What is new in UNIFIT 2016?

The aim of the improvement of the **UNIFIT 2016 software** was the development of a calculation method for the modelling of spectral background functions for XPS measurements of inhomogeneous samples. Additionally, the Five-Parameter Inelastic Electron Scattering Cross Section was introduced. The additional gap-energy parameter allows a better simulation of the loss structure of insulators. The efficient usage of the main memory by the software UNIFIT was improved, too. As the result of the software optimization the number of simultaneously processable spectra was increased from 9000 to 14400.

i) A two times more efficient usage of the main memory of the used computer system by UNIFIT is realized.

ii) The window number of the first standard window can be selected (1 - 41) and the 3D and parameter-plot windows may be displayed in the windows with low numbers (1 - 40). Thereby the used main memory by UNIFIT is reduced considerably.

iii) The maximum number of simultaneously processable spectra windows was increased to 14400.

iv) The standard-window selection dialogue was adjusted to the large number of processable spectra (see Fig. 1). The number of the selection functions has been enhanced.

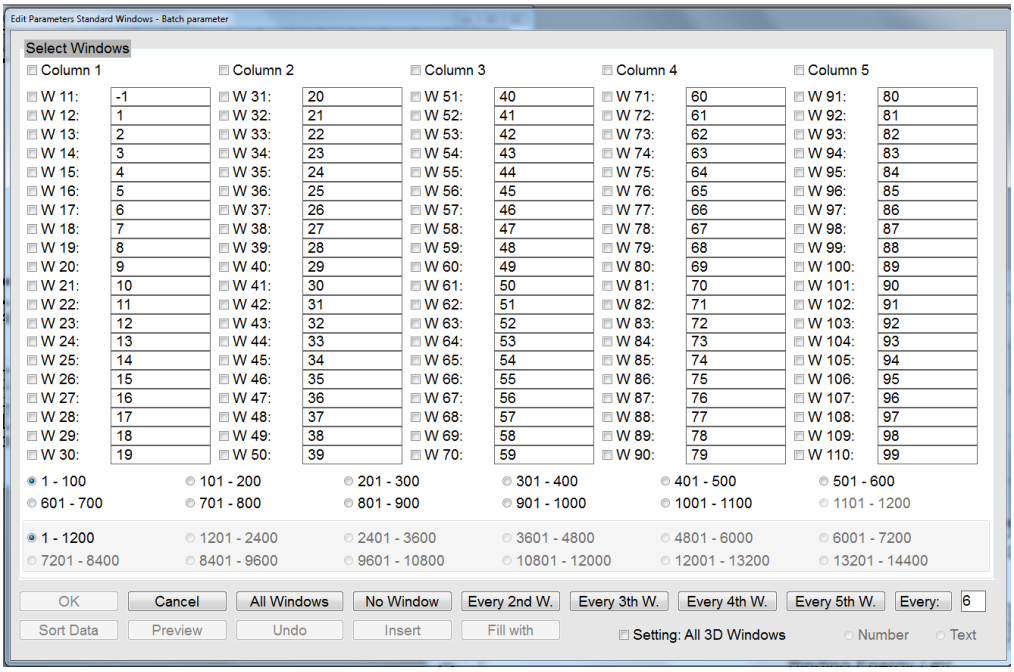

Fig. 1. The new designed selection dialogue for maximum14400 standard windows

v) The dialogue 'Hide Standard Spectra' was improved. Five new options are offered (see Fig. 2, right side).

vi) The saving of the UNIFIT projects was optimized. The storage space was halved.

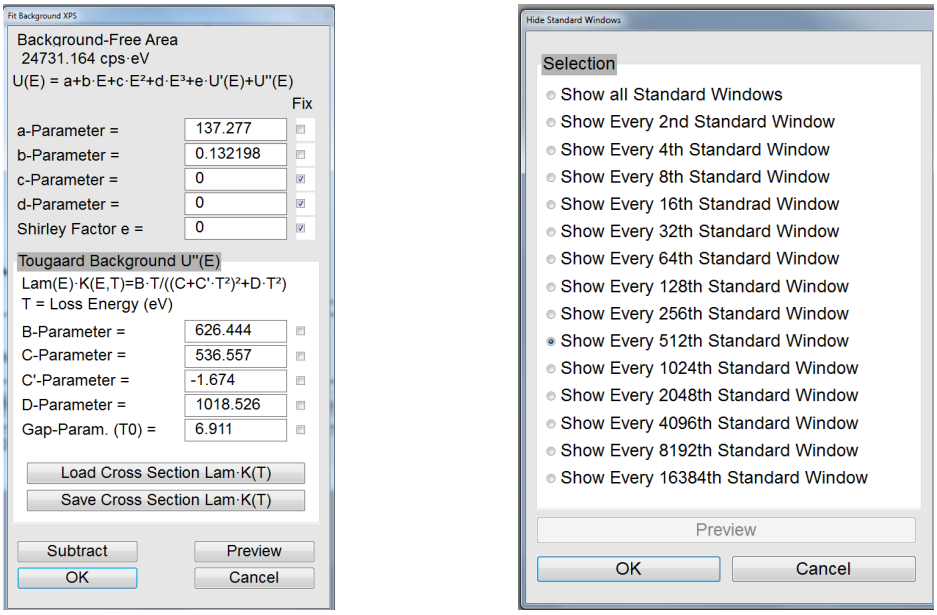

Fig. 2. Left: dialogue of the Tougaard background of homogeneous samples, right: dialogue for displaying and hiding of standard windows

