



APPLICATION NOTE SW-701

Baseline subtraction: easy correction of Raman spectra using DropView SPELEC. Part 1

Raman spectroscopy has been widely used in many fields because it characterizes the special properties of materials and provides valuable information of a variety of processes. However, Raman spectra sometimes contain the desired vibrational bands as well as undesirable elements such as background signal. This Application Note shows the "Auto baseline" tool as one of the most convenient method to correct the baseline.

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.

Raman spectroscopy provides characteristic Raman bands associated with specific vibrational modes and each molecule has a specific Raman spectrum. However, sometimes Raman spectra are not completely flat and a background signal is observed, usually associated with fluorescence. Although experimental strategies, as the laser wavelength selection, can minimize the background, often this signal cannot be removed. Although the baseline subtraction is an interesting tool that allows us correct Raman spectra, the selection of the suitable baseline must be considered.

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. SPELEC RAMAN is a fully integrated instrument available to perform electrochemical experiments, Raman characterizations and Raman spectroelectrochemical measurements. 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.

RESULTS

"Auto baseline" is an interesting tool implemented in DropView SPELEC software and it applies automatically a baseline correction at the whole spectrum. The default configuration applied is a polynomial fitting, degree of polynomial 10. Figure 1a shows the raw Raman spectrum obtained in the characterization of one powder sample. In this spectrum, not only characteristic Raman bands related to the sample are observed, but also background signal is easily differentiated. "Auto baseline" tool uses a mathematical fitting to adjust the background signal, and as Figure 1b shows, it corrects the Raman spectrum obtaining a flat response just selecting "Auto baseline" option available in DropView SPELEC.

Once the flat spectrum is obtained, the measurement of Raman bands can be easily done with "Automeasurement" tool and all the information (position, height, width, area, etc.) related to each vibrational band is collected.

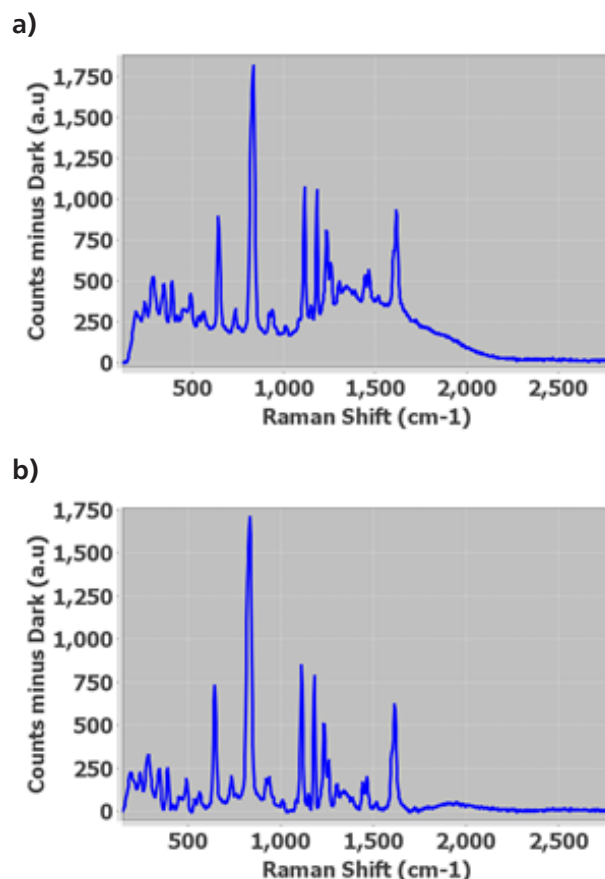


Figure 1. (a) Raw Raman spectrum and (b) Raman spectrum corrected with "Auto baseline" default subtraction.

Moreover, "Auto baseline" can be applied to a huge number of Raman spectra and is not limited to one spectrum. Figure 2a shows the raw Raman spectra recorded during a Raman spectroelectrochemical experiment. While a cyclic voltammetry is scanning the potential from -0.20 V to -0.90 V, Raman spectra are collected. As is shown in Figure 2a, there are two well-defined bands at 463 and 582 cm⁻¹ and a small band centered at 515 cm⁻¹. Figure 2b displays the evolution of this band with potential using "Spectra vs EC" tool of DropView SPELEC, when baseline is not applied. Raman intensity remains constant in the cathodic scan and only at more negative potentials than -0.70 V the intensity increases. However, in the anodic scan Raman intensity at 515 cm⁻¹ decreases during the whole scan. Then, Figures 2a and 2b lead to think that this is real behavior of this band.

