What is new in UNIFIT 2011?

The improvement of the background treatment in the spectrum fit is the main goal of the **version 2011** of the software UNIFIT.

i) The new version of the UNIFIT software allows the iterative calculation of a model function to the description of the inelastic electron scattering cross-section $\lambda(E) \cdot K(E, T)$ (λ – inelastic mean free path, E - kinetic energy, T - loss energy) during the spectrum fit. The Four parameter inelastic electron scattering cross section 4-PIESCS with fittable parameters was introduced. The new procedure gives also excellent fit results using wide range photoelectron spectra (more than 100 eV). The calculated cross sections can be plotted, stored, loaded (*.cro), as well as be integrated into the spectrum fit. Figure 1 presents the fit of As 2p (left) and Ga 2p (right) of oxidized GaAs. Figure 2 shows the estimated inelastic electron scattering cross-sections (left) and the input routine for the improved background treatment.
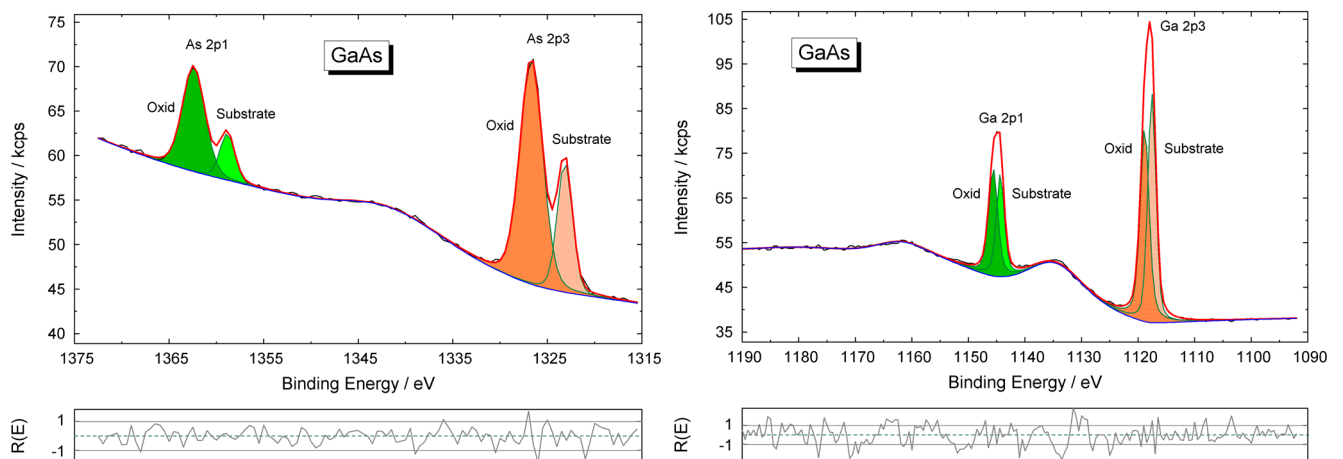

Fig. 1. Wide range spectrum fit of oxidized GaAs using improved Tougaard background mathod; images created using UNIFT 2011, exported and inserted into this Word document

ii) In the spectrum processing part of the program the correction of the spectra with the transmission function (IERF) of the used spectrometer setting was implemented. Now, in addition, the IERF can be defined by the user manually. The defined IERF can be stored and loaded. Figure 3 presents a survey of GaAs without IERF correction (left) and with IERF correction (right).

iii) In the menu point 'quantification' the lines which should be used for the calculation can be selected optionally.

iv) The maximum number of spectrum windows was increased to 200. The window selection functions were modified accordingly.

