

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

The programme permits the simultaneous handling of up to 300 windows with spectra or other presentations. The title line of the parent window shows the name of the project currently loaded. The x-axis in standard spectra windows is drawn with increasing kinetic energy (or decreasing binding energy) from the left to the right including significant information for the user in the title bar. The annotation of the x- and y-Axis will be adjusted to the chosen presentation mode. The annotation of the axes may be changed manually by the user. Eight 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 the 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 the 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. **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 (sputter time, emission angle, ...).

With the menu point **preferences** the operator can define, store and load (*.set) all setting parameters of the programme handling. The toolbar can be modified and switched on or off. The size of the icons is variable. The size, font and colour of the menu text and table export (fit parameters and quantification results) may be modified independent of the spectra windows setting. The programme language is either German or English. The user can activate an automatic restore function of the Unifit projects and define the cyclic saving time. The decimal character and delimiter of the exported data may be defined. Four options for the VAMAS input are available. The resolution of the exported images may be changed in six steps up to 1200 dpi. The number of average points for the smoothing, differentiation and background calculation is variable. The presentation of the spectra may be done in kinetic or binding energy, the intensities in counts or cps. The monitor presentation and print out is set up separately. The form, size and colour of the curves as well as the fill colours of the fitted component areas may be selected. Additionally, the form, size and colour of the coordinate axes and all other lines and symbols are adjustable. In a special menu the excitation satellites for Mg-K α and Al-K α and for two other user defined sources can be corrected and saved in up to five sets of data. The transmission function IERF can be loaded and defined manually. UNIFIT offers different mathematical backgrounds of the model function (product, sum or convolution of Lorentzian and Gaussian functions) and fit parameters (absolute or relative) to carry out the peak fit. Additionally, the user can choose from two different methods for the calculation of the fit parameter-errors.

An extended **input routine** allows the direct reading of measurement data of different kinds. All processing steps, the window sizes, positions and design elements of all opened windows, the quantification table as well as the film thickness estimation may be stored in one project. The original measurement data are saved in a separate directory. The

automatically saved backups of the projects can be opened. Auger parameters can be easily plotted as Wagner plot. The integrated test spectra enable the user to give the different functions of the programme a try without measured data. A closing function for all windows or all standard windows is available. The presentation of the active window can be transferred to the clipboard via the 'Copy – Paste – function' or exported as image taking a commonly used format (*.jpg, *.bmp, *.gif, *.wmf, ...). The resolution may be selected stepwise from the monitor resolution to 1200 dpi in four steps. 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. The output to a printer is made in a way that all important informations are clearly shown. The menus 'Select Spectra' and 'Select Blocks' allows the individual displaying of spectra from the loaded data file.

For the spectra **modification** menu there is an undo function, a copy and paste function, a correction with the IERF, 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 normalization routine with four different methods is available.

The **peak fit** is based on the non-linear least squares curve-fitting algorithm of Marquardt and Levenberg. The programme allows to choose product, sum or convolution of Gaussian and Lorentzian functions 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 hold constant, e.g. energy distances, peak widths or relative intensities of peaks during iteration. A very helpful option of the fit-parameter table is the labelling of the components with the corresponding names of the chemical species (e.g. for the C 1s components: -C-C-, -CH₂-, -CO-, -COOH, ...). The advantage of this option is the automatic transfer of the component annotations to the following processing steps (export, batch processing, parameter plot, quantification table) opening an easy way for a correct labelling of the chemical components with both the region name and the name of the chemical component (C1s -CH₂-, C1s -CO-, ...). Additionally, the fit-parameter table can be transferred to the clipboard with the 'Copy – Paste' function or exported as an image. Furthermore, it is possible to include the background parameters in the fit routine. Alternatively the background can be simulated by five different methods (or combinations of those) and subtracted from the experimental curve before initiating the peak fit. Additionally, the errors of the fit parameters can be calculated. Three separate subprogrammes permit the estimation of valence-band edges or Fermi levels. The curve-fit results can be printed including fit, acquisition parameters, and additional comments, or exported for further treatment and presentation.

The **batch-processing** submenu was implemented 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. After the batch-processing the fit parameters may be presented with respect to given batch parameters, the window numbers or on a fixed parameter point. Five different presentations of the parameter-dependent measurement are available.

A **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 transferred to the clipboard via the 'Copy – Paste' function or exported as image (1200 dpi) using a typical image format (*.jpg, *.wmf, *.gif, *.tif, ...). A parameter-plot function allows the presentations of the peak areas or atom percentages with respect to the window numbers, series parameters or manually chosen values. The film thickness can be estimated via two different methods.

Information about the acquisition parameters or the processing may be displayed any time. Identification and labelling of the peaks may be realized with the integrated data base of photoelectron lines. An additional data base of Auger parameters can be presented as chemical state plot (Wagner plot). A project comment can be used for specifying the individual treatment of the sample. The data banks integrated in UNIFIT (sensitivity factors, line positions, Auger parameters, doublet data) can be shown, edited and extended directly with special subprogrammes. Additionally, the calculated Inelastic Electron Cross-Section can be plotted.

The subroutine **Annotation/Design** gives the user the ability to manually control the scaling and labelling of the energy, intensity, and parameter axis. 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. Important remarks, comments, a title and ten marker lines may be inserted into the plot. The batch parameter (angle, sputter time, ...) may be edited in two special sub-routines for 3D windows as well as for all opened standard windows. The design setting, the spectrum title and the complete labelling of the active window can be stored (*.dsg).

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.

The **Window** handling gives the following options:

- changing the window size and position manually,
- direct selection and activation of the windows, particularly next or previous ones,
- three different tile arrangements of the windows,
- changing of the window numbers,
- two closing functions.

The window sizes and positions are saved in the UNIFIT projects.