A more detailed analysis of Raman spectra, Figure 2a, shows that this behavior is not correct since the background is moving during the experiment and its intensity changes, so it must be subtracted in order to understand the real behavior of this band. After the "Auto baseline" default subtraction is applied, obtained Raman spectra are shown in Figure 2c. These data treatment allows us to differentiate Raman intensity associated with 515 cm⁻¹ without background. Evolution of Raman intensity of this band with potential, after application of baseline correction, is shown in Figure 2d. Intensity decreases from -0.20 V to -0.90 V during the forward scan and it does not recover the initial intensity in the backward scan.

Hence, Raman spectra without baseline correction show that 515 cm^{-1} band is stable in the forward scan and decreases during the backward scan, while corrected spectra demonstrate that the real behavior of this sample consists of decreasing in the cathodic scan and remains constant during the anodic scan.

CONCLUSIONS

DropView SPELEC is a dedicated software for spectroelectrochemistry, it allows not only to perform the measurements and show in real time the information collected, but also it has specific tools for data treatment and analysis. One of these interesting tools in the baseline correction because it corrects the Raman spectra and remove the background signal. Furthermore, the selection of an adequate baseline avoids misinterpretations of the obtained results and allows us to understand the behavior of the analyzed system.

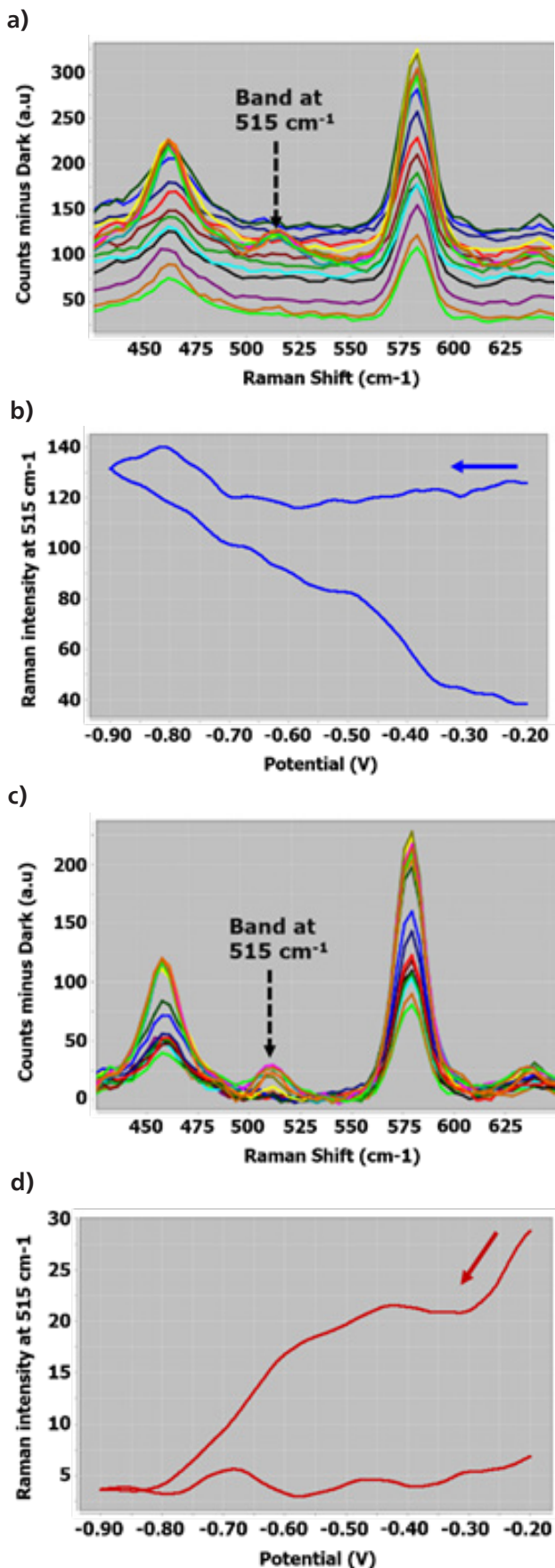


Figure 2. (a) Raw Raman spectra and (b) evolution of band at 515 cm^{-1} with potential without baseline correction. (c) Raman spectra and (d) evolution of band at 515 cm^{-1} with potential with default baseline correction applied.