

## What is new in UNIFIT 2009?

The version 2009 offers improvements of installation, data handling, design tools, and export formats. The new or improved thirteen subroutines are:

- i) realization of the user-administrator convention of Windows,
- ii) plot of the estimated fit parameters with respect to a batch parameter (Figure 1),
- iii) optional using of fill colours for the displayed components of the peak fit (Figure 2),
- iv) realization of different fill colours of the areas inside and outside the coordinate system (Figures 2 and 3),
- v) optional displaying of the residual function after the peak fit (Figures 2 and 3),
- vi) expanding of the exportable objects (activated window presentation, quantification table, fit-parameter table (Table 1)),
- vii) introduction of the 'Copy – Paste' function for a quick export,
- viii) expanding of the number of image formats using the export routines (\*.bmp, \*.wmf, \*.tif, \*.jpg, ...),
- ix) offer of four different resolutions for the exported images (monitor resolution, 400 dpi, 600 dpi, 800 dpi),
- x) introduction of variable cross sections into the Tougaard-background calculation (Figure 4),
- xi) estimation of the valence-band edge using a convolution of linear and Gaussian function optionally (Figure 5),
- xii) saving and displaying of the processing steps,
- xiii) labelling of the components of the fit-parameter table with suitable names of chemical compounds.

**i)** After the installation using the Windows-administrator mode the software UNIFIT is executable with the Windows-user mode. The first run of the software creates in the folder 'My documents' the directory 'Unifit\_2009\_User\_Files'. This folder includes all editable user files, e. g. the preferences of UNIFIT and integrated data banks and the folder 'My Unifit projects' for saving the received results.

**ii)** The parameter plot presenting the fit parameters or absolute or relative peak areas with respect to a batch parameter (e. g. sputter time or polar angle) was incorporated into the program. This new routine allows the presentation of data saved in a parameter dependent measurement format as well as data stored in a normal measurement format (with external parameter informations). Figure 1 shows the fitted peak heights of the doublet Si 2p. The ratio of the 3/2 and 1/2 peak was fixed at 2.

iii) In order to improve the design features of UNIFIT the peak areas of the fitting components can be filled optionally by colours. Figure 2 shows the As  $2p_{3/2}$  peak with five components (GaAs, As, AsO, As<sub>2</sub>O<sub>3</sub>, As<sub>2</sub>O<sub>5</sub>).

