

What is new in UNIFIT 2014?

Main focus of the advancement to the **version 2014** was in the realization of a dynamical memory management for the reduction of the necessary main memory using the software UNIFIT. As the result of the software optimization the number of simultaneously processable spectra was increased from 300 to 1200. Additionally, the source code was basically optimized.

- i) Realization of a dynamical memory management for a careful using of the hardware resources of the used computer system (see Tab. 1).

Tab. 1. Comparison of the used main memory of UNIFIT 2014 and UNIFIT 2013, folder of the tested projects: Unifit_2014_User_Files\examples and Unifit_2013_User_Files\examples, SW = standard window, 3DW = 3D window, PW = parameter window

Loaded UNIFIT project	Generated spectra windows	Used main memory by UNIFIT (MByte)		Maximal used memory by Windows and UNIFIT (MByte)	
		UNIFIT 2014	UNIFIT 2013	UNIFIT 2014	UNIFIT 2013
Without opened project	0	3	517	10	520
Sulphur_study.ufp	5 SW	9	522	20	540
Angle_Resolved_Measurement_Si.ufp	60 SW, 1 PW	36	523	110	570
BaTi-_179_spectra.ufp	179 SW 2 3DW	57	528	280	740
Stability-Measurement-Cu2p-1100-Spectra-Mono-Source.ufp (Fig. 2)	1,100 SW 1 PW	240	-	2,200	-

- ii) Implementation of an adjustment of the general program parameters on the used computer system. The maximal number of five parameters can optionally be selected (see Fig. 1).

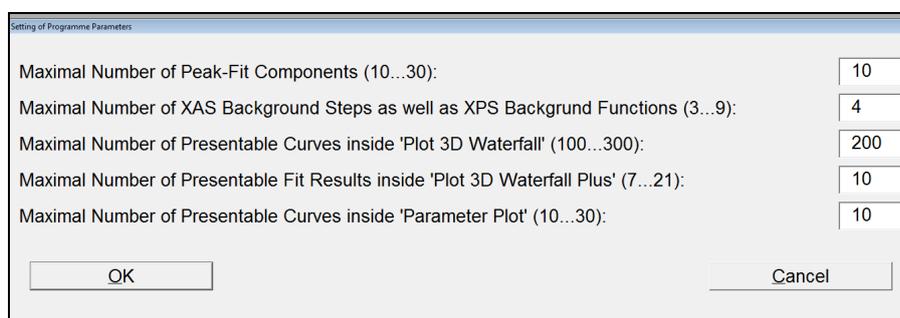


Fig. 1. Dialog for the definition of general program parameters

- iii) The maximum number of simultaneously processable spectra windows was increased to 1200.
- iv) In order to realize a comfortable handling of a large number of spectra (higher than 400) the spectra-standard windows can be generated hidden or visible. The following options are

offered: Show all windows, every 2nd, 4th, 8th, 16th, 32th, 64th, 128th, 265th and 512th window (see Fig. 2). These options can also be used to reduce the batch processing time.

