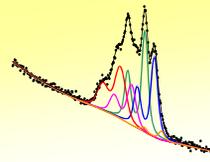




# UNIFIT 2018 – the Improved Spectrum Processing, Analysis and Presentation Software for XPS, AES, XAS and RAMAN Spectroscopy

R. Hesse, R. Denecke

Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, D-04103 Leipzig  
Website: www.uni-leipzig.de/~unifit Contact: rhesse@uni-leipzig.de



## Abstract

The improved software offers the data analysis of photoelectron spectra (XPS), Auger electron spectra (AES), X-ray absorption spectra (XAS) and RAMAN spectra. The peak fit of RAMAN spectra gives a considerably better analysis of the studied sample as compared to the traditional analysis of untreated data. In order to have more linking options for the fit parameters the fit procedures were improved. The selection of master peaks of the peak fit with relative fit parameters was extended. Now every peak-fit component can be defined as master peak. The parameters of slave peaks with succeeding component numbers can be linked to the parameters of the corresponding master peak. Two new 3D plot presentations 'XY 3D 45° Colour Profile' and 'XY 3D -45° Colour Profile' were implemented in the batch processing subroutines. The selectable processing results for the generation of XY-3D presentations were enhanced. Now, all fit parameters, the position of the maximum and minimum can be selected additionally. Three new options for the selection of standard windows were implemented: i) all windows with a defined X position, ii) all windows with a defined Y position, iii) all windows with a  $\chi^2$  greater than a defined  $\chi^2$  (after a peak fit to detect incomplete fit results).

## Example of an Analysis of RAMAN Spectra – Solar Silicon as a Case Study

1. The characterisation power of the Raman technique can be improved using the peak-fit analysis of Raman peaks.
2. During the loading procedure of the Raman spectra a transformation to equidistant step widths is made.
3. Eight different data formats are supported (e.g. \*.csv, \*.txt, \*.tvi).
4. A separate input routine allows the loading of RUFF-reference spectra.
5. UNIFIT offers a batch-processing procedure for the peak fit of a large number of Raman peaks of a multipoint measurement (micro-Raman). Figure 0 shows a typical peak fit of a Raman peak.
6. The processing time of the peak fit of 2601 Raman spectra takes less than 6 minutes.
7. The model function was a sum of Lorentzian and Gaussian peaks. The fit parameters of the spectral background were fitted parallel with the peak fit. The background model was a polynomial function of 3<sup>rd</sup> order.
8. All peak-fit parameters (peak height, FWHM, peak position, Gaussian-Lorentzian mixing ratio, asymmetry, peak area) can be displayed using different 3D presentations with respect to the x-y recording position.
9. The peak-fit analysis of a multipoint micro-Raman measurement of a solar silicon wafer gives information about (Ref. G. Sarau et al., book "Advanced Aspects of Spectroscopy", Chapter 8, open access):
  - a) Defect density using FWHM of the peak fit (Figs. 1 and 2, A1 and A2)
  - b) Internal stress using the position of the peak fit (Figs. 1 and 2, B1 and B2)
  - c) Doping information using the asymmetry of the peak fit (Figs. 1 and 2, C1 and C2)
  - d) Grain orientation using the intensity of the peak fit (Figs. 1 and 2, D1 and D2).

