# 3D Chemical State Plots of XPS Multipoint Measurements using UNIFIT 2015

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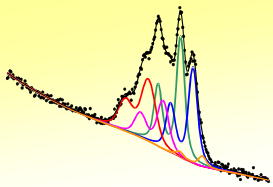


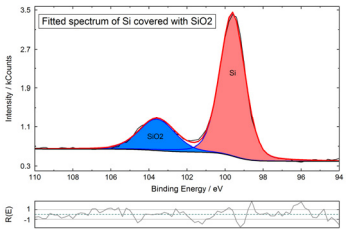
**Abstract:** Main focus of the advancement of the **UNIFIT 2015 software** was the implementation of new processing and presentation features for the treatment of a very large number of spectra of line scans and multipoint (area) scans. This requires the more efficient usage of the main memory by the software UNIFIT and an optimised presentation routine of the spectrum windows. As the result of the software optimisation the number of simultaneously processable spectra was increased from 1200 to 9000. The three new functions 'XY 3D Plot 45°', 'XY 3D Plot -45°' and 'XY 3D Colour Profile' allow the presentation of the element distribution or the plot of the distribution of the chemical components with respect to the x and y values of the recording position on the sample.

## NEW FEATURES

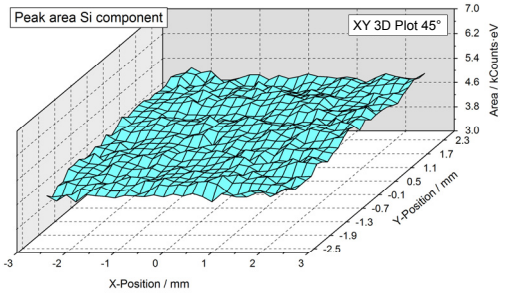
i) Realization of a more efficient usage of the main memory of the used computer system by UNIFIT.
ii) The maximum number of simultaneously processable spectra windows was increased to 9000.
iii) The selection of presentable curves including the 3D plots has been expanded. The spectrum, the modified spectrum and the background can be plotted. Additionally, after the peak fit the sum curve and the fit components (chemical states) may be displayed.
iv) The menu for editing the spectrum parameters has been completely refreshed. A special additional sub-menu ('Fill With' button) allows the easy manipulation of the values.
v) The quantification table was adjusted to the large number of spectra.
vi) The layout of the controls has the common Windows design.
vii) Now the software can use more than 3 GByte main memory (Large Address Flag).
viii) The acquisition parameters x and y of line or multipoint scans can be used as abscissa of the parameter plot.
ix) The direct activation of the spectra windows was changed and adjusted to the large spectra number.
x) The three new functions 'XY 3D Plot 45°', 'XY 3D Plot -45°' and 'XY 3D Colour Profile' allow the presentation of the distribution of the elements or chemical components with respect to the x-y position for the measurement of the sample. Five different display options are offered:
   1. Maximum of the intensity of the spectrum,
   2. Minimum of the intensity of the spectrum,
   3. Background-free area,
   4. Area of the sum curve after a peak fit,
   5. Area of the chemical component i (i = 1 to n, n - number of components during the peak fit).

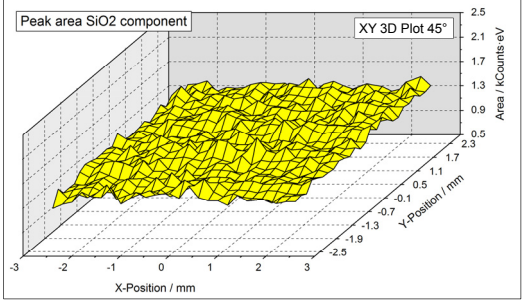
## EXAMPLE: SPUTTER CRATER CHARACTERIZATION

**Aim:** The position and size of the sputter crater of the spectrometer ESCALAB 220 iXL shall be estimated.
**Measurements:** Two multipoint (area) scans of the untreated and sputtered sample (26x26 recording points) and a line scan over the sample edge were carried out. Note, during the measurement of the sputtered sample the X-ray source switched off.
**Spectrometer setting:** x-y step width of the manipulator: 0.2 mm, analysis area: 0.16 mm (see measurement 2)
**Data processing:** Peak fit of the Si components. Presentation of the fit results using the 'XY 3D Plots' and 'Parameter Plots'.
**Results:** 1. The sputter crater is shifted about 1.5 mm in both directions with respect to the normal recording position x = 0 and y = 0.
2. Because the sputter crater was not complete recorded, the size could not correctly estimated. The size is about 2x2 mm².
3. The zero intensities from the positions y = 1.5 mm to y = 2.5 mm represent the measurements without X-ray excitation.