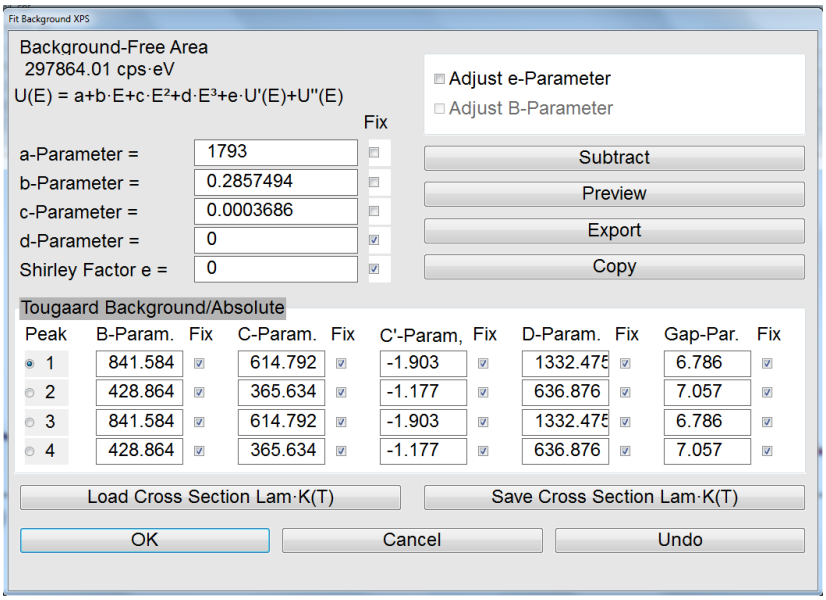

Fig. 3. Dialogue for the Advanced-Tougaard background, input and display of all background parameters, four background functions are used (imply four peak-fit components), parameters peak 1 and 3: Al_2O_3, parameters peak 2 and 4: SiO_2 (see Fig. 4 and 5)

vii) The Legend/Select Curves dialogue may be selected by clicking the right mouse button of a legend displayed in the active window.

viii) The number of marker lines was increased to 15.

ix) The Five-Parameter Inelastic Electron Scattering Cross Section is introduced. The additional gap-energy parameter allows a better simulation of the loss structure of insulators (Fig. 2, left).