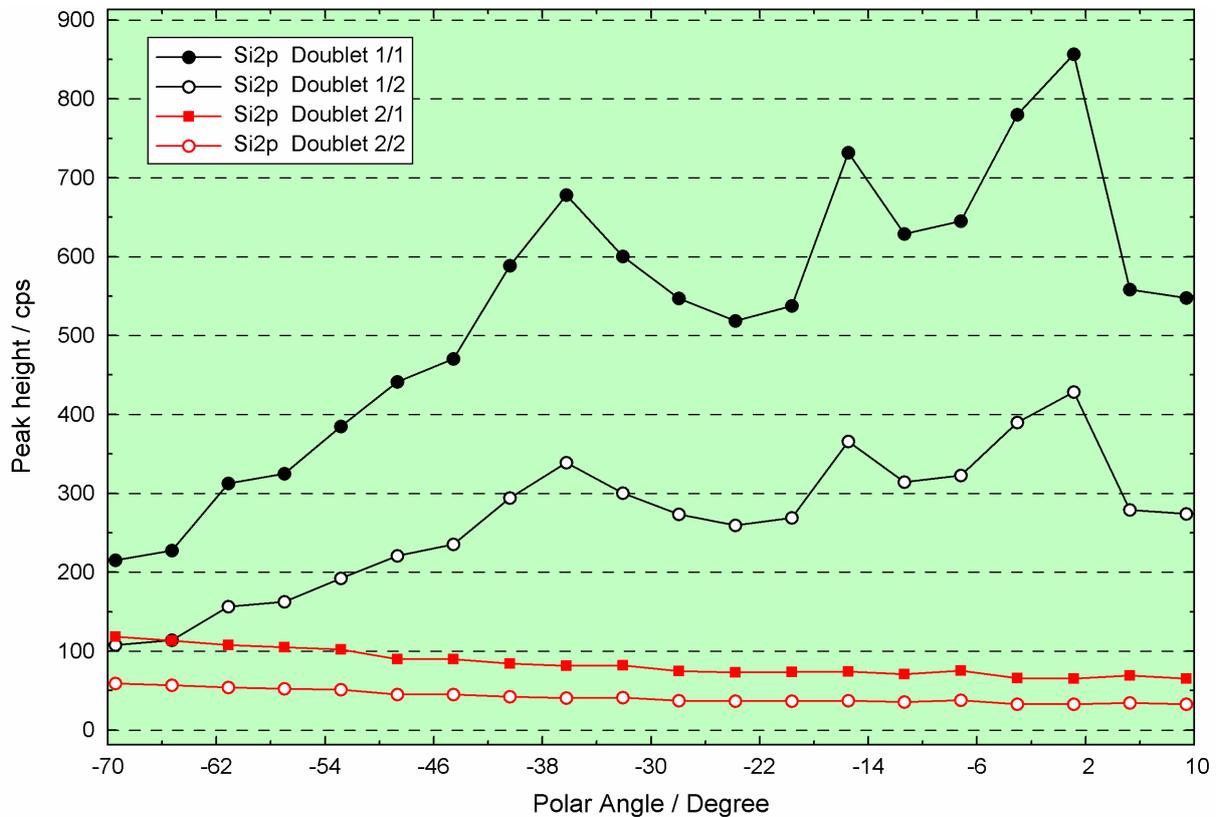


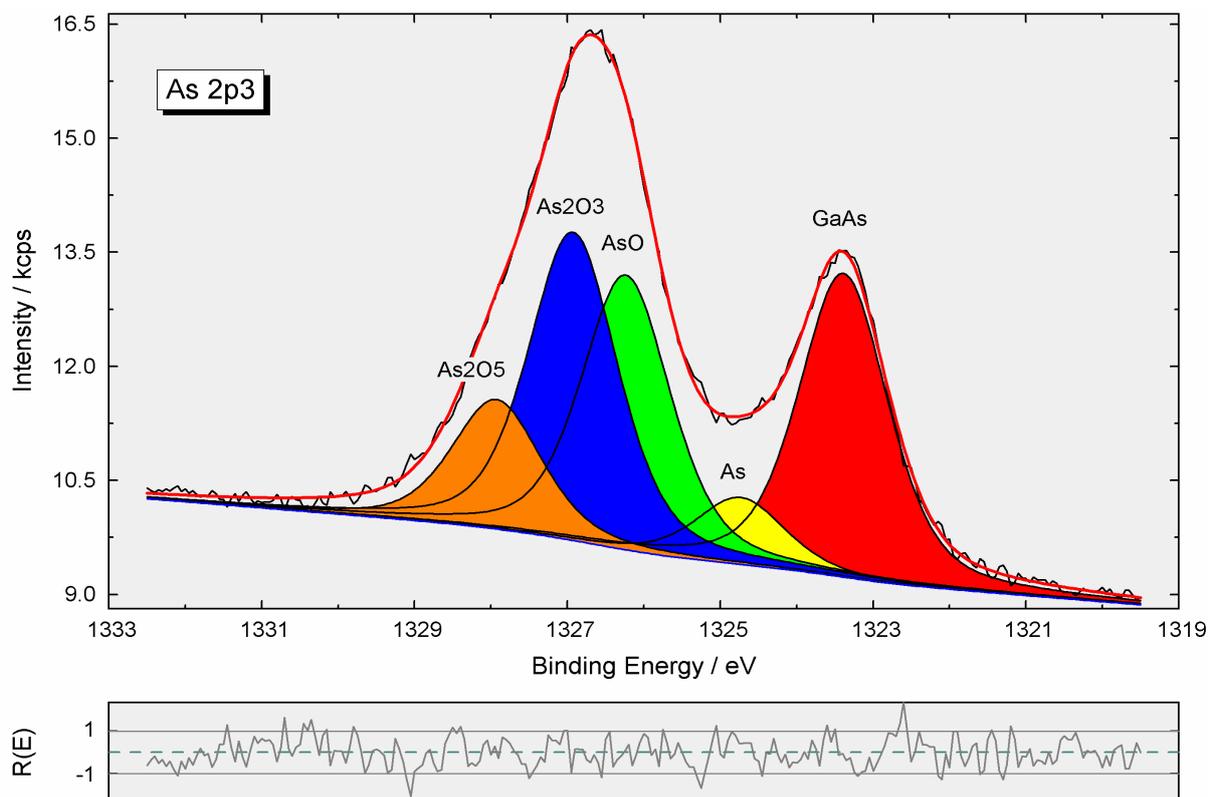
Fig. 1. Parameter plot (peak height) of an angle resolved measurement (\*\Unifit 2009\examples\projects(ufp)\Angle\_Resolved\_Measurement\_Si.ufp) of naturally oxidized Si; image created using UNIFIT 2009, exported and inserted into this Word document

iv) The colours of the areas inside and outside the coordinate system can be selected separately. Figure 2 shows a yellow fill colour inside the coordinate system and green colour outside.