v) Because parameter representations are connected with the window numbers, a function was introduced to exchange the numbers of two windows.
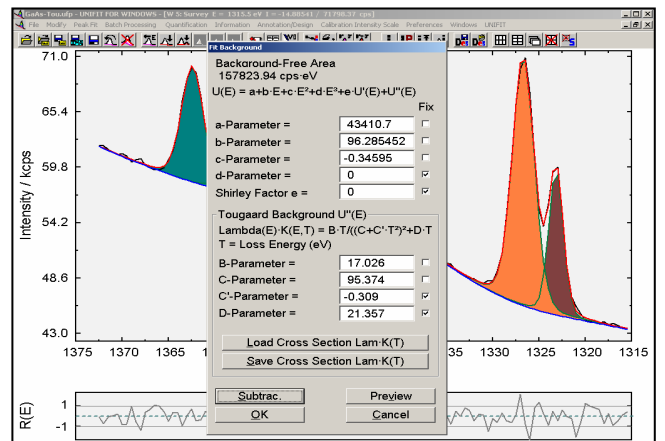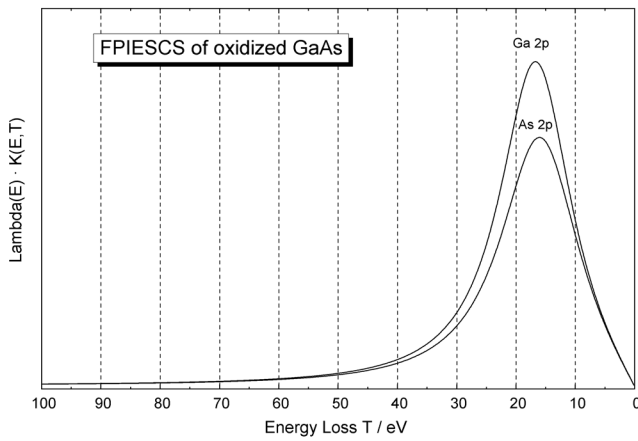
Fig. 2. Left: Calculated FPIESCS of oxidized GaAs deviated from the Ga 2p and As 2p peak, right: Fittable-background input dialog for the determination of the background-fit parameters parallel to the peak fit
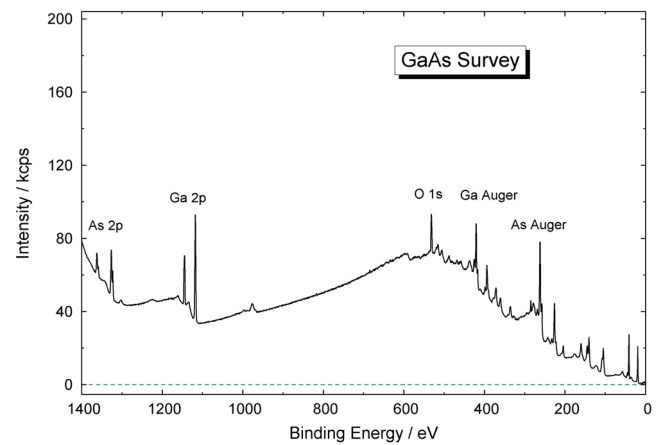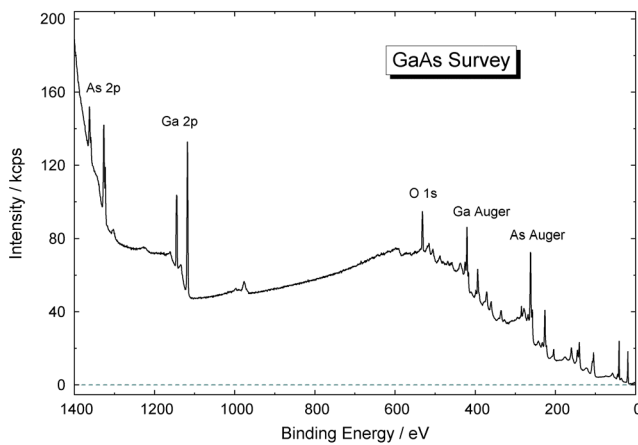

Fig. 3. Left: GaAs survey untreated, right: GaAs survey after correction with IERF

vi) With the representations 3D-Waterfall 45° and 3D-Waterfall -45° the energy-intensity wall, intensity-parameter wall and energy-parameter wall can be indicated optionally. The colour setting of three walls can be chosen in the preferences. Figure 4 shows 3D-presentations with and without wall plotting.
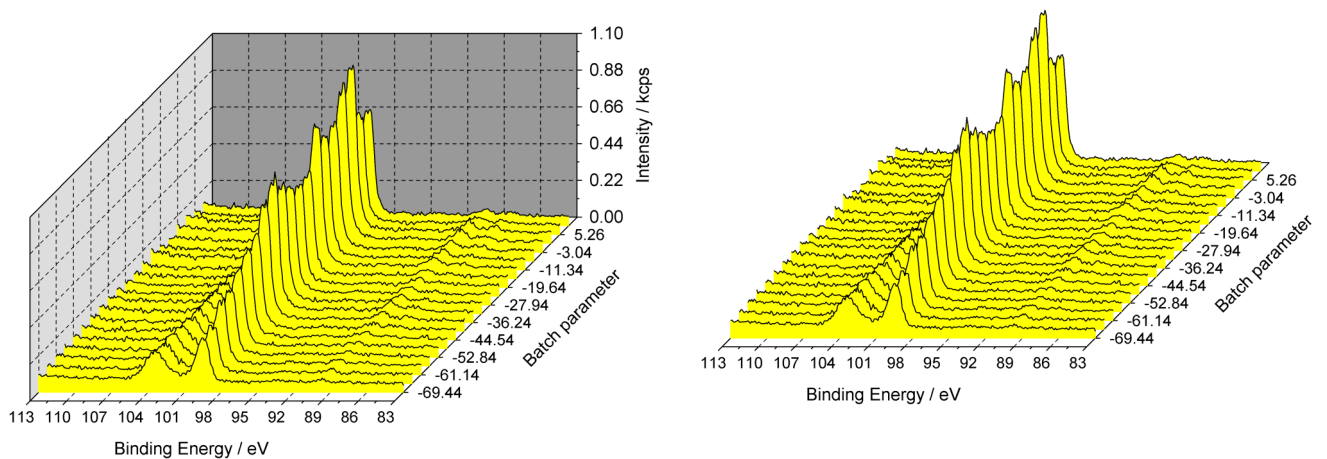