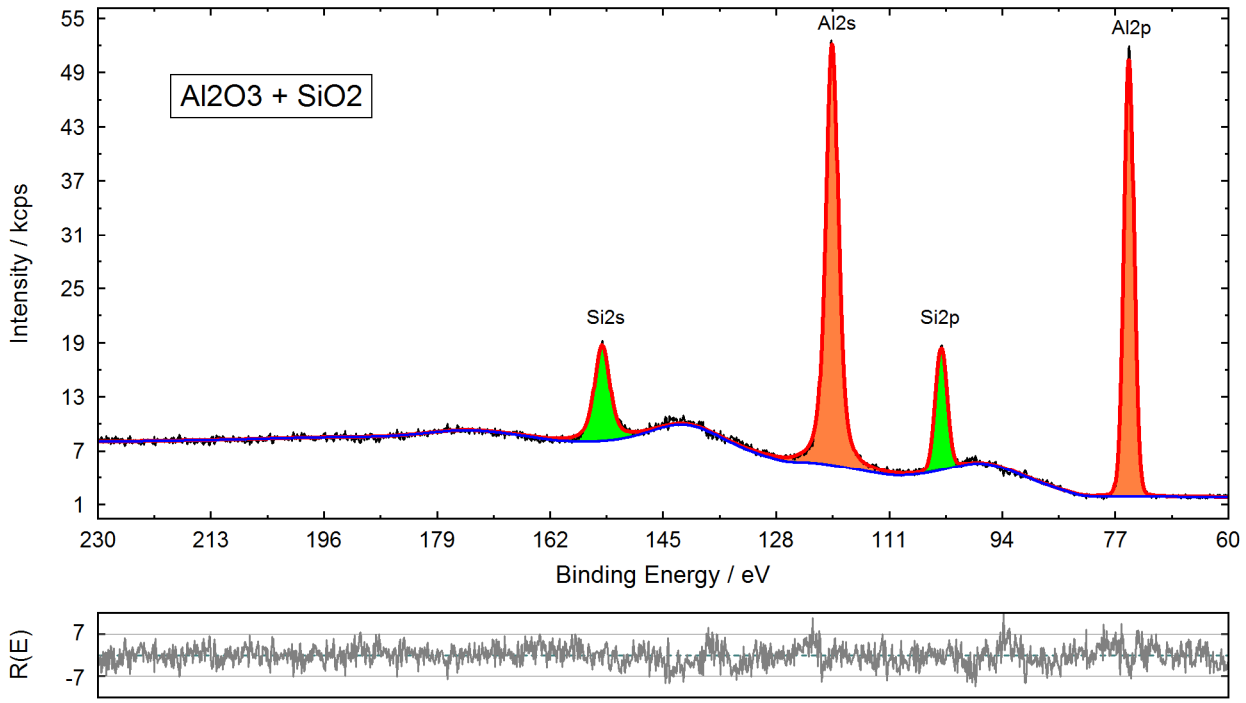

Fig. 4. Peak fit of the 2s and 2p lines of Al_2O_3 and SiO_2 using the Advanced-Tougaard Background method, parameters of the background functions are shown in Fig. 3, the corresponding λ·K(T) functions are plotted in Fig. 5

x) The Advanced-Tougaard Background was developed for a better modelling of the spectral background function of XPS measurements of inhomogeneous samples. The spectral background of every peak-fit component is calculated separately (see Fig 3, 4 and 5).

xi) After the loading of spectra all acquisition parameters can be modified. A special interpolation routine is started if the step width, the start or end energy are changed. Modified spectra are calculated.

xii) A new input routine of measurement data files recorded at the Laussane Nanolab (XAS) was implemented.

xiii) The input routine of measurement data files recorded using the Scienta SES spectrometer software was revised. The sum of the intensities of all slices per energy step (number of saved regions = number of loaded spectra) or the intensities of all saved slices (number of regions · number of slices = number of loaded spectra) may be loaded.

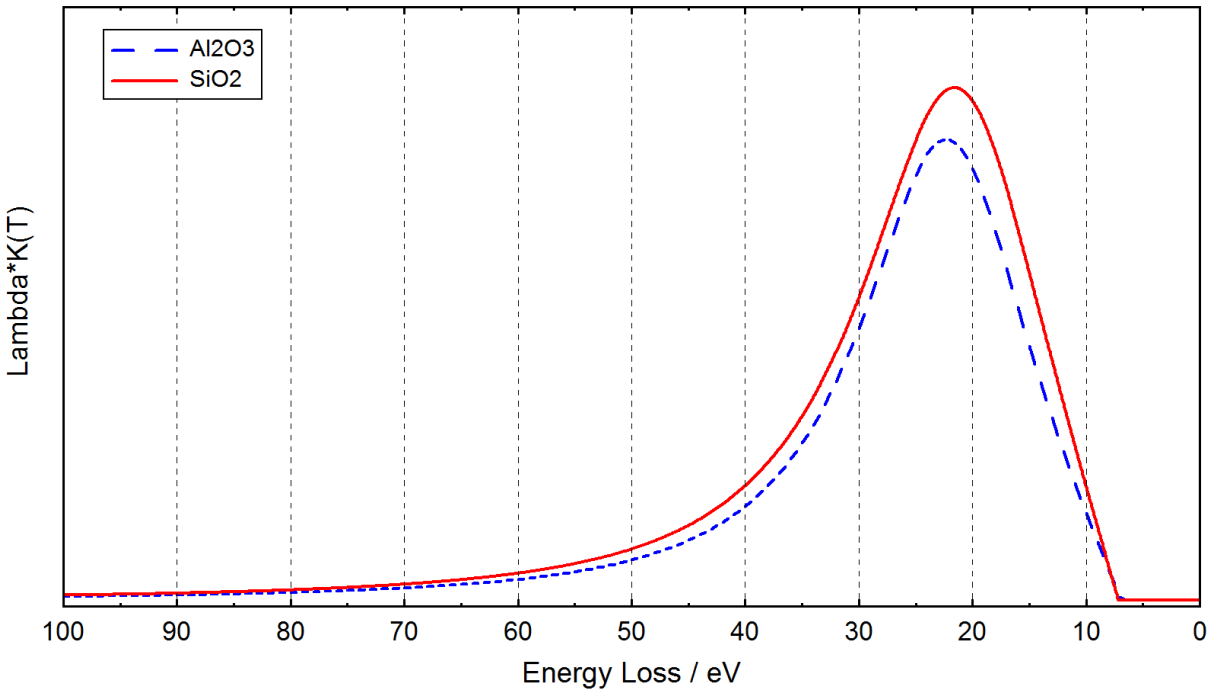

Fig. 5. Plot of the λ·K(T) functions of Al_2O_3,and SiO_2, corresponding parameters are shown in Fig. 3