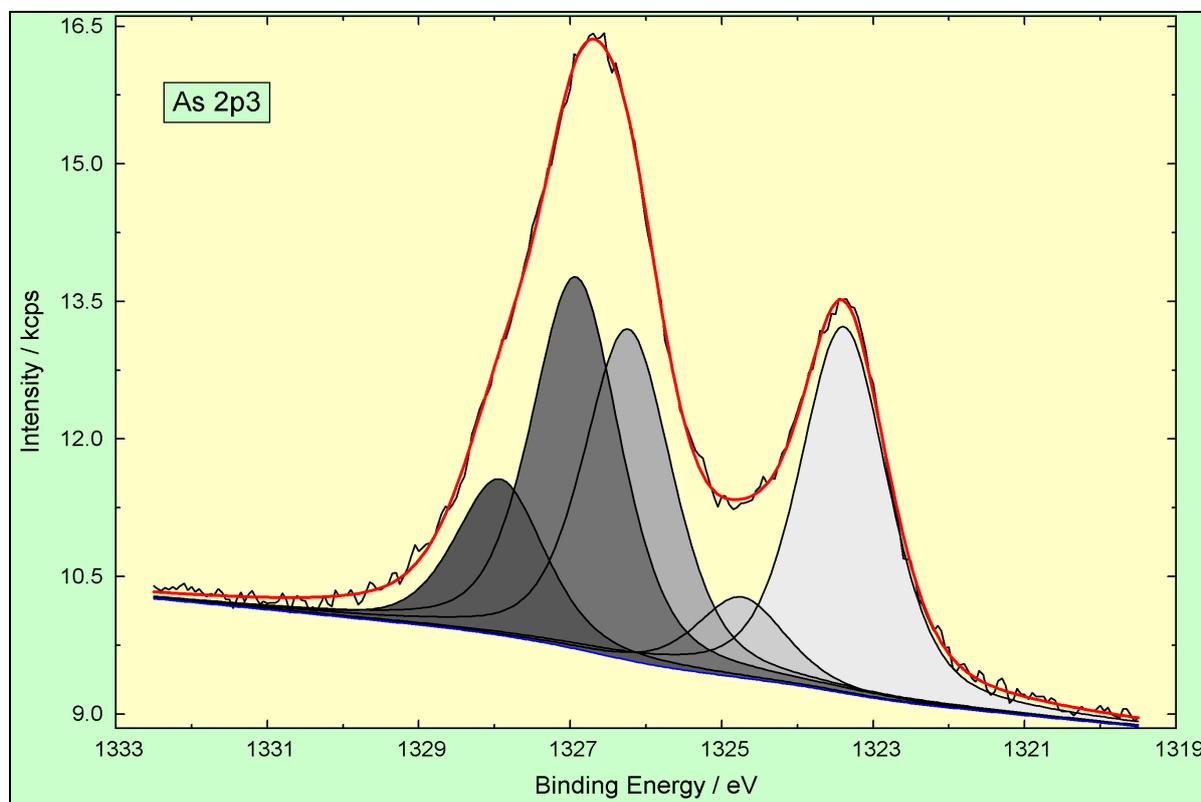
v) The new software offers the optional plotting of the residual function  $R(E)$  (Figures 2 and 3).

vi) Three different objects can be exported: 1. the activated window presentation, 2. the quantification table, 2. the fit-parameter table. Table 1 shows the fit-parameter table of the peak fit shown in Figures 2 and 3.

vii) In order to permit a very quick export of the presentable results from UNIFIT to other softwares (e. g. Word, Origin, ...) the 'Copy-Paste function' was integrated. With the call 'Copy Image' the currently activated window presentation can be exported to the clipboard and with the call 'Paste' inserted into a Word document.



**Fig. 2.** Plot of an As 2p<sub>3/2</sub> peak fitted with 5 components, component areas filled by different colours, red: GaAs, yellow: As, green: AsO, blue: As<sub>2</sub>O<sub>3</sub>, orange: As<sub>2</sub>O<sub>5</sub>, image was created using UNIFIT, exported and inserted in this Word document



