What is new in UNIFIT 2013?

Main focus of the advancement to the **version 2013** was the implementing of the spectrum processing of X-ray absorption spectra (XAS). The following innovations and changes were necessary during the programme development:

1. Separate spectrum input for XPS and XAS measuring data.
2. Programming of new input routines for XAS data (also for non-equidistant and non-monotonous step width, step width, start- and end energies can be selected manually, data can be normalized optionally).
3. Implementing of a new model function (sum from error and Arc tangent function) for the modelling of the spectral background for XA spectra (see Fig. 1 and Fig. 2).
4. Adaptation of the calculation of the asymmetry with the description of XA spectra line shapes.

i) Now Photoelectron- (XPS) and X-ray absorption spectra (XAS) can be analysed parallel with the programme UNIFIT 2013.
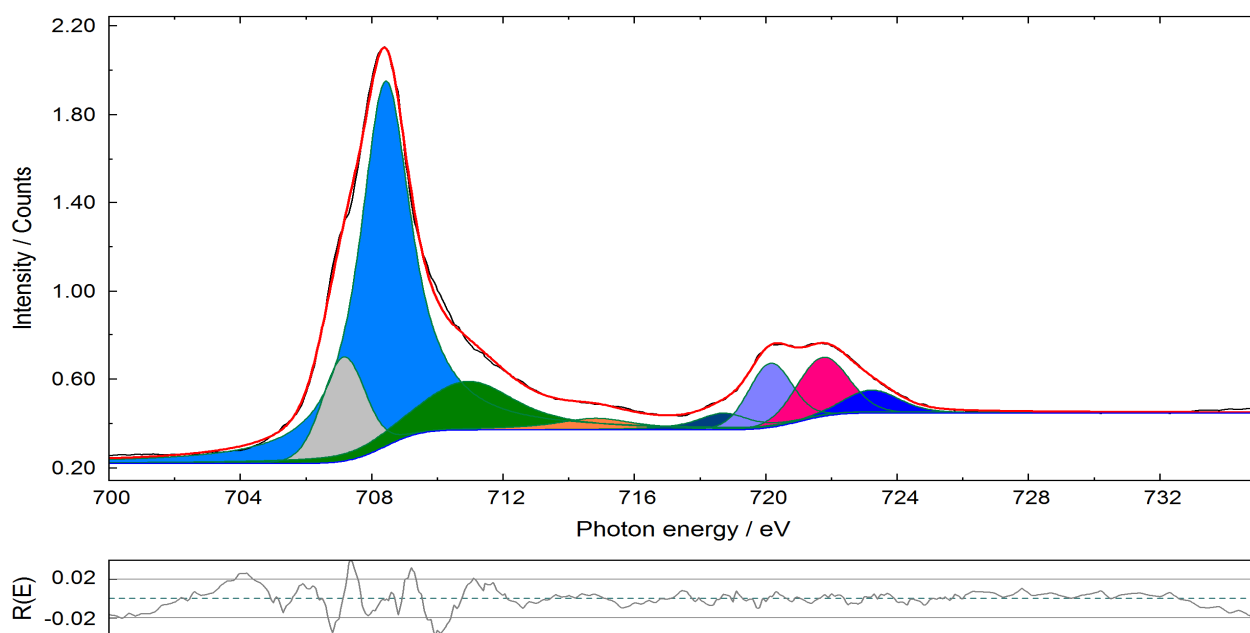

Fig. 1. Peak fit of the L edge XAS signal of Fe in Fe_xO_y using UNIFIT, background: step function (sum of error and Arc Tangent function) with two steps

ii) During the fit of the valence band or Fermi edge the model function (root, linear or Theta function) may be displayed without broadening by the Gaussian function (see Fig. 3).

iii) Five at last loaded projects are indicated in the programme and can be quick opened by mouse click.

iv) Now the fit-parameter table contains additionally a button for switching to absolute or relative parameters. By changing the parameter form the used iteration sub-routine will be switched, too.

