What is new in UNIFIT 2019?

The aim of the improvement of the UNIFIT software is the expansion of the support for the users to optimize the processing, analysis and presentation of a large number of spectra. The automatically loading of a set of data files including spectra of standard measurements (e.g. survey and 5 narrow spectra), the optimized quantification with a new optional 100% normalization tool as well as the saving of all design and processing steps of the selected spectra of the standard measurement improves the efficiency of the data analysis. Additionally, an automatic spike correction of all loaded spectra was implemented. Special new design options were developed and integrated into the software UNIFIT 2019.

i) A batch loading of files with measurement data was implemented. The special file names must be a combination of the same basic name and a batch parameter. The bath parameter is a number with maximal five digits (Test_00001.txt, Test_00002.txt, Test_00003.txt,,,). The following data formats for single-region and multi-region measurements are supported:

a) XPS: PHI spe-format *.spe

b) RAMAN: Wave Number increasing (*.csv, *.txt, *.dat)

c) RAMAN: Wave Number decreasing (*.csv, *.txt, *.dat)

d) XPS: VAMAS vms-format (*.vms)

e) XPS: Scienta txt-format (Sum of Slices) (*.txt).

The names of the loaded regions are a combination of the original region names (e.g. S 2p, C 1s) and the batch names of the files (e.g. S 2p_00001, C 1s_00001 from the file Test_00001.txt, S 2p_00002, C 1s_00002 from Test_00002.txt...).

ii) Typically in the UNIFIT software is that all peaks in the quantification table are used for the calculation of the at-% values. The sum of all selected peaks has to be 100%. Now, an additional option can calculate the at-% values related to the peaks with the same batch parameter. That is a very important feature in case of the loading of more than one standard measurement (see chapter i and Fig. 1).

iii) The resolution of the XY-3D Plots can be improved. The number of the data points in the X and Y direction can be stepwise increased with two. The intensities of the additional points are calculated using linear interpolation (see Fig. 2).

iv) The annotation function has a new option. Now, the denoted annotation can be used for the active window, for all windows or for selected windows.