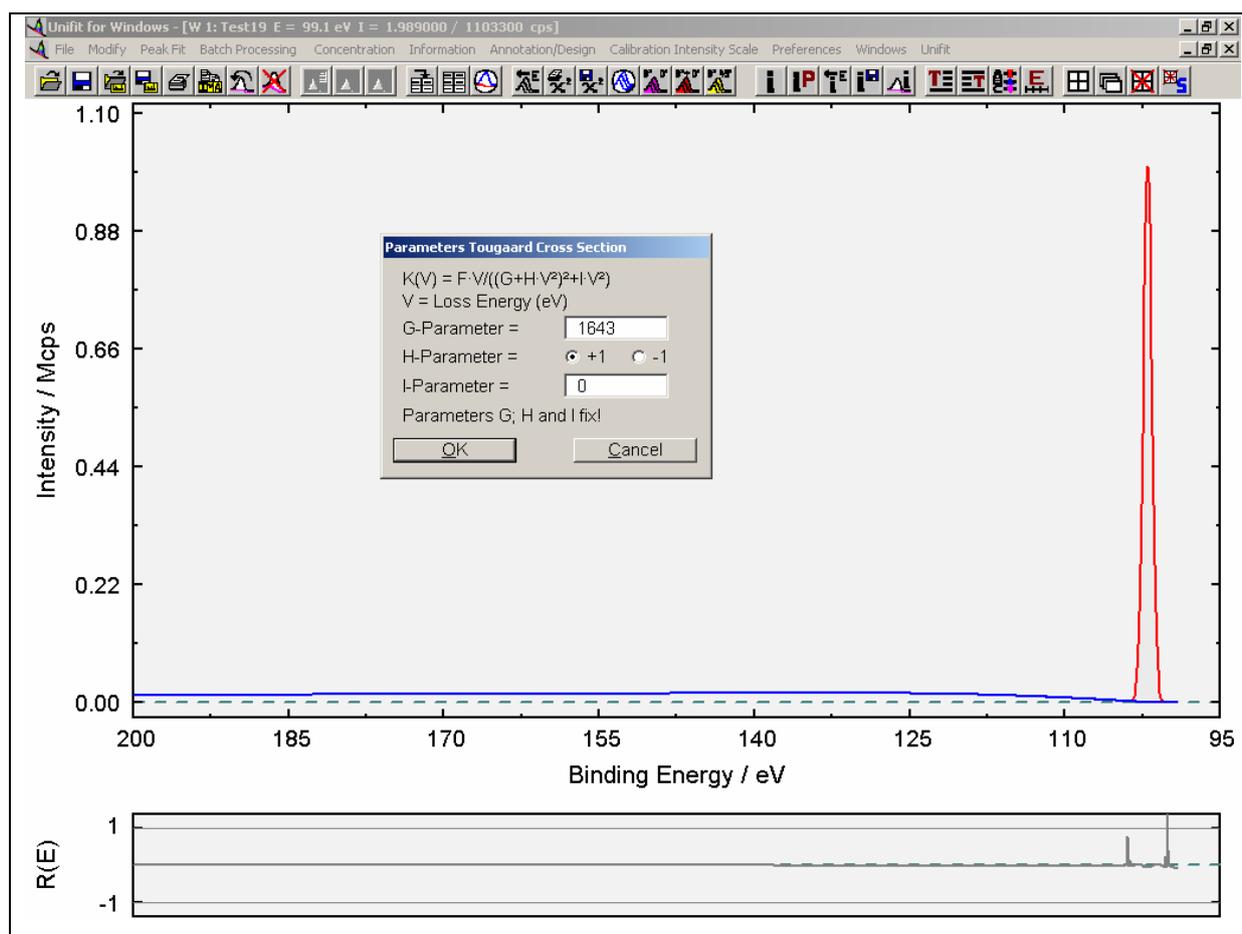
**Fig. 3.** Plot of a fitted GaAs peak (compare Fig. 2), the residual function  $R(E)$  is hidden, image was created using UNIFIT, exported and inserted in this Word document

**Tab. 1.** Fit-parameter table of the As 2p<sub>3/2</sub> peak shown in figure 2 and 3, table was exported from UNIFIT and inserted in this Word document

Peak name	Peak height/ cps	L-G mixing	Position/ eV	FWHM/ eV	Peak area/ cps·eV	rel. Peak area/ %
GaAs	3998,1	0,4354	1323,3889	1,37902	6876	28.04
As	882,6	0,4354	1324,7342	1,37902	1520	6.2
AsO	3612,9	0,4354	1326,2368	1,37902	6220	25.37
As2O3	4058,1	0,4354	1326,928	1,37902	6980	28.47
As2O5	1703,2	0,4354	1327,9294	1,37902	2923	11.92

viii) The usable export formats were increased offering the following formats: TIFF, BMP, WMF, AFI, VST, EMF, TGA, ICO, PPM, JPG, PGM, GIF, PBM, PNG, DCX, PCX, PCC, PDF.

ix) The resolution of the exported or copied images can be changed in four steps: monitor resolution, 400 dpi, 600 dpi, 800 dpi. The copy function with the highest resolution demands 2 GByte main memory or more.

