



APPLICATION NOTE SW-702

Baseline subtraction: easy correction of Raman spectra using DropView SPELEC. Part 2

As Raman spectroscopy and Raman spectroelectrochemistry are used to study a huge variety of systems, the spectra are also very assorted and show different vibrational bands and background signals. This Application Note explains different procedures to obtain the best adjustment of the baseline to each spectrum. In that way, background subtraction allows to obtain spectra accurately corrected.

INTRODUCTION

Raman spectroscopy and its combination with electrochemistry, known as Raman spectroelectrochemistry, are powerful techniques used in a huge number of different applications, such as characterization of materials, sensing, corrosion studies, electrocatalysis, life science, geology, memory and storage devices, etc. due to outstanding results are obtained.

This Application Note shows the important effect that the baseline correction has on Raman spectra and it demonstrates how the selection of an adequate baseline could avoid misinterpretations of the obtained results.

INSTRUMENTATION AND SOFTWARE

Raman spectra are recorded with SPELEC RAMAN and DropView SPELEC software. DropView SPELEC is a dedicated software that acquires simultaneously and in real-time spectroelectrochemical information as well as includes specific tools for data treatment and analysis. In this Application Note, the "Auto baseline" subtraction will be explained in detail.

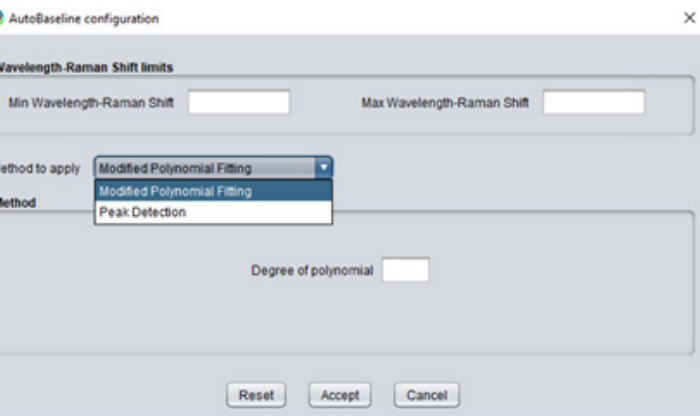


Figure 1. "Auto baseline" configuration.

RESULTS

"Auto baseline" configuration

Correction of Raman spectra requires different baseline adjustments depending the background signal and sometimes "Auto baseline" default configuration is not suitable. For that reason, configuration of "Auto baseline" can be changed in DropView SPELEC following the route: Menu bar > Curves > Baseline > Config auto baseline. The next menu (Figure 1) is observed:

"Auto baseline" configuration allows us to:

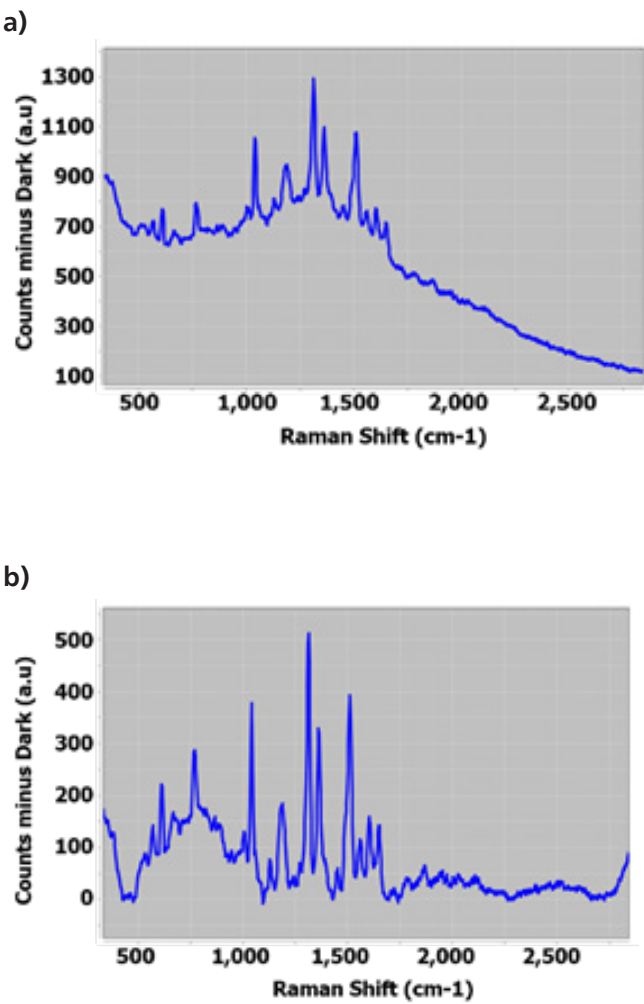
- Define the limits of the spectral region, min and max wavelength-Raman Shift, where baseline correction will be applied.
- Select the correction method: modified polynomial fitting or peak detection. As it will be explained in the next examples, each method has specific parameters to generate the baseline.