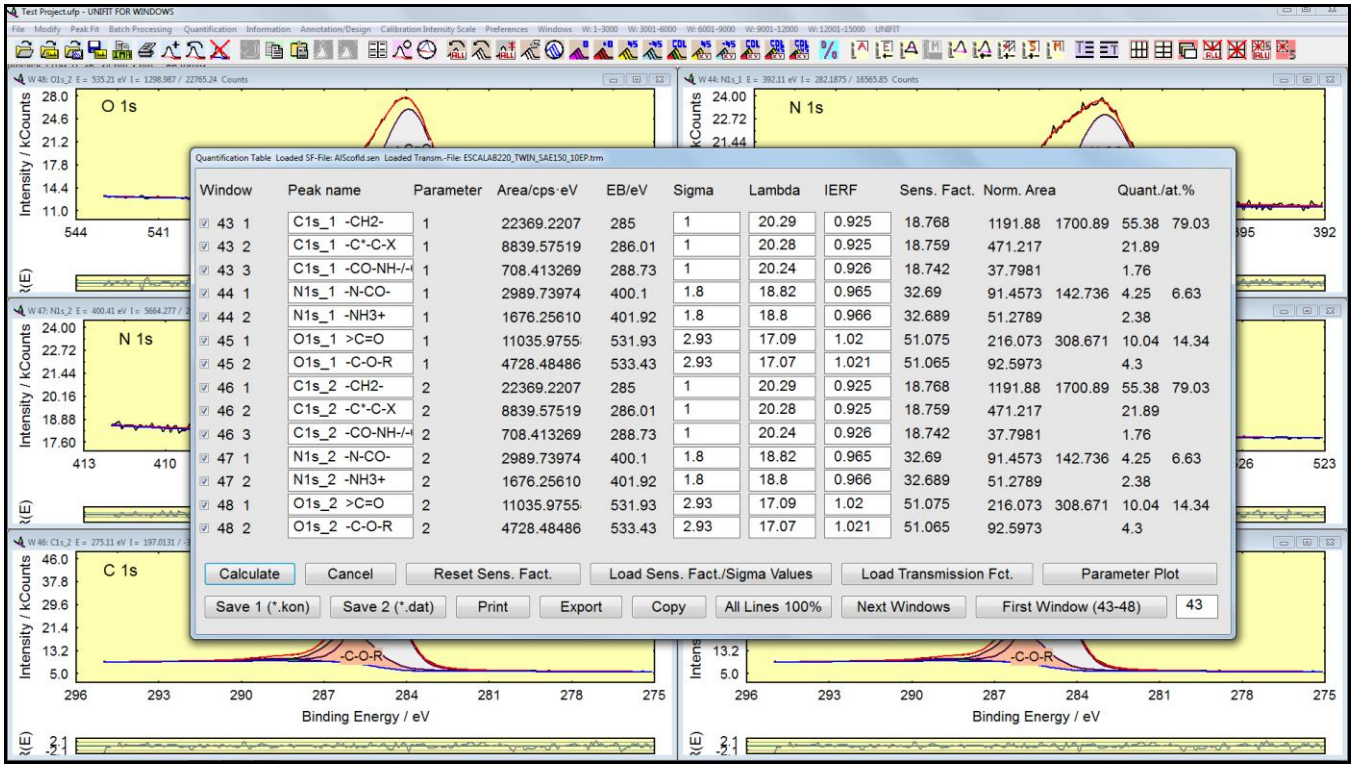

Fig. 1 Screen shot of the quantification table: with the button 'All lines 100%' or 'Par. Lines 100%' the calculation of the at-% values (column: Quant./at.%) takes all lines or the lines with the same batch parameter, the figure illustrates the 100% normalization of the windows 43, 44 and 45 (parameter = 1) and 46, 47 and 48 (parameter = 2)