v) The maximum number of components for the generation of the model function at the peak fit has been increased from 15 (doublets: 30) to 30 (doublets: 60, Fig. 4).
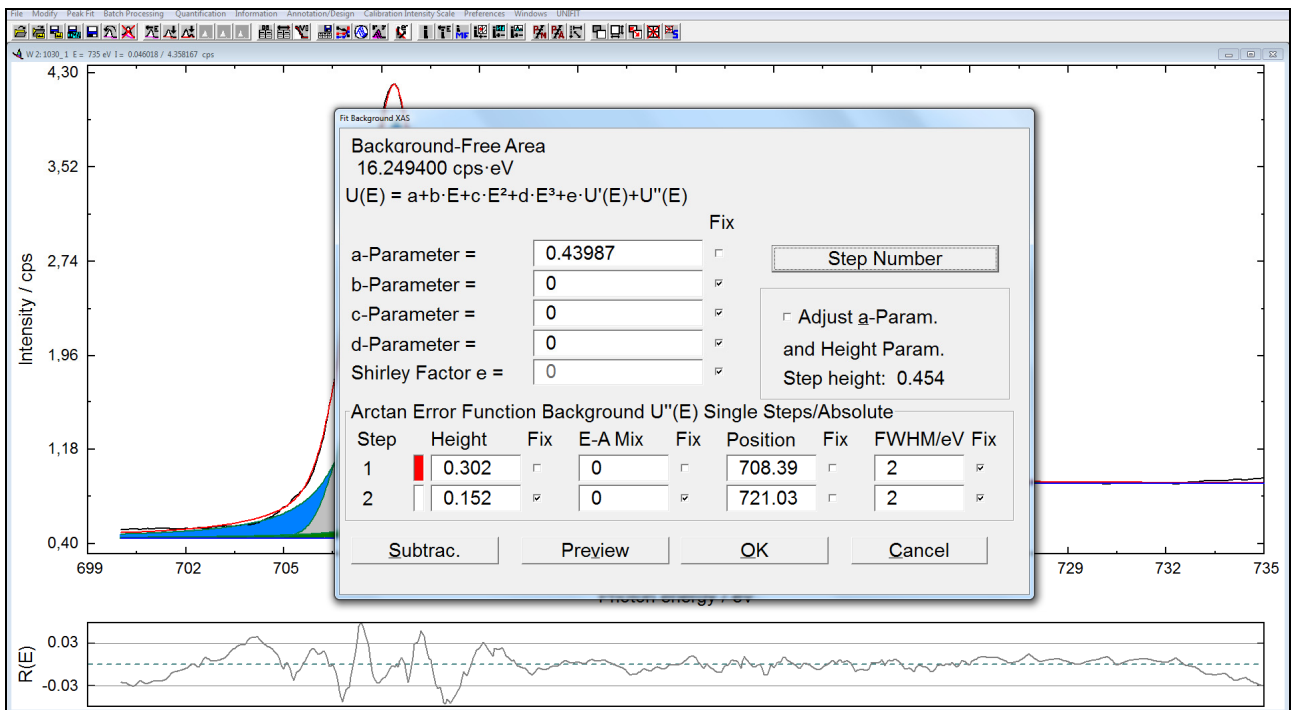