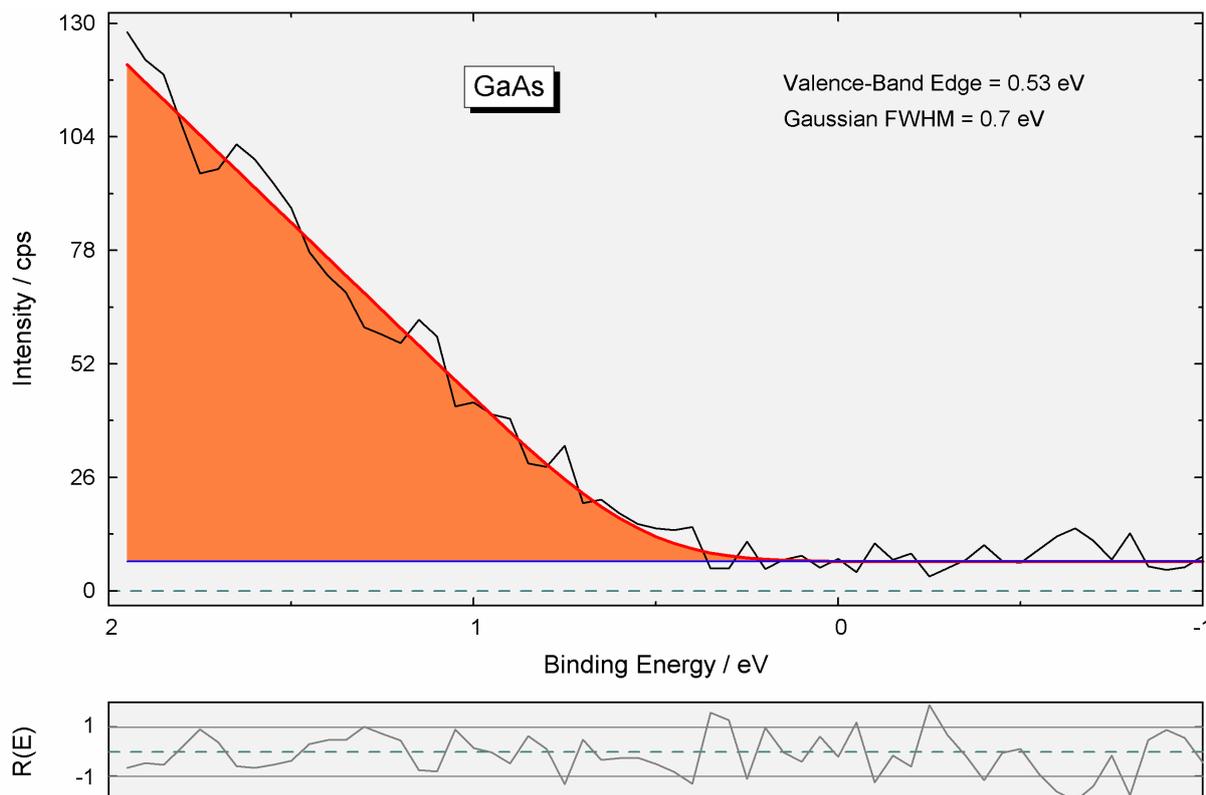


**Fig. 4.** Hot shot of the dialog 'Parameters Tougaard-Cross Section', the parameters V, G, and I are fixed, the F-parameter is fitted parallel to the peak fit

x) The using of the Tougaard-background function demands an appropriate adjustment of the so-called Universal cross section. The new introduced Four-parameter cross section

combines the Two-parameter cross section and the Three-parameter cross section (Figure 4). The correctness of the developed program code can be tested by using the new created test function 'Test19-Tougaard-Background.ufp'.

**xi)** A lot of users recommend a linear approximation of the valence-band edge. Additional to the model function calculated by the convolution of square root and Gaussian functions the convolution of linear and Gaussian functions for creating the model function was implemented (Figure 5).



**Fig. 5.** Estimation of the Valence-band edge of a GaAs sample, model function: convolution of linear and Gaussian functions, image created using UNIFIT, exported and inserted in this Word document

**xii)** In order to give the operator the informations about the processing steps the information call 'Information – Processing Steps' was implemented in the software.

**xiii)** A new 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-, -CH<sub>2</sub>-, -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) and therefore a easy way for a correct labelling of the chemical components with both the region name and the name of the chemical component (C1s -CH<sub>2</sub>-, C1s -CO-, ...).