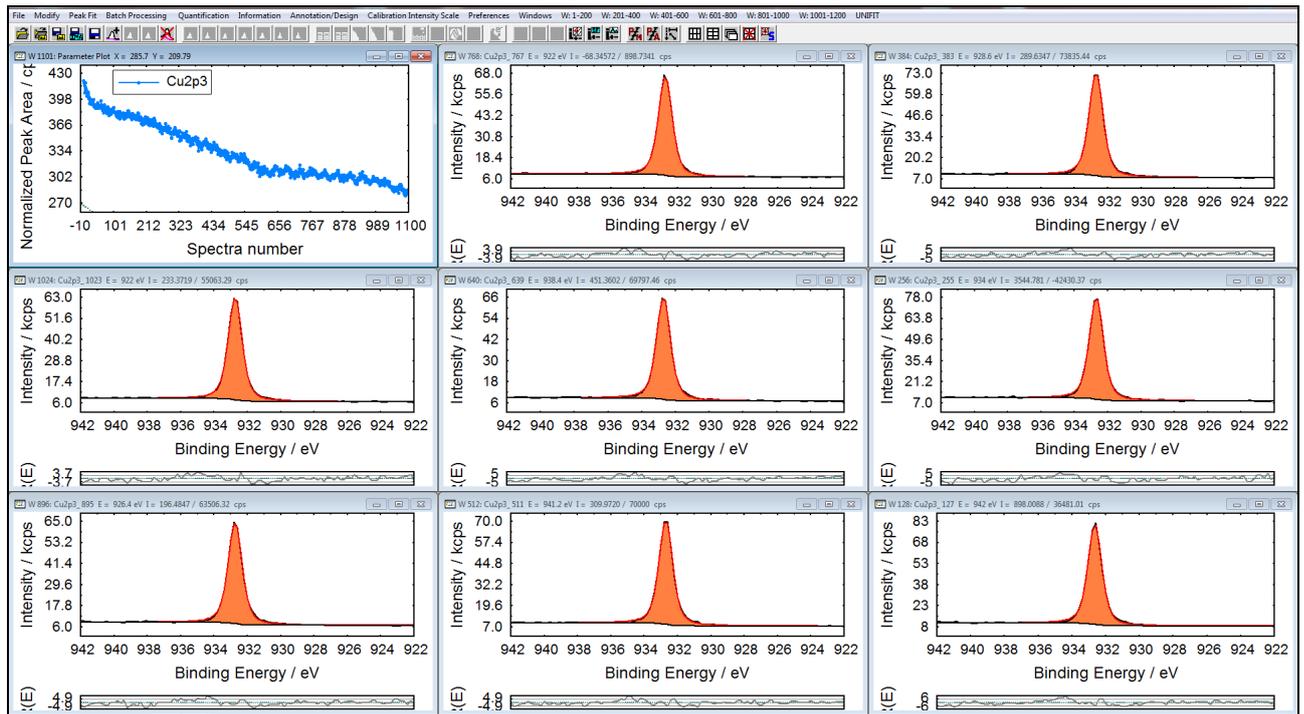


Fig. 2. Validation experiments of the stability of the mono source: measurement time: 6 hours, number of spectra: 1100, every 128th spectrum standard window is displayed, a strong reduction of the intensities can be observed (parameter plot: top, left)

- v) The standard-spectra selection dialog as well as the direct-activation function of standard windows (e.g. necessary for the 3D plots, batch processing, and concentration) was adjusted on a larger number of spectra standard windows (see Fig. 3).
- vi) The changing of the energy scale from XP and XA and vice versa was optimized. The x-axis of the XA spectra is invariably displayed (photon-energy scale). The x-axis of the XP spectra can be changed between binding and kinetic energy.
- vii) The new preference option 'Display Setting ==> Printer Setting' deactivates the pull down menu point 'Printer' for a separate layout definition of plotted spectra (directly from UNIFIT). The printing out has the same layout as displayed on the monitor.
- viii) The additional preference option 'Open Project and show Quantification and Film Thickness Table' activates or deactivates the plot of saved quantification and film thickness results during the loading of projects.
- ix) The number of decimal places of the values on all axes (energy, intensity and parameter axis) can be fixed.
- ix) The plot of the zero line of all window types may be activated or deactivated optionally.
- x) The new option 'Refresh Plot' was implemented in the dialog 'Parameter Plot'.

xi) A new mouse option allows a quick activation of the annotation and design dialogs. If the mouse is at the appropriate position in the window, the following dialogs may be activated by clicking the right mouse button:

