UNIFIT 2019 – the Improved Spectrum Processing, Analysis and Presentation Software for XPS, AES, XAS and RAMAN Spectroscopy

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Abstract

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 automatic 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. Now, the batch-file loading is available for a lot of different data-file types.

Automatic Spike Correction

- A very important feature for the processing of a large number of spectra is the automatic spike correction (e.g. for Micro-RAMAN Spectroscopy).
- The basic of the new developed spike correction is a modified Laplace method (see Fig. 1, [1]).
- The threshold *T* for the identification of the spikes has to be defined manually.
- Optionally, the spectra modified using the discrete Laplace Operator *L(i,j)* can be displayed.
- The maxima *Lmax(i,j)* > *T* define the spikes. *L* is defined by

$$L(i,j) = 4 \cdot M(i,j) - M(i-1,j) - M(i+1,j) - M(i,j-1) - M(i,j+1)$$

with *M* = intensity, *i* = number of the measuring point (channel), *j* = number of the spectrum.

- All boundary issues (first or last point of the spectrum, first or last spectrum of the series) are considered, resulting in a modified Laplace operator (see Fig. 2, Case b … Case i).
- The automatic spike correction has to be carried out using all loaded spectra.
- The corrected intensity *M'* of spikes is calculated by (Case a):

$$M'(i,j) = (M(i-1,j) + M(i-1,j-1) + M(i-1,j+1) + M(i,j-1) + M(i,j+1))/5$$

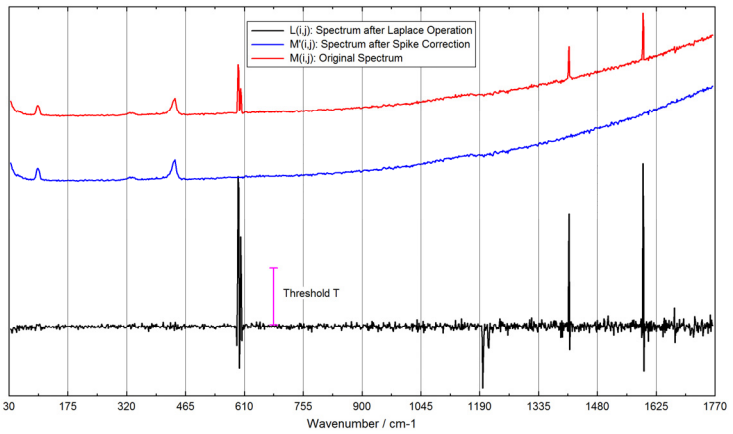

Fig. 1 Illustration of the spike correction using the modified Laplace method, **red:** original spectrum with spikes, **black:** spectrum after the Laplace operation, **blue:** spectrum after spike correction

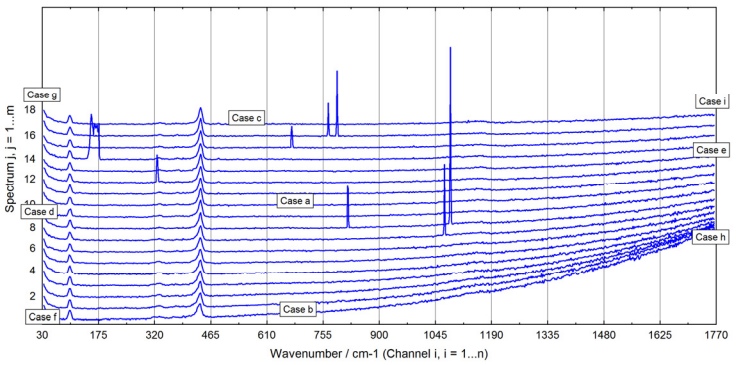

Fig. 2 Illustration of the special issues of the calculation with the Laplace operator, case a: normal case, case b to case i: modified Laplace operator is used