In the following examples, several Raman spectra will be

"Wavelength-Raman Shift limits"

Figure 2a shows a raised Raman spectrum because the background signal is high for all Raman Shift. Using the default "Auto baseline", Raman spectrum displayed in Figure 2b is obtained. Although this tool provides a well-corrected spectrum from 1100 cm-1 to longer Raman Shift, the rest of Raman Shift (up to 1100 cm-1) is not completely flat.

However, as was previously explained, DropView SPELEC enables to change the configuration of "Auto baseline" parameters. Taking into account that in this example Raman bands are only located from 500 to 1700 cm-1, only changing the region where the correction will be applied (Figure 2c) is more than enough to obtain a completely flat spectrum in the interest region (Figure 2d).



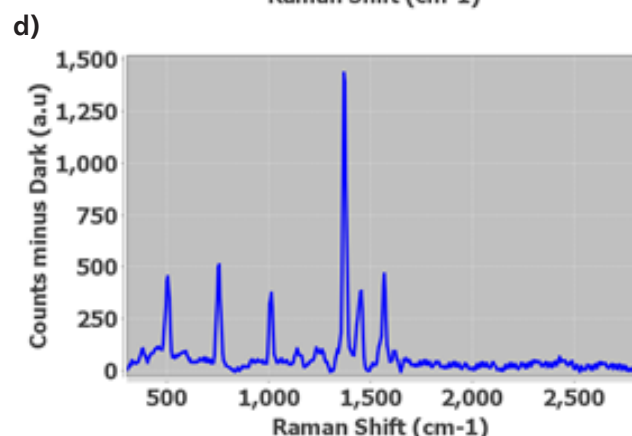
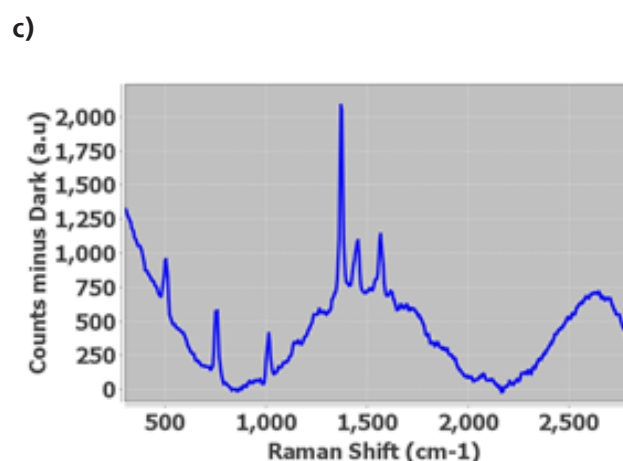
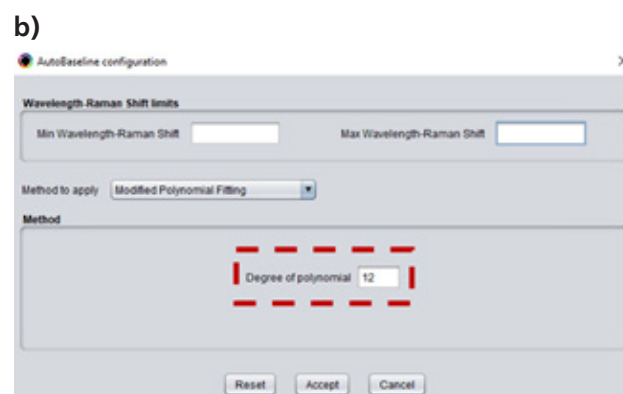
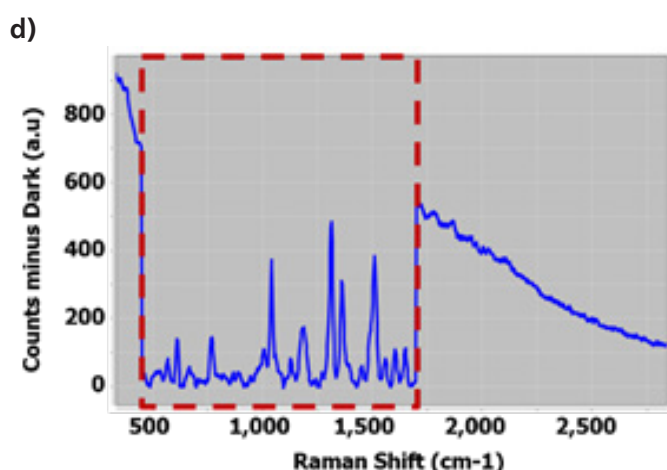
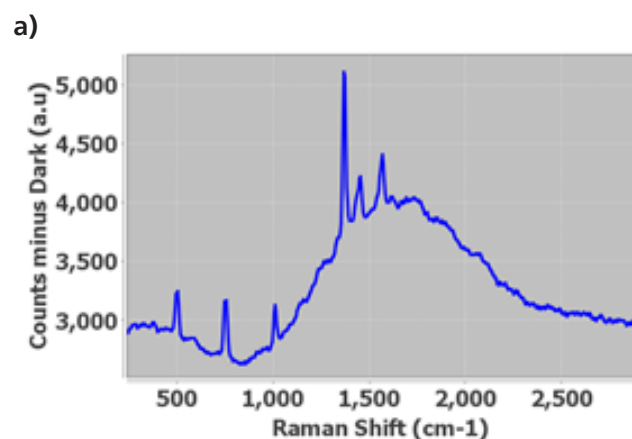
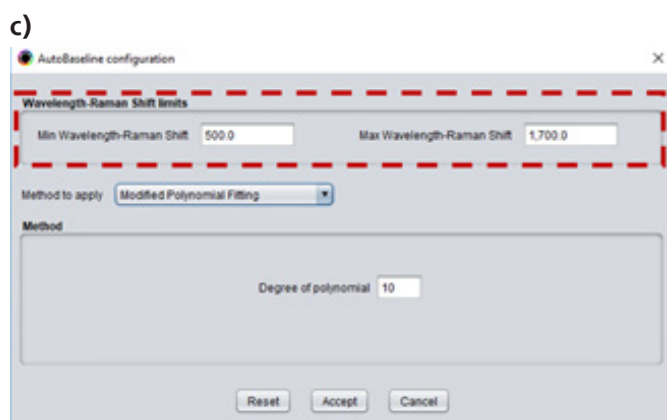


