Unifit 2001 – The New 32-bit Program for XPS
Peak Fitting under WINDOWS

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1. Motivation
An adequate modelling of experimental photoelectron spectra containing several different components has been possible since the introduction of the program UNIFIT. A further improved level for easy handling and sensitivity of parameters has been obtained. The program is used for more detailed information on binding energy and intensities of components. To avoid measuring energy distance can be gained. In order to obtain the desired information from raw data various peak appearance curves have been developed in the past that base on the description of experimental data by synthetic model functions.

The typical advantages of commercially available software with curve-fitting capabilities and statistical design options. However, they often exhibit excessive costs in data modeling. On the other hand, user-developed programs are only suitable for single applications and special applications. In many cases they have been written for use by insiders only.

In order to fill this gap, a program for peak shape analysis of experimental photoelectron spectra has been developed. A test function was created by ORIGIN (Fig. 1) and fitted with UNIFIT. The iteration start parameters were selected consecutively rough (Fig. 2). The parameters of the calculated curves correspond very well to those of the original test function. The line convergence was with non-optimal start parameters in obvious.

3. Fit of a Test Function
A test function was created by ORIGIN (Fig 1) consisting of two Voigt functions with different parameters. After transfer of the raw curve data to UNIFIT, the parameters were optimized. The iteration start parameters are selected consecutively rough (Fig. 2). The parameters of the calculated curves correspond very well to those of the original test function. The line convergence even with non-optimal start parameters is obvious.

4. Batch Processing
The batch-processing sub-menu serves as fast and convenient way to carry out a series of curve fits with the same settings. However, they often exhibit excessive costs in data modeling. On the other hand, user-developed programs are only suitable for single applications and special applications. In many cases they have been written for use by insiders only.

Further important features:
- User defined preferences for fit procedure, fit parameters, languages, details of presentation (colors and symbols) on the desktop as well as for printing, etc.
- Acceptance of VAMS (Nors and SNI) and NPL format.
- Load function chosen on user demand for several data formats provided e.g. by VG/GC/SCI.
- Simultaneous handling of up to 32 windows.
- Background subtraction by five different methods or combinations of them.
- Including the background in parallel.
- Different background functions such as e.g. change correction, variable subtraction, spike correction, differential subtraction, background correction, polynomial manipulation and spectrum operation.
- Description of the experimental curves by up to 15 single peaks or doublets.
- Different options in order to keep e.g. energy distance, peak width or relative intensity of peaks during iteration.
- Peak parameters may be varied linearly, varied within a chosen interval or fixed in certain intervals.
- All options for spectra modification and peak fit can be utilized in batch processing.
- Quantitative analysis using surveys, single spectra or special mathematical functions calculated either by Wagner or Scalfoni or defined individually by the user.
- Save, print, saving parameter tables and graphs including acquisition parameters and additional comments.
- Export for further treatment and presentation.
- Creation of different satellite functions, chi-square analysis.
- Improved handling.
- Integration of data by peak positions and chemical shifts.

References:
Website: www.uni-leipzig.de/~unifit

6. Adaptation of a Typical Synchrotron Text Function
The typical features of a synchrotron spectrum are:
- The intensity varies significantly between the different peaks.
- The intensity ratios of corresponding transitions in an XPS peak are not exactly the same.

For a test a doublet function (Tab. 2, Fig. 5) was generated with the software ORIGIN. A peak fit with the program UNIFIT 2001 and a special option was used to find the best adaptation for this complicated problem. The chosen start parameters were very rough (Fig. 8). The results are presented in Table 2 and Fig. 6.