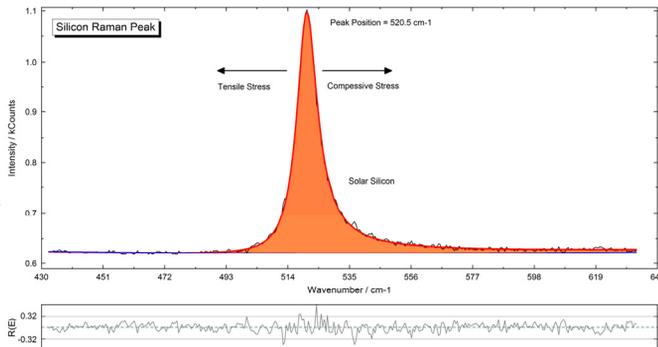
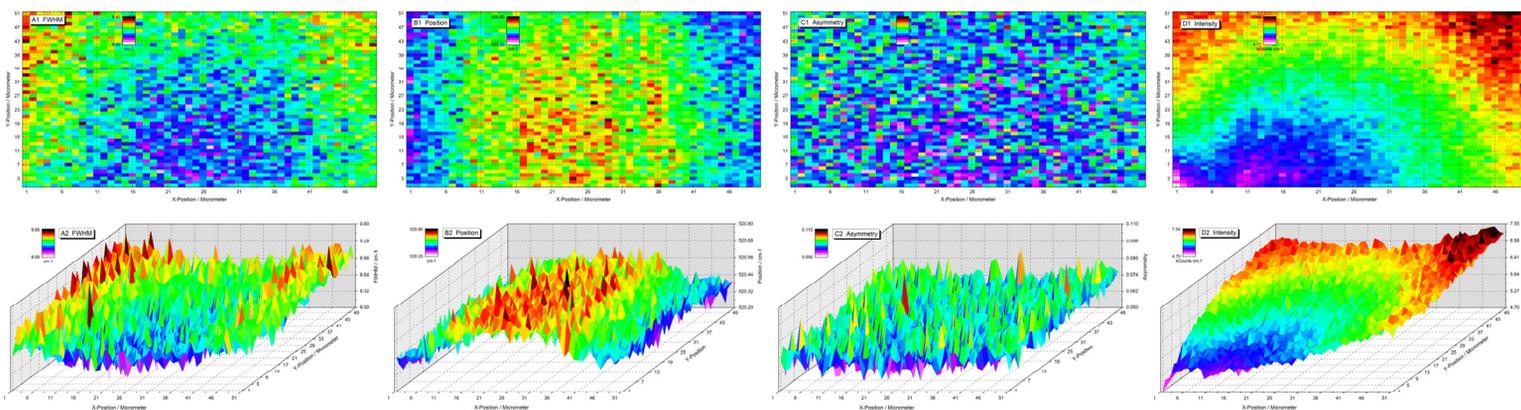


Fig. 0 Peak fit of the Silicon Raman peak, the peak asymmetry caused by doping, the reference peak position of the stress free silicon line is 520.0 cm-1



Figs. 1 and 2 Peak-fit results of a multipoint-RAMAN measurement of solar silicon, A1 and A2: FWHM – defect density map, B1 and B2: peak position (520,2 to 520,8 cm-1) - internal stress map, the gradient shows compressive stress, C1 and C2: asymmetry – doping map, D1 and D2: intensity – grain orientation map shows a strong gradient from X|Y = 1|1 to 50|50

## Improved Fit-Parameter Selection

In former versions of the UNIFIT software the definition of the master peak of the peak fit with relative fit parameters was fixed and settled to the first component. Now, every peak-fit component can be defined as master peak. The parameters of slave peaks with a higher component number can be linked to the parameters of the corresponding master peak. A colour code in the fit parameter table informs the operator of the component status:

1. RED: Master peak, activated for input,
2. GREEN: Master peak, not activated for input,
3. BLUE: Slave peak, activated for input,
4. WHITE: Slave peak, not activated for input (Fig. 3).

The XPS-background parameters for inhomogeneous samples and the XAS-background parameters may be defined in the same way.

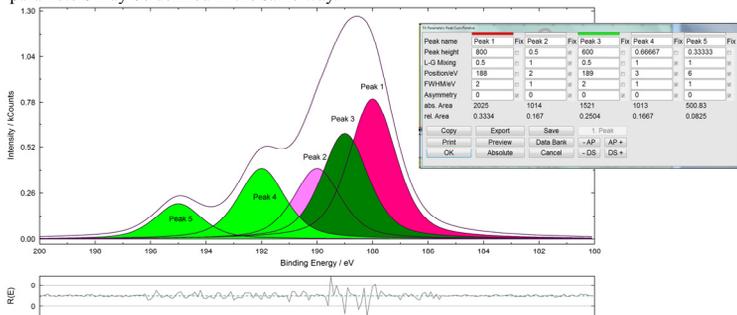


Fig. 3 Peak fit of a test spectrum with five components, right: Fit-parameter table of five single peaks of the test spectrum, fit conditions: sum of Gaussian and Lorentzian peaks, relative fit-parameters, peak 1 (dark red) and peak 3 (dark green) defined as master peaks, peak 1 activated for input, parameters of peak 2 are relative to the parameters of peak1, parameters of peak 4 and peak 5 are relative to the parameters of peak 3

## Additional Presentations to the Results of Figures D1 and D2

