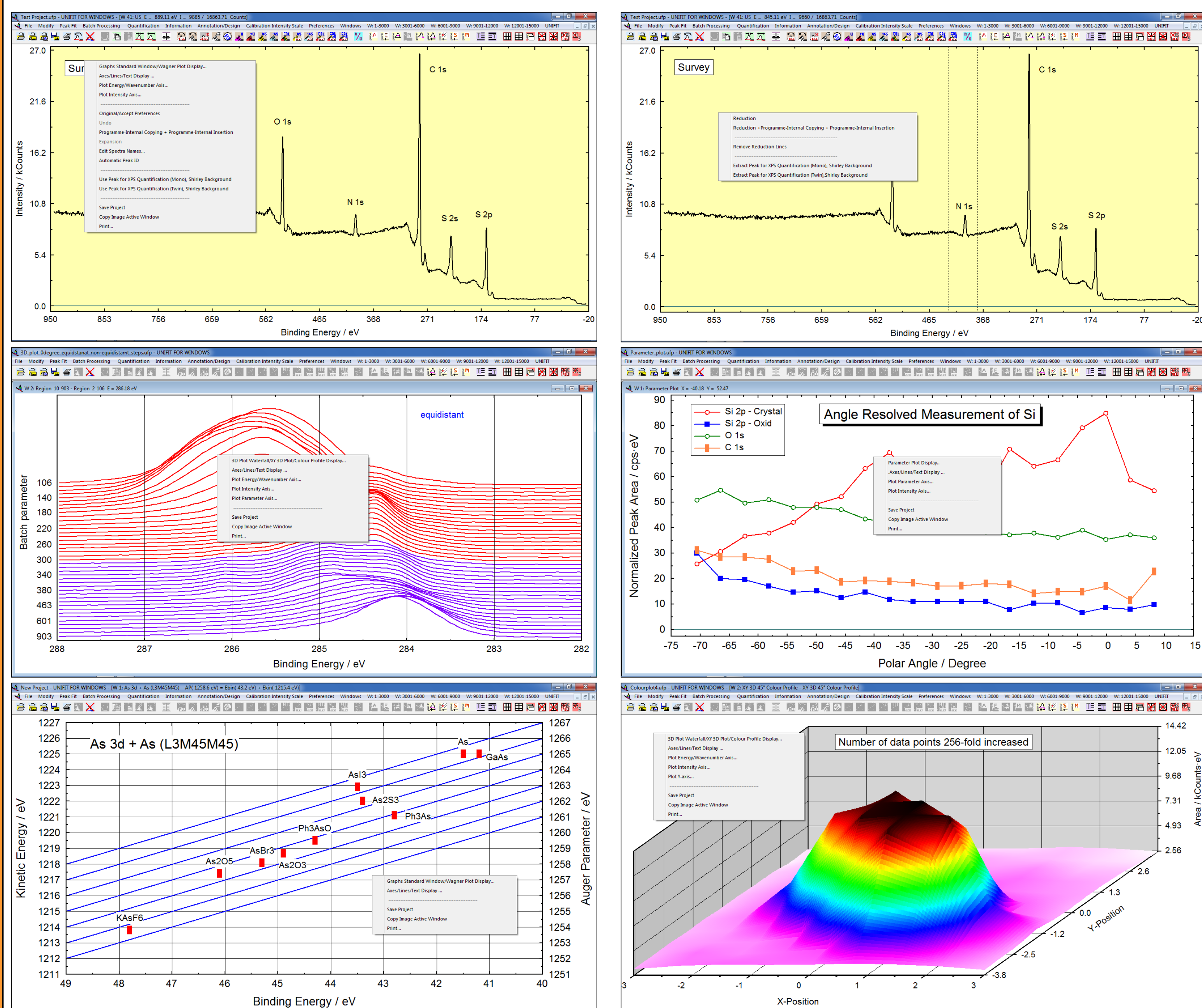


Fig. 1 Examples of the popup menus of six different UNIFIT window types: **top left**: standard window, **top right**: standard window with defined reduction-marker lines, **central left**: 3D Waterfall 0°, **central right**: parameter plot, **bottom left**: Wagner plot, **bottom right**: XY 3D 45° colour profile