Fig. 2. Dialogue for the definition of the XAS-background model function (example: 2 steps)
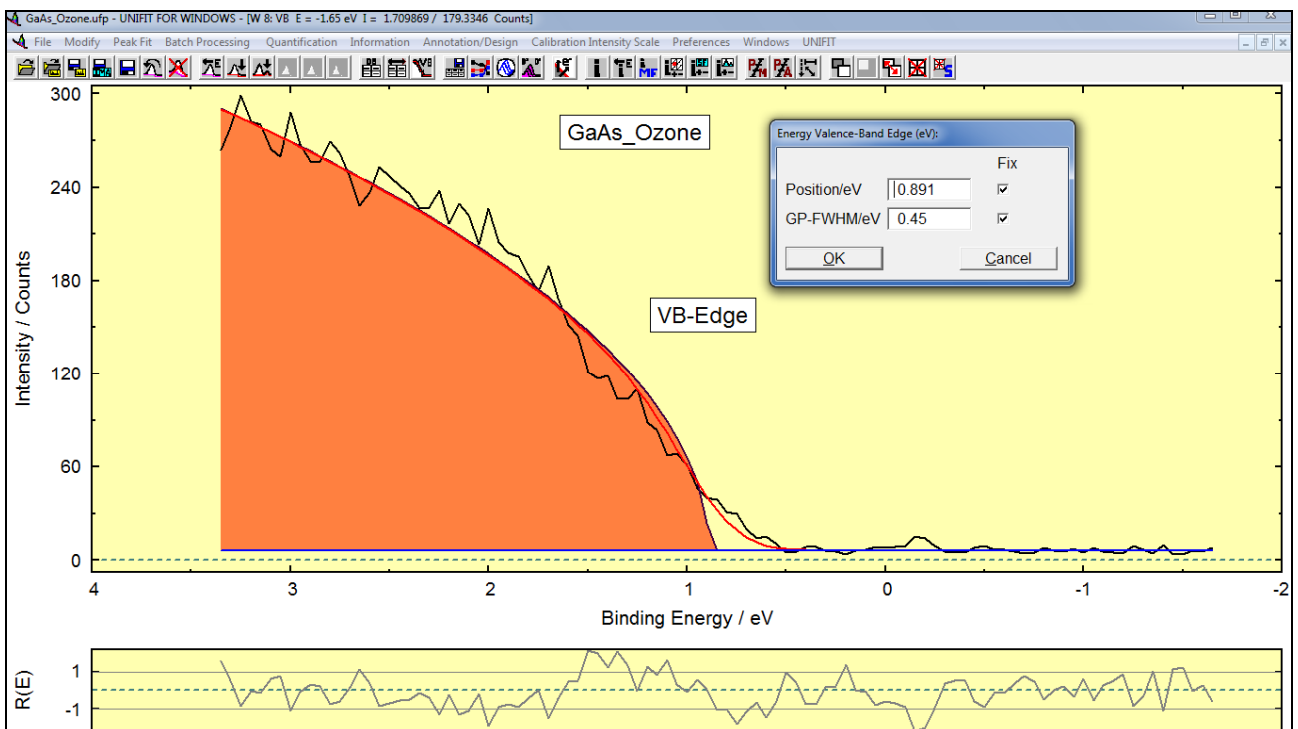