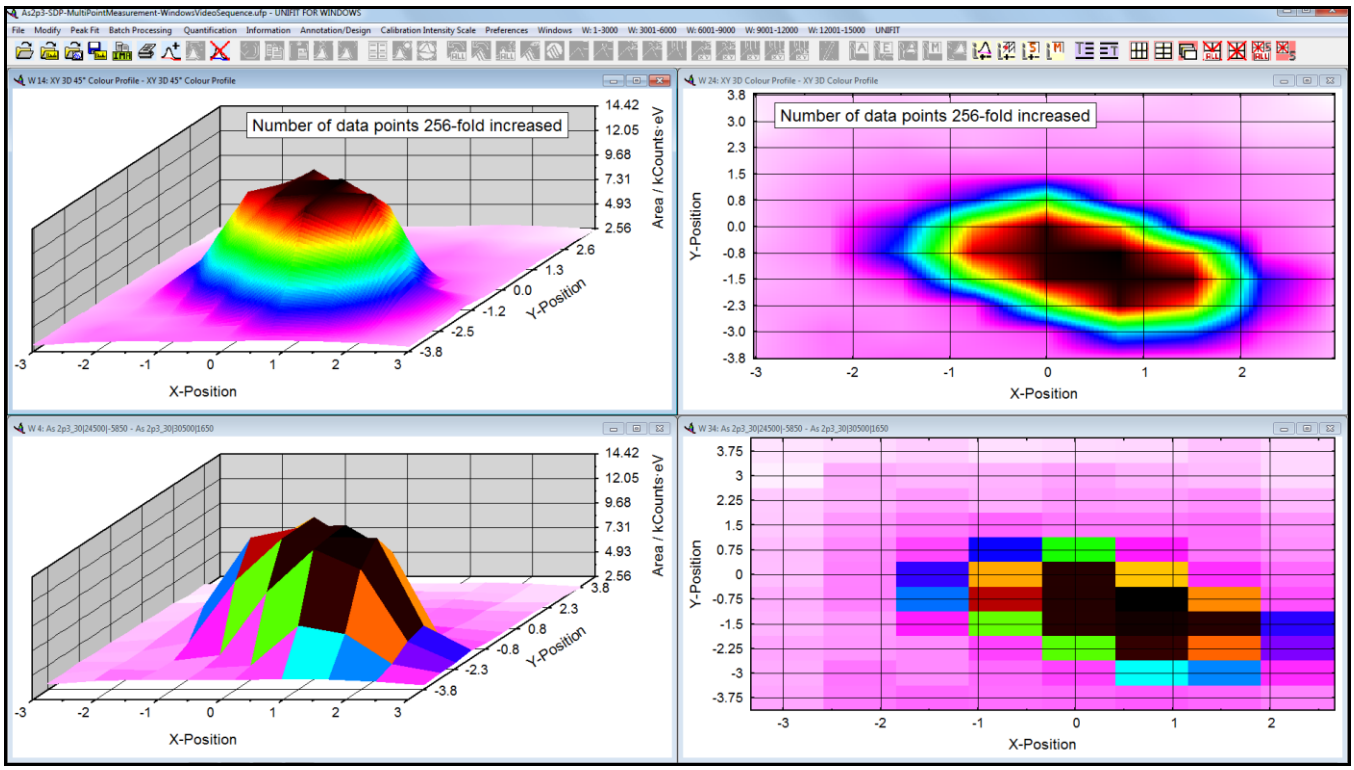

Fig. 2 Screen shot of four 'XY 3D Colour Profiles': bottom left: 'XY 3D 45° 3D Colour Profile' without modification, top left: 'XY 3D 45° Colour Profile' after 256-fold increasing of data points, bottom right: 'XY 3D Colour Profile' without modification, top right: 'XY 3D Colour Profile' after 256-fold increasing of data points

vi) Now, the measurement data-file names have also the correct name of the files after a batch-file loading. A separate new measurement-file names field was implemented into the software. In former versions all spectral regions had the same measurement-file name of the first loaded file.

vii) A important new feature is the saving of all processing steps and design features of before selected regions. The extension is *.ppd. After loading of a *.ppd file a selection box is opened and the regions for the operating with the saved design features and processing steps can be defined. Only regions that have the same name (without the batch parameter, e.g. _01) as the saved processing step block can be used. Formatted titles and labels, interpolation operations and charge corrections are not saved. Tab. 1 illustrates a possible example.

Tab. 1. Left hand side: Two multi-region measurements with four regions, loaded using batch-file input, right hand side: example for saved processing steps

Loaded regions	Saved Processing Steps
1. Survey_01	Survey:
2. C1s_01	- Annotation
3. O 1s_01	O1s:
4. S2p_01	- Reduction
5. Survey_02	- Satellite Subtraction
6. C1s_02	- Fittable Background
7. O1s_02	- Peak Fit, Sum, Relative
8. S2p_02	C1s:
	- Reduction
	- Satellite Subtraction
	- Fittable Background
	- Peak Fit, Sum, Relative
	S2p;
	- Background Subtraction

viii) An additional manual setting of the plot of the curves was implemented (see Fig. 3). For points, crosses, circles, squares, rectangles the following definitions are possible:

1. Automatic selection,
2. all channels
3. every 2nd, 3rd or 4th channel.

ix) **Now, t**he manual hidden windows saved in an Unifit project *.ufp will be not shown after reloading of the Unifit project. Former versions have neglected this special windows hidden feature.