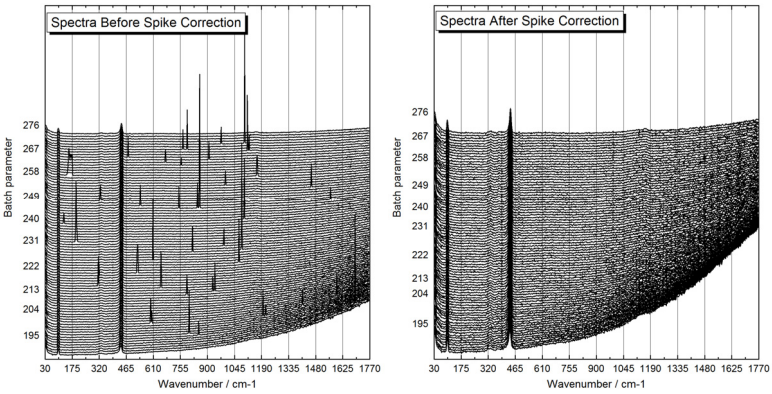

Fig. 3 Left: Original RAMAN spectra of a parameter-depended measurement (with spikes), right: spectra after automatically spike correction.

Improved Presentation of XY-3D Plots

- The number of plotted points of theXY-3D plots can be stepwise increased.
- The X-axis and Y-axis can be changed separately.
- In all cases the factor of the increasing of points is two.
- The intensities of the additional points are calculated using a linear interpolation.
- Fig. 4 illustrates a sputter crater of GaAs, recording area: 9x11 points.

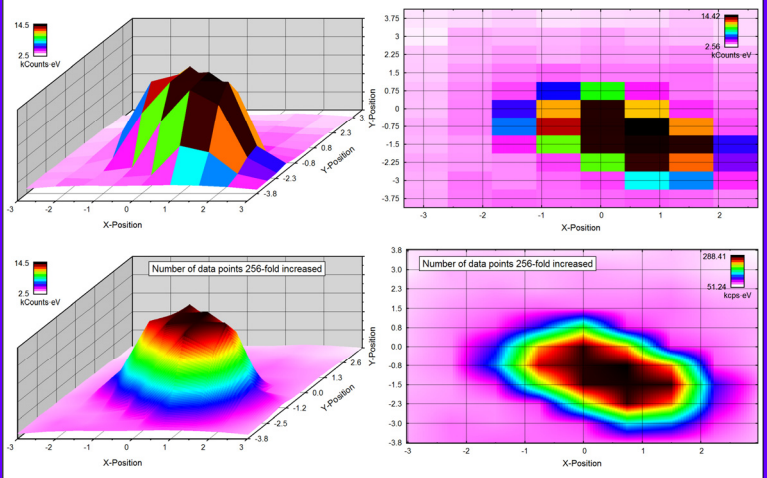

Fig. 4 XY-3D presentations of the sputter crater of GaAs. Illustrated signal: Peak area of the peak-fit component of the oxides of As 2p3 signal, **top:** 9x11 points, **bottom:** 144x176 points.

Saving, Loading and Applying of Processing Steps and Design Features

- **Idea:** All processing steps and design features of the analysis of a multi-region measurement may be saved in one file (*.ppd). The saved processing and design steps can be reloaded and applied for other multi-region measurement of similar samples with the same region names.
- **Requirements:** The master template of processing steps and design features of the displayed and selected regions with different names can be saved (e.g. multi-region measurement of GaAs: Survey, O 1s, C 1s, As 2p3, Ga 2p3, As 3d, Ga 3d).
- **Benefits:** The processing, analysis and design time can be reduced clearly.
- **Batch-File Loading:** Files with the same name and a batch parameter (e.g. Test_01.vms, Test_02.vms) are loaded together. The regions are marked with the file-batch parameter.
- **Not saved:** Charge corrections, interpolation procedures, formatted annotations.
- **Left:** Loaded regions of two files **Right:** Saved, reloaded and applied processing steps

Loaded Regions

1. Survey_01
2. C1s_01
3. O1s_01
4. S2p_01
5. Survey_02
6. C1s_02
7. O1s_02
8. S2p_02

Saved Processing Steps

Survey:
- Annotation

O1s:
- Reduction
- Satellite Subtraction
- Fittable Background
- Peak Fit, Sum, Relative

C1s:
- Reduction
- Satellite Subtraction
- Fittable Background
- Peak Fit, Sum, Relative

S2p;
- Background Subtraction

Lit: [1] Chemometrics and Intelligent Laboratory Systems, 155, (2016) 1-6

Printed by URZ (University Leipzig)