Fig. 4. 3D-Waterfall 45° plot left: with energy-intensity, energy-parameter and intensity-parameter wall and right: with energy-parameter wall only

vii) Now all design settings can be assigned to every window separately (Fig. 5) or all windows. All design settings of every open window will be stored in the project. With the loading of projects these saved settings are used, regardless of the loaded pre-setting. With the exception of the stored language and tool bar settings, the stored preferences can be loaded by open windows too.

viii) The design setting, the title, the annotation and the legend can be stored separately from the active window (*.dsg). The saved settings can be loaded and used for the active window.

ix) In addition, the values of the layer thickness can be printed out.

x) Now, the width and height of the spectra windows can be calibrated additionally to the x- and y-axis of the coordinate system.

xi) The position and size of the parent window is stored if the program UNIFIT is closed. A reopening of the UNIFIT software activates the saved position and size.

xii) The options of the input of the measurement data stored in the VAMAS format were improved. The intensities or the first corresponding variables can be loaded optionally. During the loading the data can be normalized by the first corresponding variables. Additionally, a sum spectrum may be created using the spectra from all blocks of a spectral region.
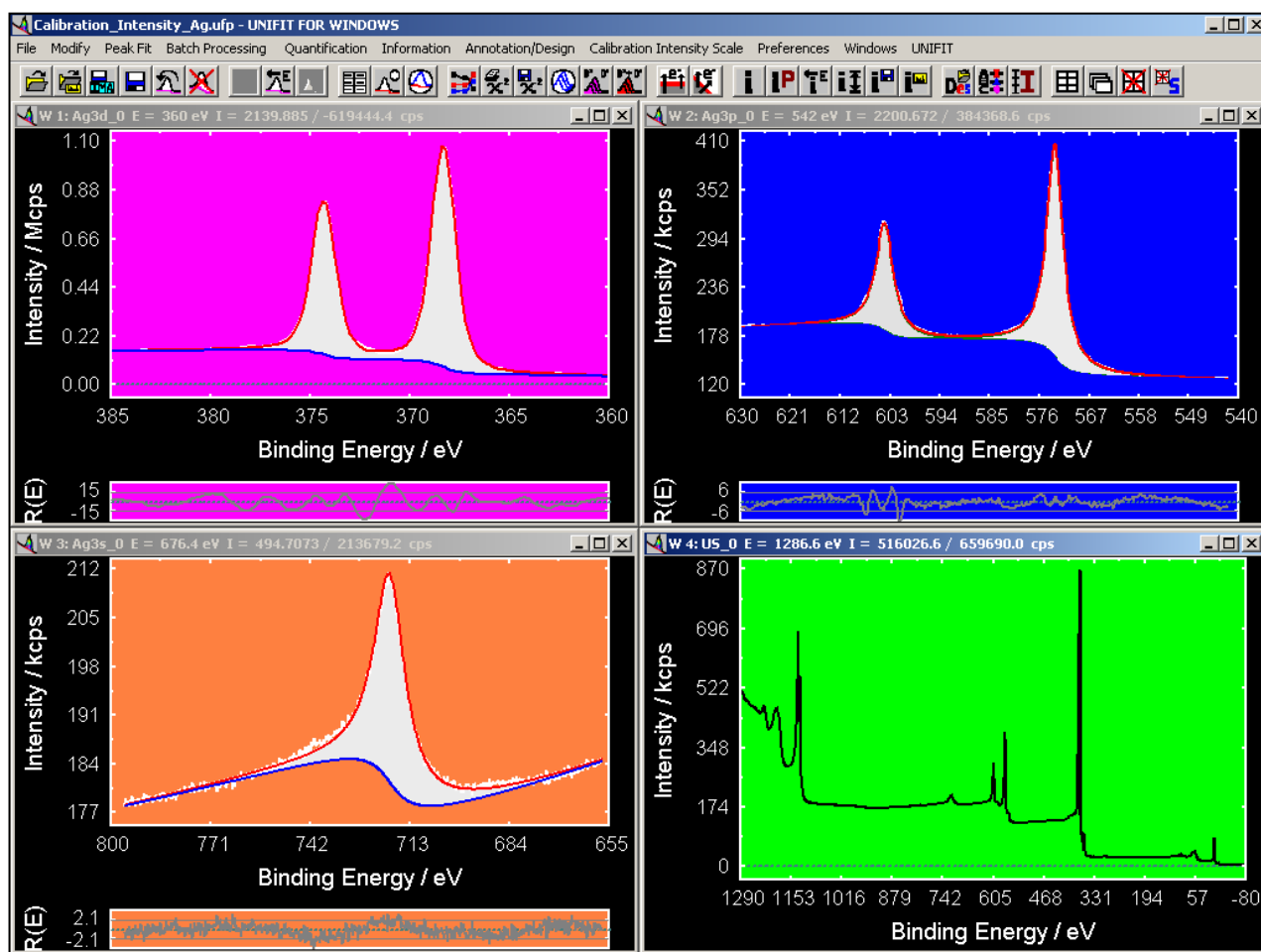

Fig. 5. Four UNIFIT windows with four different background colours