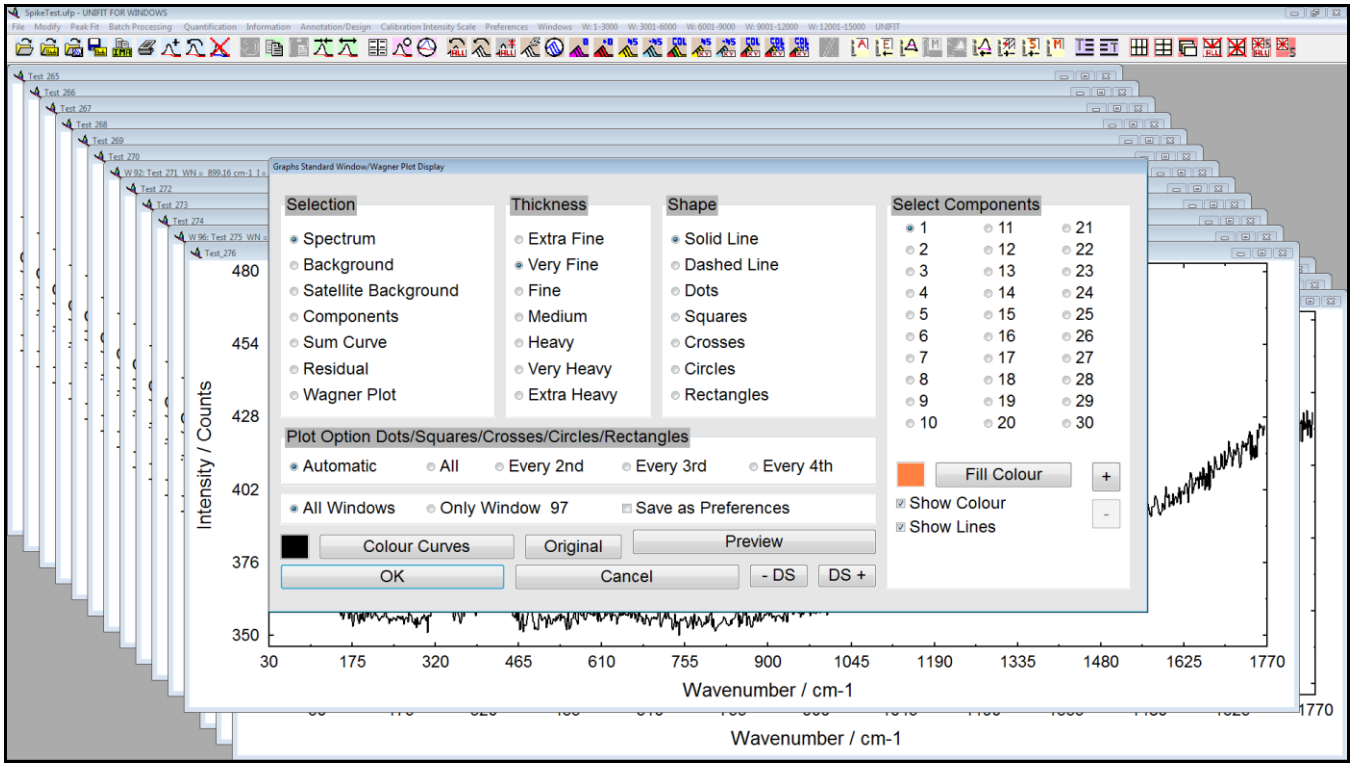

Fig. 3. Screen shot of the dialogue for the definition of the graphs of standard windows, the option 'Plot Option Dots/Squares/Crosses/Circles/Rectangles' is new