Figure 2. (a) Raw Raman spectrum and (b) whole Raman spectrum corrected with default "Auto baseline". (c) "Auto baseline" configuration menu and Raman spectrum corrected with baseline subtraction between 500 and 1700 cm⁻¹. Red dash line indicates the specific region corrected.

"Modified Polynomial Fitting"

Depending on the background signal, the degree of polynomial used to generate the baseline plays a key role. Figure 3a shows a Raman spectrum recorded with DropView SPELEC with background signal. As can be seen in Figure 3b, configuration of "Auto baseline" can be easily changed and allows us to modify the default parameters, as in this case the degree of polynomial.

Figure 3c and 3d show the Raman spectrum corrected using different degrees, 5 and 12, respectively. Figure 3c demonstrates that the spectra corrected with polynomial of degree 5 does not provide a good adjustment of the baseline and the spectrum is not well-corrected. However, Figure 3d shows that baseline configuration using a polynomial of degree 12 provides a close fitting correction and the background contribution of the Raman spectrum is removed.

Figure 3. (a) Raw Raman spectrum. (b) "Auto baseline" configuration menu. Red dash line indicates the degree of polynomial selected. (c) Raman spectrum corrected with polynomial fitting, degree 5. (d) Raman spectrum corrected with polynomial fitting, degree 12.

“Peak Detection”

An additional option available is the selection of other method to correct the optical signal. In the next example, “Peak Detection” instead of “Modified Polynomial Fitting” is used for the simultaneous peak detection and the baseline correction. Figure 4a shows the Raman spectrum obtained with a fluorescent sample.