1. Annotation/Design - Spectrum Title 1
2. Annotation/Design - Spectrum Labelling 1
3. Annotation/Design - Plot Energy Axis
4. Annotation/Design - Plot Intensity Axis
5. Annotation/Design - Plot Parameter Axis
6. Preferences - Display - Graphs Standard Windows/Wagner Plot
7. Preferences - Display - 3D Plot Waterfall 0°/45°/-45°/Color Profile
8. Preferences - Display - 3D Plot Waterfall 0° Plus
9. Preferences - Display - Parameter Plot
10. Preferences - Display - Axes/Lines/Text

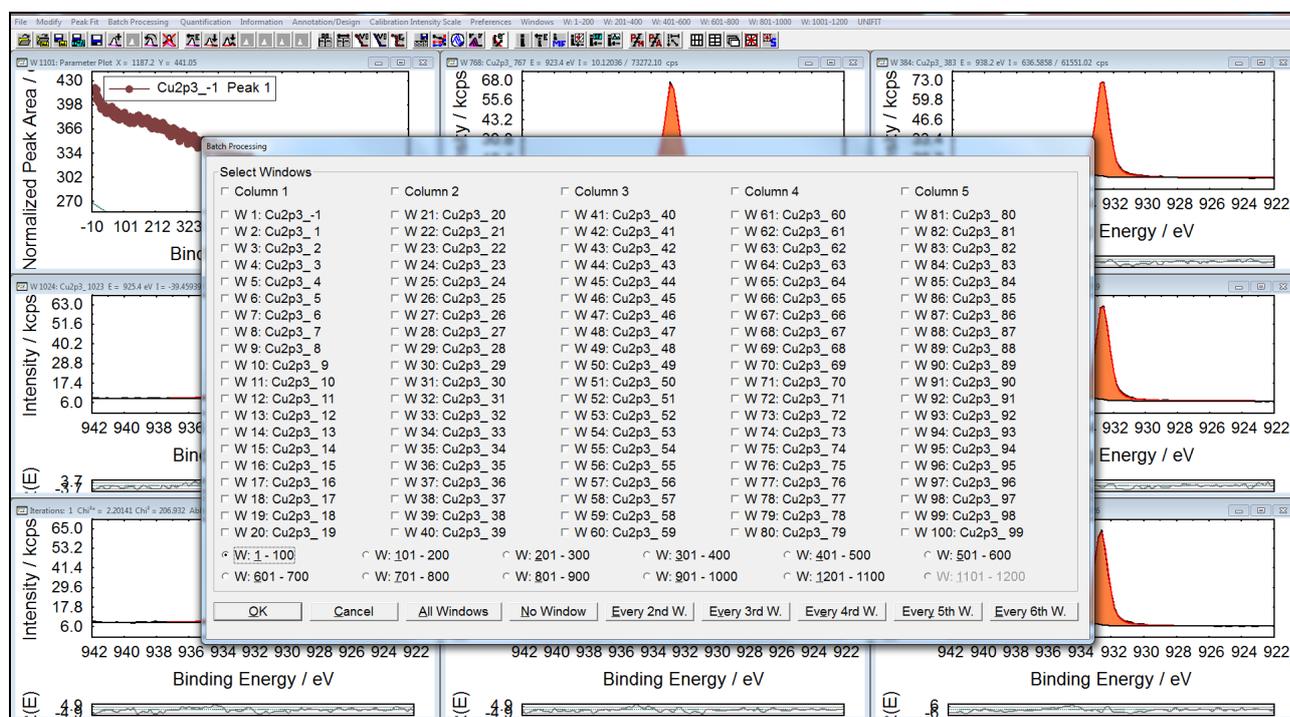


Fig. 3. Dialog for selecting the standard windows (3D plots, batch processing ...)

- xii)** The copy and export function was implemented in the dialogs 'Fit-parameter errors' and 'Fit Background XAS'.
- xiii)** The dialog 'Select Spectra' was extended by two additionally options. These options allow the loading of every 2nd or 4th spectra of a large number of data.
- xiv)** The number of the fitted spectra shown using the 'Plot 3D Waterfall 0° Plus' was increased to 21.