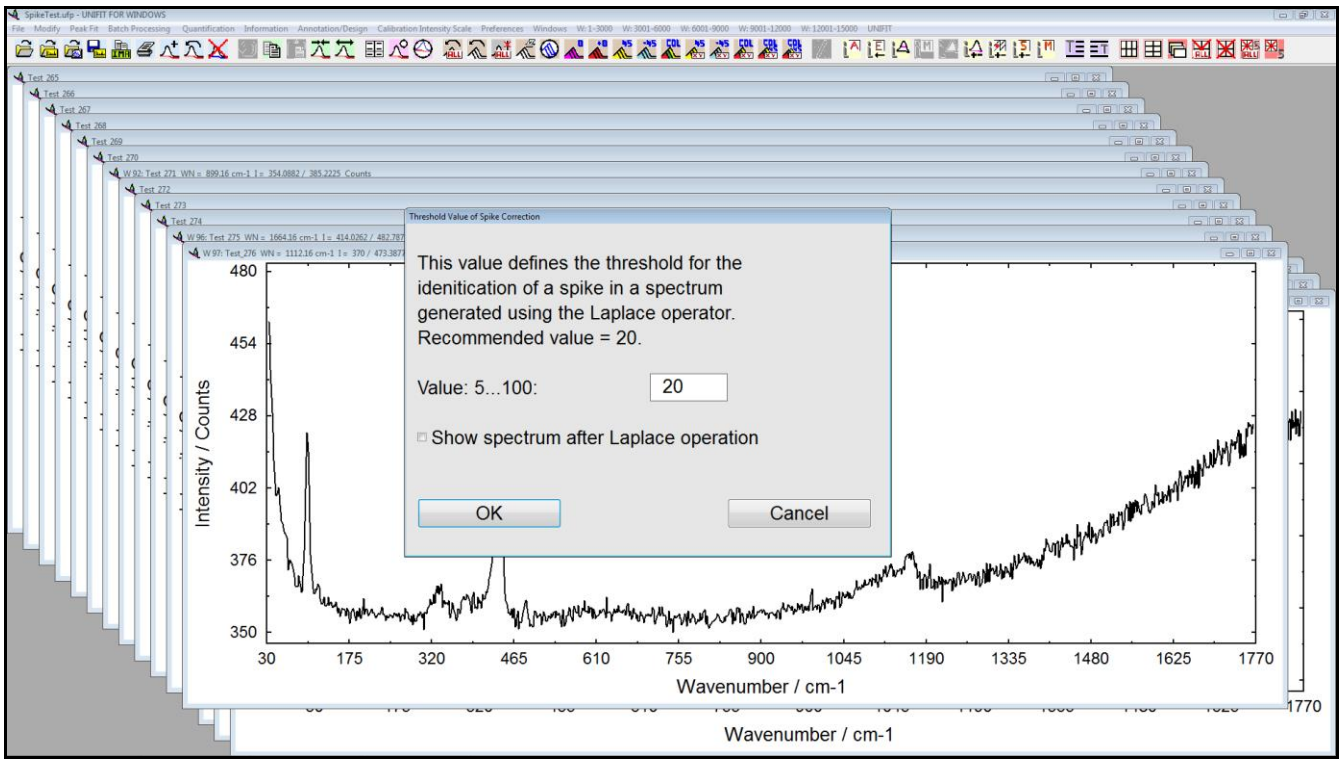

Fig. 4. Screen shot: Setting for the threshold for the identification of the spikes, option: show the spectra after Laplace operation

x) A very important feature for the processing of Raman spectra is the spike correction. In case of a micro Raman measurement (multipoint map) a well working automatically routine is necessary. The basic of the new developed automatically spike correction is a modified Laplace method. The

threshold for the identification of the spikes has to be defined manually. Optionally, the spectra modified using the discrete Laplace Operator can be displayed (see Fig. 4). Because the procedure works with neighbouring channels and spectra, only all loaded spectra can be used together.