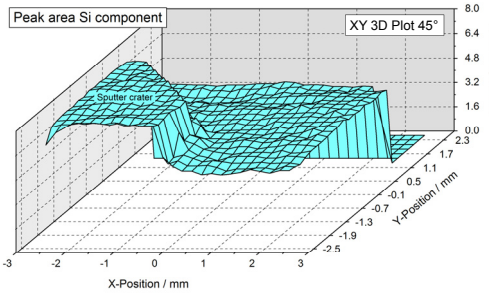


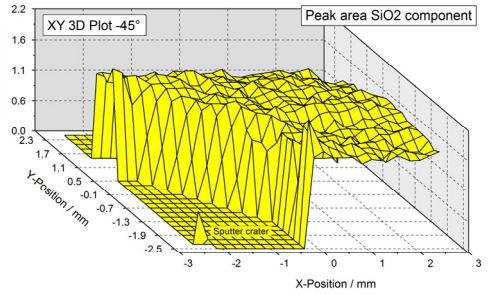

### Measurement 1: Before sputtering

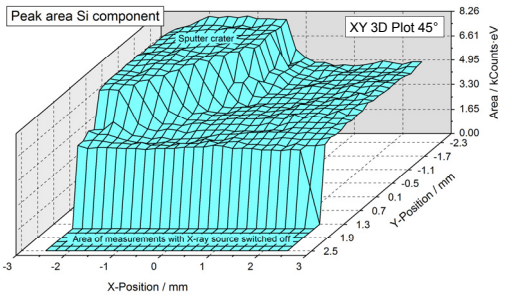


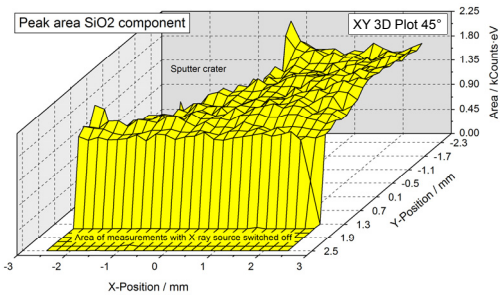




### Measurement 3: After sputtering

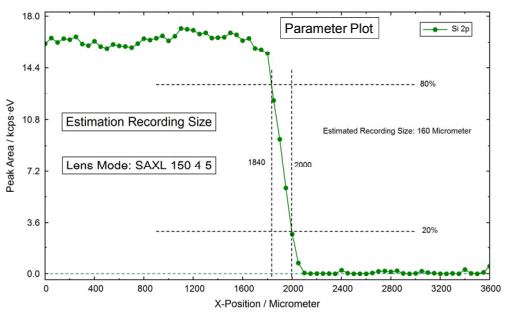


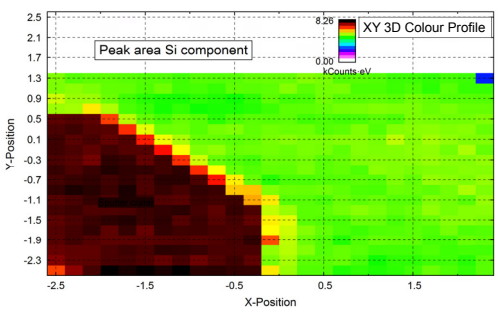



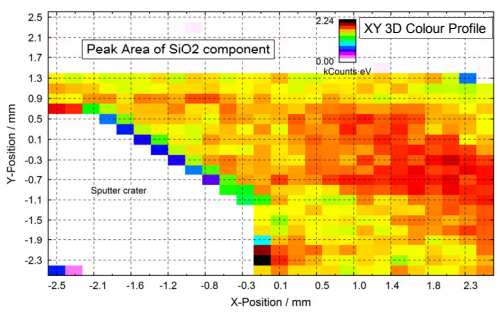




### Measurement 2: Line Scan

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