Fig.3. Dialogue of the determination of the valence-band edge position of the ozone treated GaAs (model function: convolution of square root and Gaussian functions *SQR(E)*G(E)*) (screen shot), orange: Square root function without Gaussian bordering, red: sum curve, blue: background curve
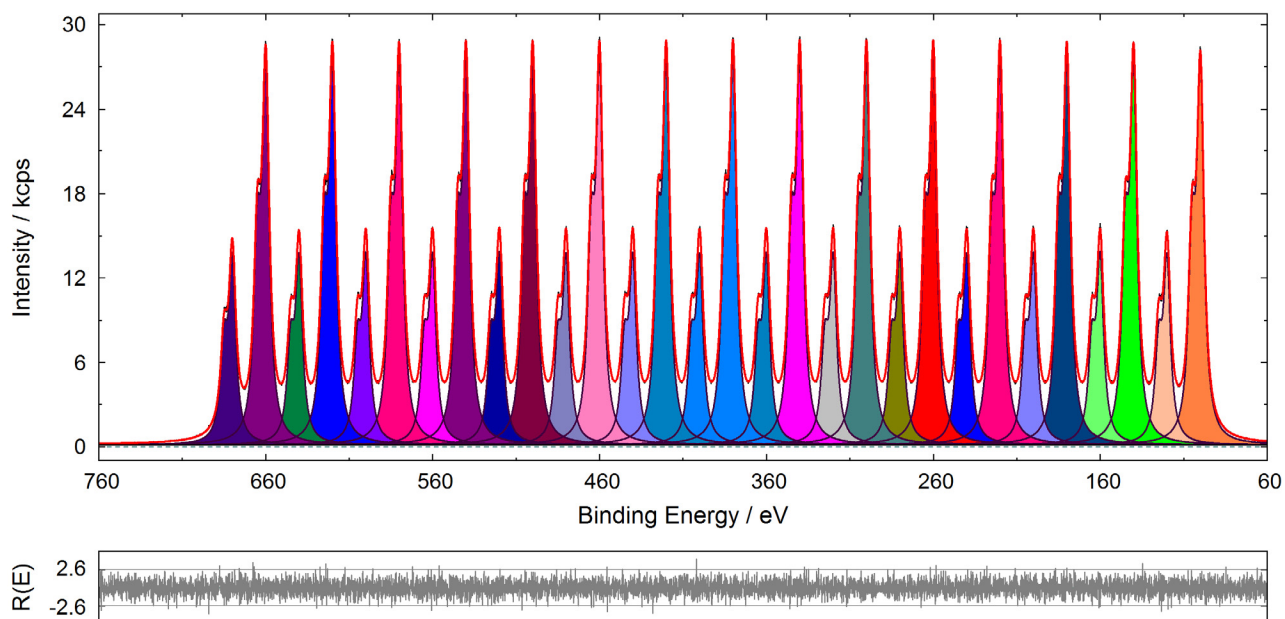
Fig. 4. Peak fit of a synthetically generated test spectrum (Unifit_2013_User_Files\test spectra\Test 32_30Doublets-Convolution-Absolute_Result.ufp) with 30 doublets (60 peaks)
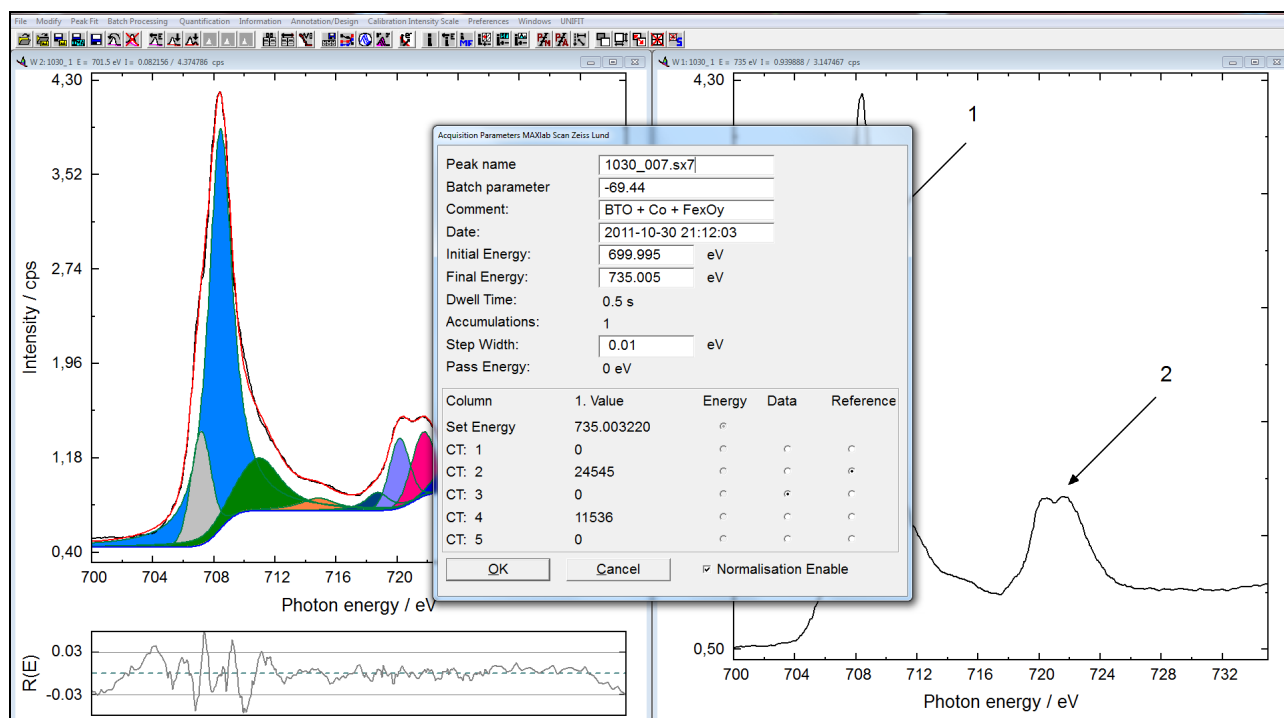

Fig. 5. Input dialogue for XAS data, acquisition parameters can be changed manually, the allocation of counter (CT) columns to the energy, intensity or references is variable. the data can be normalized optionally

vi) Now a legend can be indicated for all window types (standard window, 3D-window...) of the programme.

vii) The internal calculation of the Tougaard background was changed. The estimated polynomial will be subtracted before the Tougaard background is calculated.

viii) Now in the quantification table includes additionally the sum of the standardised peak areas of every spectrum region. These can be also plotted with the parameter plot sub-routine.

ix) Additional data formats were integrated into the input routine of the programme:

1. XPS: SSI-XPS (University Stanford), SPECS Phoibos 225, croissant format (PESP)

2. XAS: BESSY/EMP-2, Zeiss MAXlab Scan (Lund), NEXAFS and two standard formats (2 columns: Photon energy and intensity (see Fig. 5).