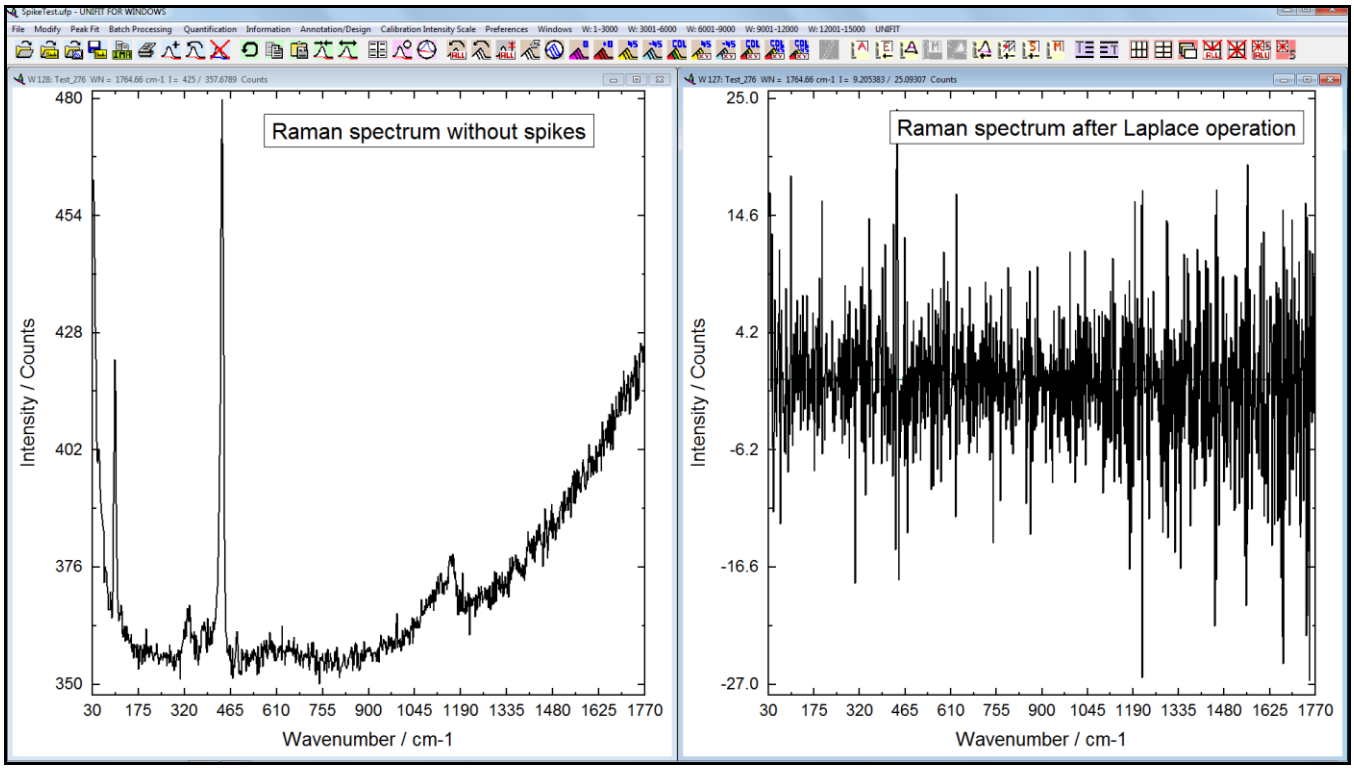

Fig. 5. Screen shot: Left: Raman spectrum without spikes, right: corresponding Raman spectrum after the improved Laplace operation

