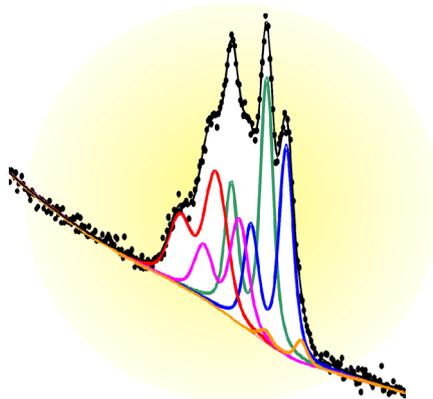# unifit FOR WINDOWS

Spectrum Processing, Analysis and Presentation Software for Photoelectron Spectra (XPS), Auger Electron Spectra (AES), X-ray Absorption Spectra (XAS) and RAMAN Spectra

General Characteristics:

- Curve fitting algorithm of Marquardt
- Selection of product, sum or convolution of Gaussian and Lorentzian functions (Doniach-Sunjic function)
- Background simulation by different models
- Calculation of inelastic electron scattering cross sections
- Valence-band edge and Fermi energy calculation
- Batch processing for treatment of parameter-dependent series
- Calibration of the transmission function and intensity scales
- Peak ID is supported by a data bank with 15000 XPS lines and AES transitions
- Quantification using cross section and sensitivity factor data bases
- Data bases of binding energies, doublet data, Auger parameters
- 32-bit and 64-bit MS Windows based programme
- Simultaneous display and handling of up to 75600 windows
- Individual preferences (language, export format, curve fitting, graph display and design, printing, etc.)
- I/O routine reads 350 data formats and user demand formats
- Extensive graphical design tools
- Fit parameter and 3D plots including quantification results
- Comfortable data export from all windows presentations
- High resolution export (1200 dpi) for all window presentations, the quantification table and fit-parameter table
- Copy – Paste function for transferring processing results to other generally used softwares (Word©, Excel©, Origin©)
- Saving and loadung of projects
- Generation and presentation of 'Windows Video Sequences'

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UNIFIT - an Universal Programme for XPS, AES, XAS and RAMAN Spectra Peak Fitting, Analysis and Presentation Based on WINDOWS

The programme permits the simultaneous handling of up to 75600 windows with spectra or other presentations. The windows may be generated hidden or visible. All generated windows (visible or hidden) may be used for the following operations (e.g. 3D presentation, quantification, parameter plot). The title line of the parent window shows the name of the project currently loaded. The X-axis of XP spectra in standard spectra windows is drawn with increasing kinetic energy or decreasing binding energy from the left to the right. The title bar includes significant information for the user. The X-axis of XA spectra is always presented with increasing photon energy. The X-axis of Auger electron spectra is presented with increasing kinetic energy. The X-axis of RAMAN spectra is presented with increasing wave number (cm-1). The annotation of the energy, intensity or parameter axis will be adjusted to the chosen presentation mode. The annotation of the axes may be changed manually by the user. Eleven presentations are available:

1. **Standard:** presentation of spectra, saved transmission or loss functions,
2. **Wagner plot:** presentation of Auger parameter,
3. **3D-Waterfall 0°:** presentation of spectra, modified spectra or sum curves (after peak fit) of parameter dependent measurements in one window without x-shift,
4. **3D-Waterfall 0° Plus:** presentation of fitted spectra of parameter dependent measurements without x-shift in one window,
5. **3D-Wasserfall 45°:** presentation of spectra, modified spectra or sum curves (after peak fit) of parameter dependent measurements in one window with x-shift to right,
6. **3D-Wasserfall -45°:** presentation of spectra, modified spectra or sum curves (after peak fit) of parameter dependent measurements in one window with x-shift to left,
7. **3D-Colour Profile:** presentation of the intensities of spectra as brightness, modified spectra or sum curves (after peak fit) of parameter dependent measurements in one window,
8. **XY 3D Plot 45°:** presentation of the maximum or minimum of the intensities of spectra or the areas of background free spectra, areas of sum curves (after peak fit), chemical components (after peak fit) or fit parameters of the peak-fit components (after peak fit) with respect to the x and y coordinates of multipoint (area) scans in one window with x-shift to right,
9. **XY 3D Plot -45°:** presentation of the maximum or minimum of the intensities of spectra or the areas of background free spectra, the area of sum curves (after peak fit), chemical components (after peak fit) or fit parameters of the peak-fit components (after peak fit) with respect to the x and y coordinates of multipoint (area) measurements in one window with x-shift to left,
10. **XY 3D Colour Profile:** presentation of the maximum or minimum of the intensities of spectra or the areas of background free spectra, the area of sum curves (after peak fit), chemical components (after peak fit) or fit parameters of the peak-fit components (after peak fit) with respect to the x and y coordinates of multipoint (area) measurements as brightness in one window,
11. **XY 3D 45° Colour Profile:** presentation is a combination of 'XY 3D Plot 45°' and 'XY 3D Colour Profile',
12. **XY 3D -45° Colour Profile:** presentation is a combination of 'XY 3D Plot -45°' and 'XY 3D Colour Profile',
13. **Parameter Plot:** presentation of fit parameters (peak height, line position ...) or the results of quantification (peak areas, normalized peak areas ...) with respect to the parameters,
14. **Show Windows Video Sequence:** presentation of a short windows video sequence of standard, 3D or parameter windows (maximal 75600 frames using standard windows, maximal 100 frames using 3D or parameter plot windows). Only visible standard windows can be included into this presentation.