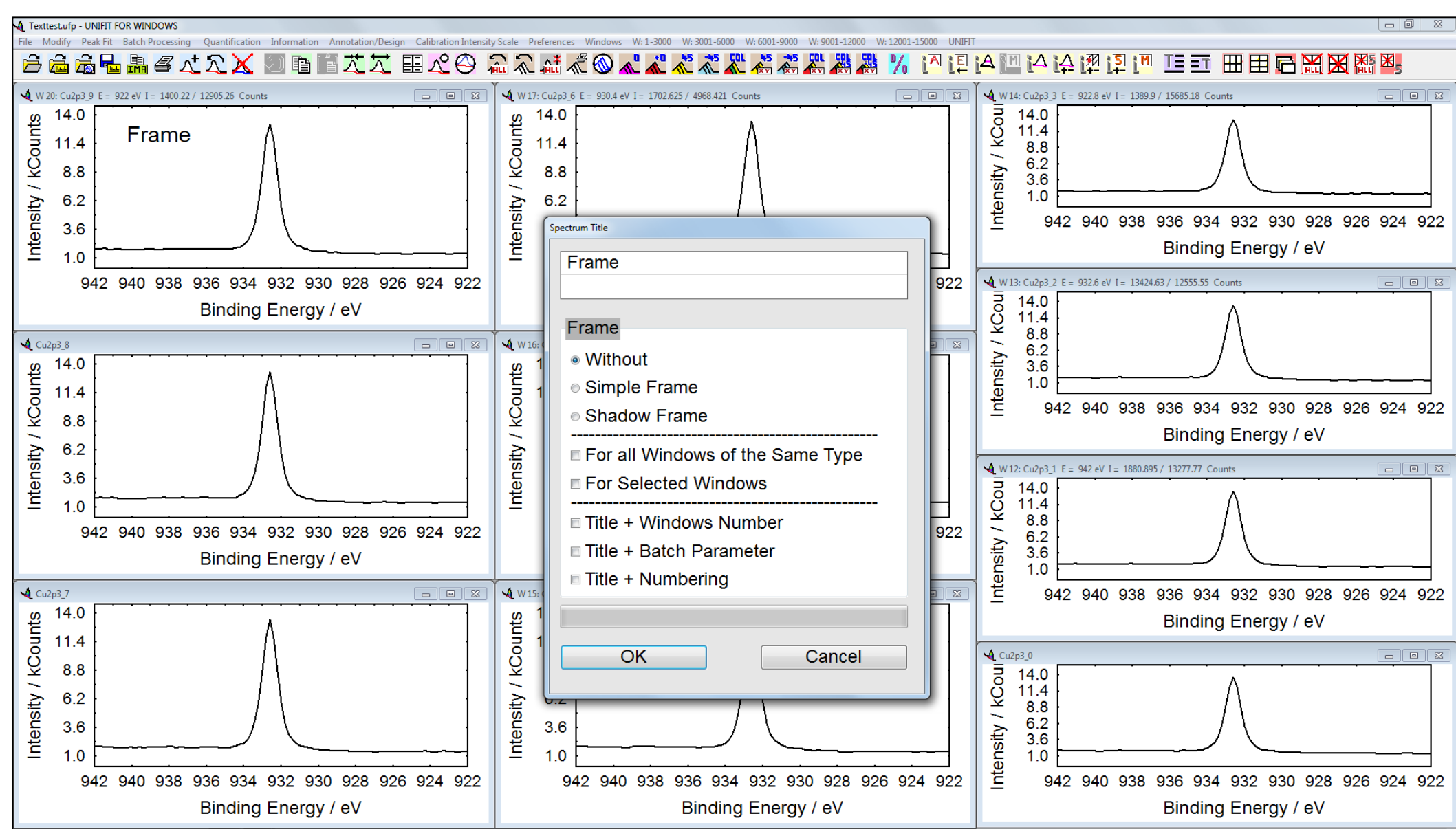
Batch Export of Images

1. All displayed windows can be exported using three options.
2. The names of the images are: Selected name + " " + windows number (five digits (e.g. GaAs_00001.gif, GaAs_00002.gif, ...)).
3. An normalization of the intensities and windows sizes of all exported windows should be carried out before the image export (Video-Display function of the UNIFIT software).
4. Export options:
 - a) Active window,
 - b) All windows,
 - c) Selected windows.