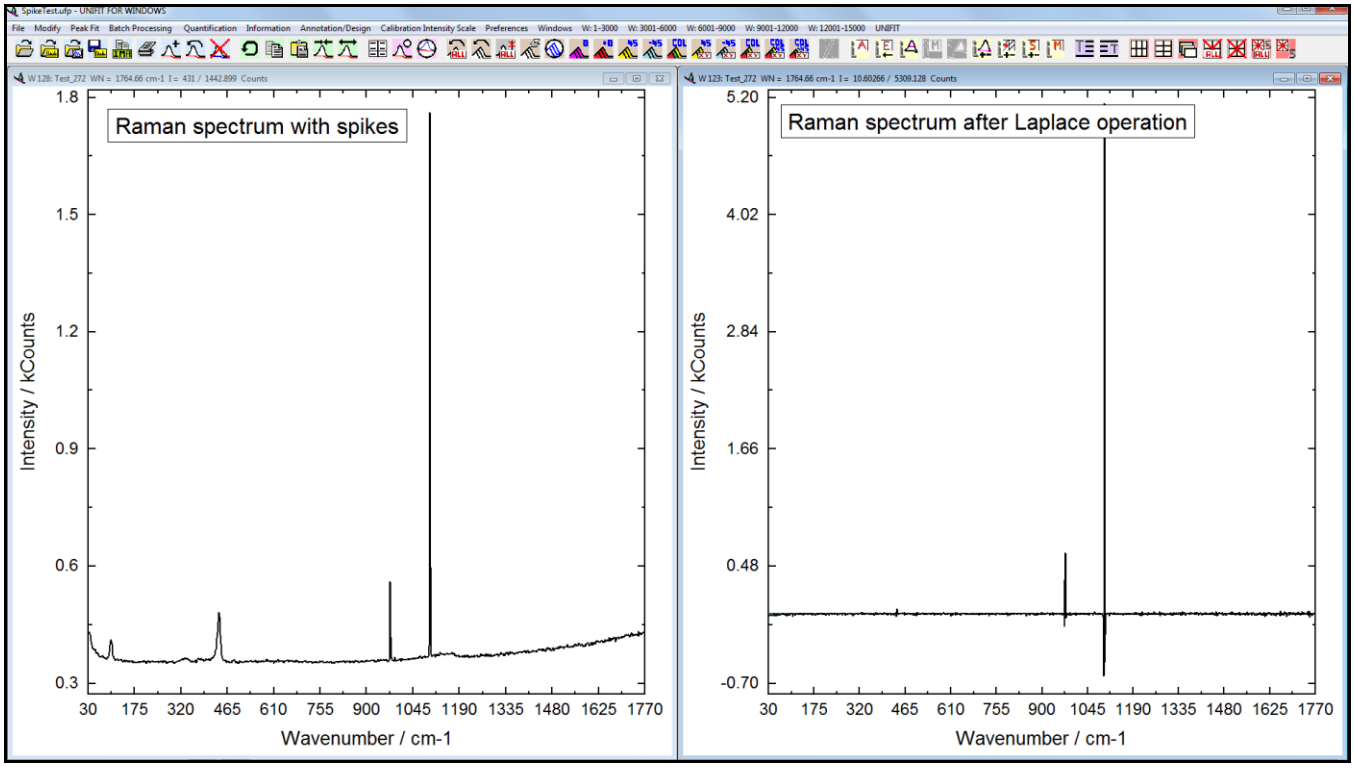

Fig. 6. Screen shot: Left: Raman spectrum with spikes, right: corresponding Raman spectrum after the improved Laplace operation, the sharp positive peaks show the position of the spikes

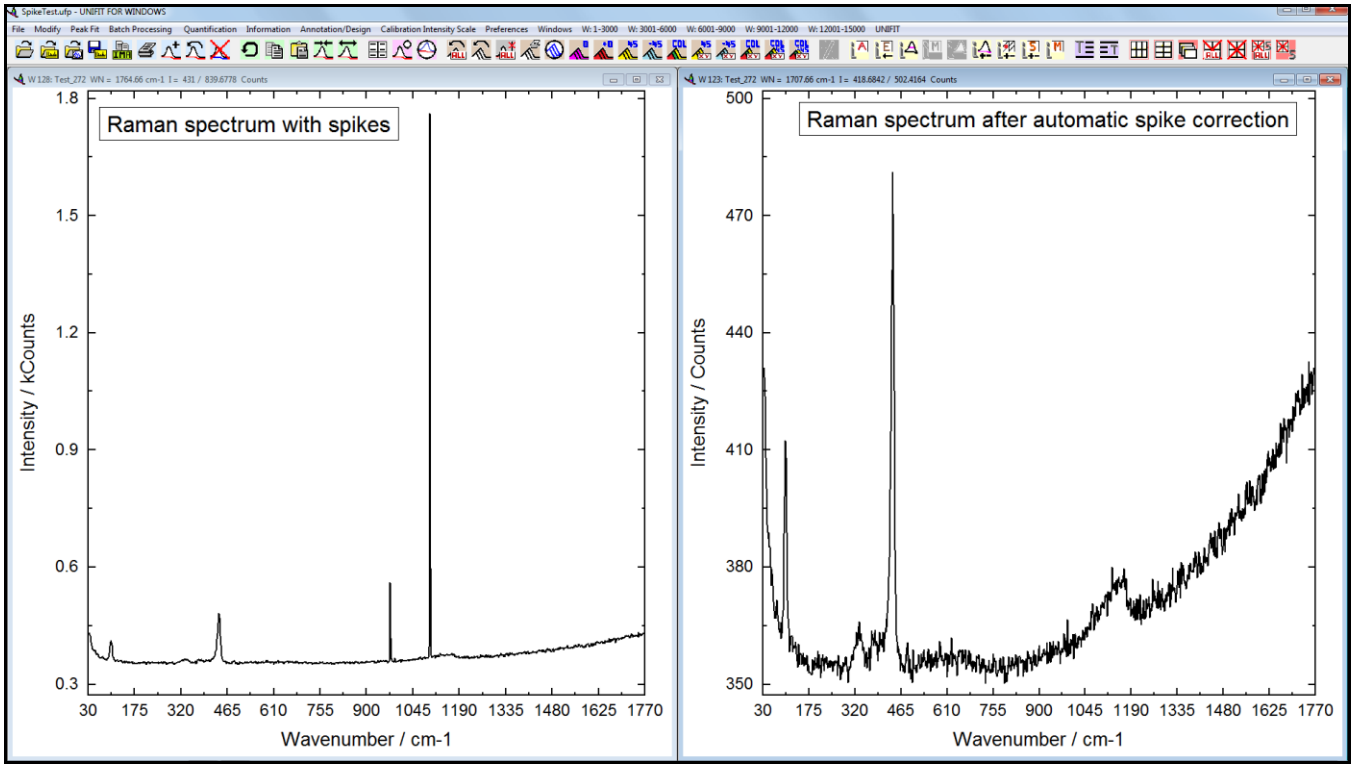

Fig. 7. Screen shot: Left: Raman spectrum with spikes (se also Fig. 6), right: Raman spectrum after the automatic spike correction