Individual preferences can be selected for the mathematical background of the model function (product, sum or convolution of Lorentzian and Gaussian functions), fit parameters (absolute or relative), language (German or English), text style of dialogs and exported tables, details of presentation (line colours, line form, thickness of lines, text style of annotation) on the desktop as well as for printing. There are two methods for the error analysis of the calculated fitting results. In a special menu the parameters of the excitation satellites for MgKα and AlKα can be edited and saved in up to five sets of data. The Tougaard background can be calculated for homogeneous or inhomogeneous samples.

An extended input and output routine allows the direct reading of measurement data of different kinds. The fast transfer of the data achieved in the spectra analysis to the standard spreadsheet software (i.e. Excel©, Origin©) is given by an export routine. All processing steps of all opened windows as well as the quantification table and the film thickness estimation may be stored in one project. The original measurement data are saved in a separate directory. Auger parameters can easily be presented as Wagner plot.

The active window presentation can be copied or exported as an image with different resolutions (400 dpi, 600 dpi, 800 dpi, 1200 dpi) and formats (tiff, gif, emf, jpg, bmp, etc.) The output to a printer is made in a way that all important information are clearly shown. The provided test spectra give the user the possibility to test the different functions of the programme without measured data. For the spectra modification menu there are options for charge correction of the active window, several procedures for the background calculation, satellite subtraction, smoothing, differentiation, and spike correction as well as the chance for spectra manipulation and operation. Additionally, a normalisation routine with four different methods is available.

The peak fit is based on the non-linear least squares curve-fitting algorithm of Marquardt. The programme allows choosing product, sum or convolution of Gaussian and Lorentzian functions (in case of assymetrie the Doniach-Sunjic function) for the calculation of the model function. All peak parameters may be varied freely, varied within a chosen interval or fixed at certain values. Moreover, parameters may be determined on absolute scales or they may be treated as relative parameters i.e. related to the leading peak of a doublet or to the first out of a group of peaks. Different options are available, enabling the user to keep, e.g. energy distances, peak widths or relative intensities of peaks constant during iteration. Furthermore, it is possible to include the background parameters in the fit routine. Besides this inclusion in the minimization procedure, the background can be simulated by five different methods (or combinations of them) and subtracted from the experimental curve before initiating the peak fit. The fit-parameter table can be saved, copied or exported. UNIFIT permits the estimation of valence-band edges or Fermi edges. The error of the fit parameters can be calculated.

A batch-processing submenu was supplemented for fast analysis of parameter-dependent series of spectra (e.g. depth profiles, angle dependent measurements). All options for spectra modification and the peak fit can be included in batch processing. Ten different presentations of the parameter-dependent measurement are available. Additionally, the estimated fit parameters can be plotted with respect to the window numbers, batch parameters or a freely chosen values.

The quantitative analysis is possible from survey or single spectra using cross sections as given by Scofield, empirical sensitivity factors by Wagner or defined individually by the user. The quantification table may be copied or exported as an image (1200 dpi). A parameter-plot function allows the presentations of the peak areas or atom percentages with respect to the window numbers, batch parameters or manual chosen values. Remarks and comments may be included in the spectrum presentation. **The integrated data bases** of photoelectron lines, Auger electron transitions and Auger parameters can be used for peak identification, labelling and chemical-state plot (Wagner plot) respectively. A project comment can be used for specifying the individual treatment of the sample. The data banks integrated in UNIFIT can be shown, edited and extended directly with special subprogrammes. The AES emission yield can be estimated using a special calculaion tool. The binding energies of the target atom subshell are saved in a data bank.

The subroutine "Annotation/Design" gives the user the manual controlling of the scaling and labelling of the energy, intensity, and parameter axis. The energy axis in every window is drawn with increasing kinetic energy (or decreasing binding energy) from the left to the right and significant information for the user in the title bar. Additionally, the spectrum may be entitled and labelled. Optionally a grid for all axes can be plotted. For standard spectra and parameter plots a legend for specifying the plotted curves can be shown. All acquisition parameters can be changed after loading the spectra.

The menu "Calibrate Intensity Scale" allows the determination of the transmission function of the spectrometer in two different ways. The calculated functions can be shown, saved and used for quantification