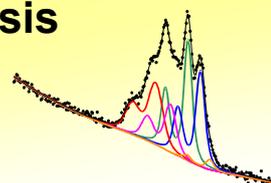


UNIFIT 2014 - the new spectrum processing, analysis and presentation software for XPS and XAS



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Abstract: The main focus of the advancement to UNIFIT 2014 is 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 used main memory can be reduced up to 100-fold. Therefore the number of simultaneously processable spectra could be increased from 300 to 1200. With the new implemented adjustment of the general program parameters (e.g. maximal number of peak fit components, maximal number of curves of 3D plots) the used main memory can be additionally reduced. In order to realize a comfortable handling of a large number of spectra (higher than 400) the standard spectra windows can be generated hidden or visible. The source code was basically optimized. The examples are experiments with a large number of spectra.

NEW FEATURES

- i) Realization of a dynamical memory management for a careful usage of the hardware resources of the used computer system.
- 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).
- 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 standard spectra windows can be generated hidden or visible. The following options are offered: Show all windows, every 2rd, 4th, 8th, 16th, 32th, 64th, 128th, 265th and 512th window. These options can also be used to reduce the batch-processing time (see Fig. 2).
- v) 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 printout has the same layout as displayed on the monitor.
- vi) 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.
- vii) The number of decimal places of the values on all axes (energy, intensity and parameter axis) can be fixed.
- viii) The plot of the zero line of all window types may be activated or deactivated optionally.
- ix) A new mouse option allows a quick activation of the annotation and design dialogs. If the mouse has the appropriate position in the window, the related dialogs may be activated by clicking the right mouse button.
- x) The number of the fitted spectra shown using the 'Plot 3D Waterfall 0° Plus' was increased to 21.
- xi) The copy and export function was implemented in the dialogs 'Fit-parameter errors' and 'Fit Background XAS'.

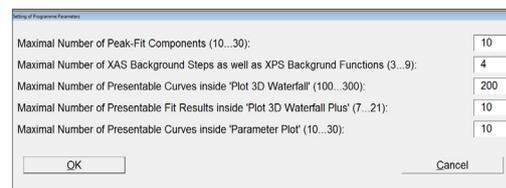


Fig. 1. Dialog for the definition of general program parameters

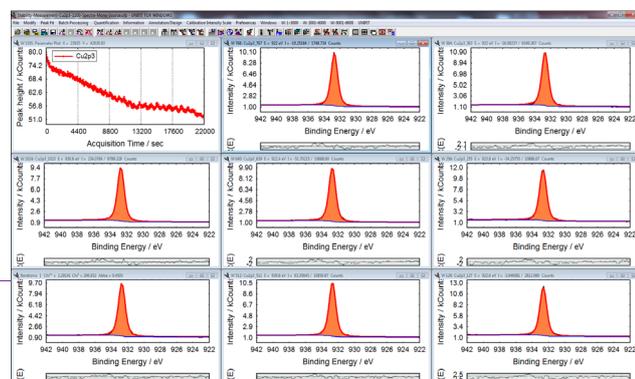


Fig. 2. Screen shot: Validation experiments of the stability of the mono source: measurement time: 6 hours, number of spectra: 1100, every 128th standard spectrum window is displayed, a strong reduction of the intensities can be observed (parameter plot: top, left)

EXAMPLES: LONG-TERM MEASUREMENTS

In order to check the long-term stability of a spectrometer ESCALAB 220 iXL measurements of the manipulator arm (oxidized Cu) using the twin and mono x-ray sources were carried out. For both experiments the measurement period was 6 hours and the number of spectra 1,100. Typical spectrometer settings were used. The 1,100 spectra were fitted with UNIFIT 2014 (fitting time: 55 seconds) and the intensities, peak positions and the FWHMs of the Gaussian and Lorentzian functions were plotted. During the peak fit (one component, convolution of Gaussian and Lorentzian functions) every 128th spectra were displayed.

Example 1: Al/Mg Twin Anode

1. The peak height increases from 8.1 to 9.4 kCounts (16%). The oxide on the anode are reduced.
2. The peak position changes from 932.75 to 932.79 eV ($\Delta E = 0.04$ eV). This is a typical shift of the electronic measuring equipment.
3. The GP- and LP-FWHM show a statistical behavior. This results from the peak fit.

Example 2: Monochromatized Al Source

1. The peak height decreases from 78 to 53 kCounts (32%). The heating of the monochromator crystals and e-gun change the focus position (LAXL lense mode).
2. The peak position changes from 932.59 to 932.74 eV ($\Delta E = 0.15$ eV). This strong shift results from the heating of the monochromator crystals. The Bragg angle is changed during the measurement.
3. The GP- and LP-FWHM show a statistical behavior. This results from the peak fit.