Two parameters must be defined in this method, smallest and largest window size for peaks width and smallest and largest window size for minimums and medians in peak removed spectra. After optimizing these two parameters associated with “Peak Detection” method (Figure 4b), the resulting spectrum is very well-corrected and the fluorescence background is completely removed as can be seen in Figure 4c.

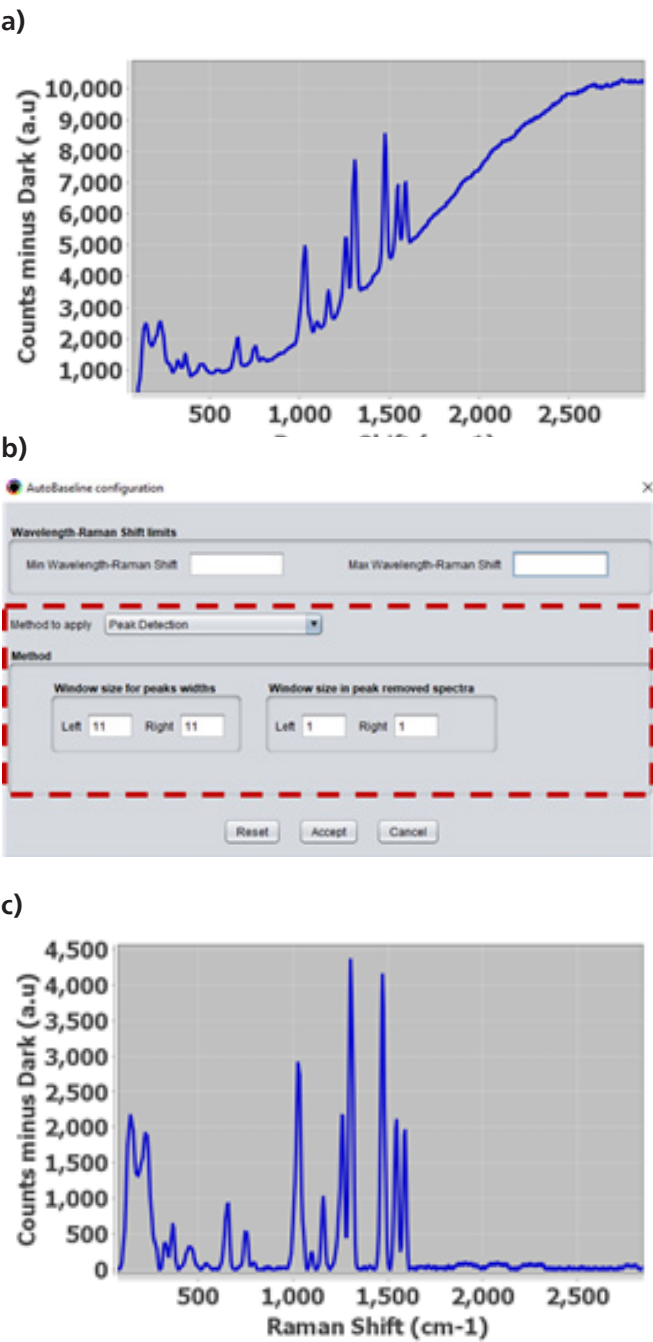
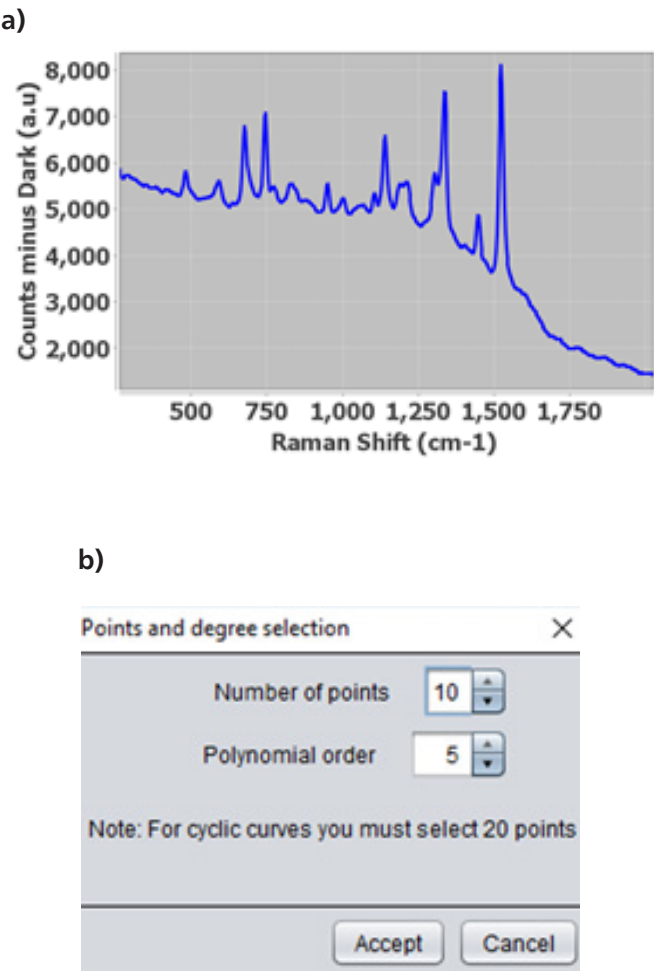