Improved Menu 'Spectrum Title 1'

The menu 'Spectrum Title 1' was extended by three new batch functions:

1. Title + Windows Number,
2. Title + Batch Parameter,
3. Title + Numbering.

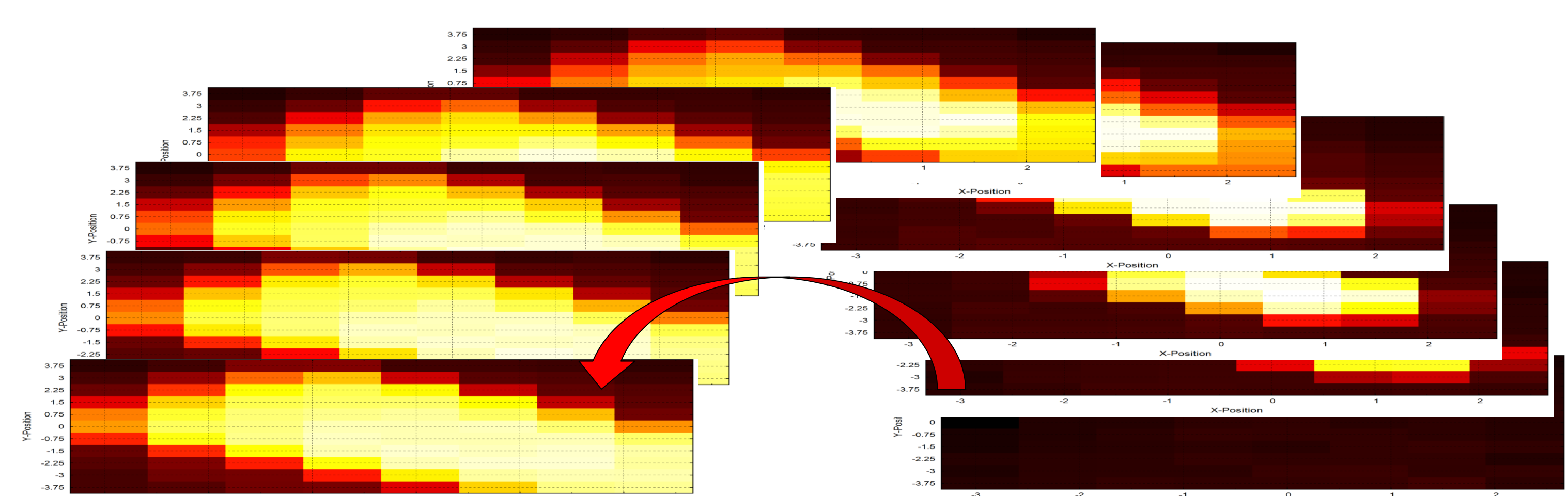


Generation of Animated-Gif Presentation

A dynamic presentation tool was already implemented in the software UNIFIT 2017. All available windows types (e.g. standard spectra, 3D presentations) can be presented as windows video sequence. But, the generated video sequence could only be presented using the UNIFIT software only.

Now, the windows video sequence can be exported as animated Gif and implemented in a PowerPoint presentation. The following steps are necessary:

1. Generation of a UNIFIT video sequence.



2. Batch export of images using all or selected UNIFIT windows as Gif-images.
3. Select all exported Gif files and load the files via drag and drop into the software gifanimator.exe (included the UNIFIT software package).
4. Select all images, define the frame dwell time and save the animated gif file with a appropriated name.
5. The animated Gif file can be displayed separately or implemented into a PowerPoint presentation using the drag and drop function.