Figure 4. (a) Raw Raman spectrum. (b) “Auto baseline” configuration menu. Red dash line indicates “Peak Detection” as selected method and the parameters used to correct the spectrum. (c) Raman spectrum corrected.

“Manual baseline”

Furthermore, Raman spectra can be also corrected by generating a “Manual baseline”. Raman spectrum shown in Figure 5a was selected to create a new baseline with the parameters displayed in Figure 5b. Although in this case the polynomial degree is 5 and 10 points are selected in the spectrum to create the baseline, these parameters can be adapted depending on each spectrum.

As can be checked in Figure 5c (black line), manual baseline generated in this example provides a close fitting to the Raman spectrum. As a result of the “Manual baseline” correction, background signal of the initial Raman spectrum (Figure 5a) is removed and a flat resulting spectrum is obtained (Figure 5d).



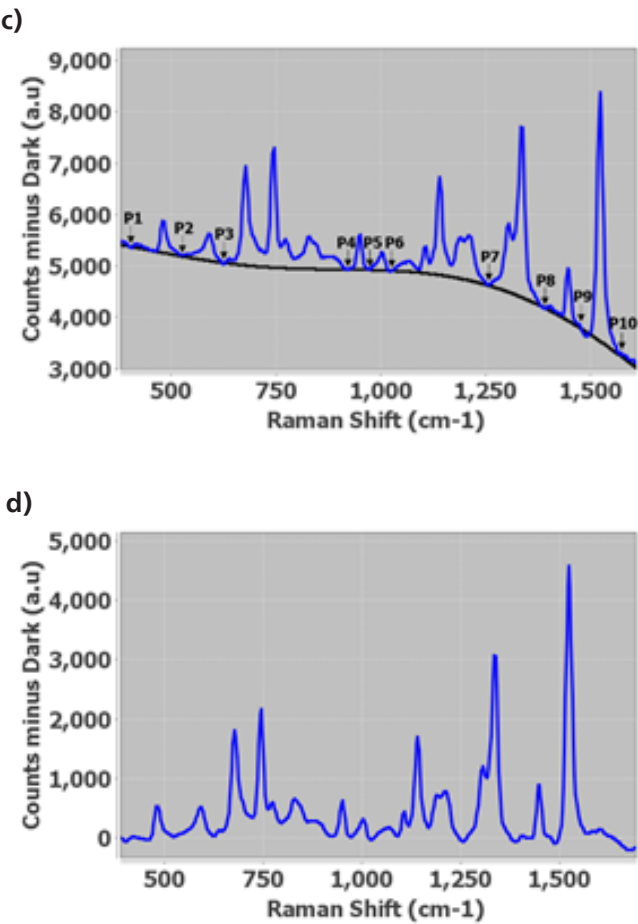


Figure 5. (a) Raw Raman spectrum. (b) “Manual baseline” configuration menu. (c) Raw Raman spectrum and baseline manually generated (black line) (d) Raman spectrum corrected with “Manual baseline”.

CONCLUSIONS

DropView SPELEC software offers interesting tools to correct raw Raman spectra. In order to obtain the best adjustment of the baseline to each spectrum, optimization of “Auto baseline” configuration improves the background correction. Flat spectra facilitate the measurement of Raman bands and in that way, obtain the information of the studied system.

Method:

Electrochemistry,
Spectroelectrochemistry

Industry:

R&D