Automeasurement tool: fast procedure for extracting the information in DropView SPELEC

DropView SPELEC is a dedicated software that allow us to obtain electrochemical, spectroscopic and spectroelectrochemical curves. In addition, it offers interesting tools for data treatment and analysis. In this Application Note, the "Automeasurement" tool is explained in detail.

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INTRODUCTION

Electrochemistry, spectroscopy and spectroelectrochemistry are powerful techniques that provide interesting information related to different systems and processes. Although they are used in a wide variety of fields, the analysis of the obtained results is not always as easy as would be desired. Especially complicated and even tedious is the analysis of complex electrochemical and spectroscopic responses.

This Application Note shows the usefulness of the "Automeasurement" tool to obtain automatically the information related to electrochemical peaks as well as spectroscopic bands. Different examples demonstrate that the optimization of "Automeasurement" configuration enables to gather as much information as possible in a single measurement.

INSTRUMENTATION AND SOFTWARE

Spectra shown in this Application Note are obtained with SPELEC instruments and DropView SPELEC software. These instruments are fully integrated equipments available to perform electrochemical, optical and spectroelectrochemical measurements in different spectral ranges. DropView SPELEC is a dedicated software that acquires real-time spectroelectrochemical information and also includes specific tools for data treatment and analysis. In this Application Note, "Automeasurement" tool will be explained in detail.

RESULTS

"Automeasurement" is a suitable tool implemented in DropView SPELEC software to perform automatic measurements on a curve. Applying this tool is as easy as select the electrochemical or the spectroscopic curve in which will be applied and then select the "Automeasurement" tool.

When the measurement is done, the information related to each electrochemical peak or spectroscopic band is shown in the Measurements tab in the Parameters and Measurements Area. In this tab, all the measurements done will be shown and is not limited to only one measurement.

Furthermore, not only the information obtained in one measurement can be individually exported as a .csv file, but also the information of all the measurements will be recorded in a single file.

"Automeasurement" tool is specifically interesting for Raman measurements. Taking into account that Raman spectra usually show numerous bands, the automatic and simultaneous measurement of all of them facilitates the acquisition of information related to Raman bands. Figure 1 shows a Raman spectrum in which the "Automeasurement" has been applied. As can be observed, this tool recognizes the Raman bands and the specific information associated with each them is displayed.
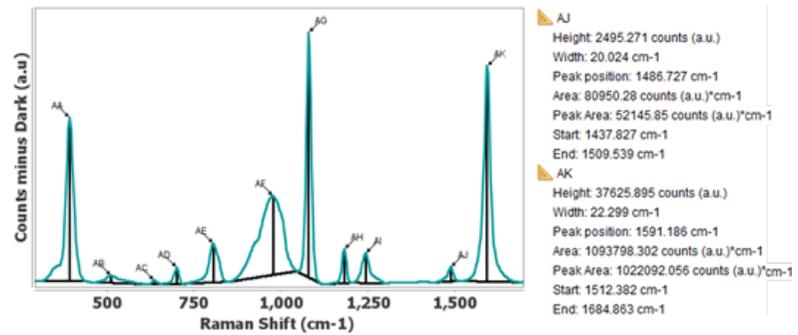

Figure 1. Raman spectrum measured by "Automeasurement" default tool and the information related to AJ and AK bands.

"Automeasurement" provides the value of height, width, peak position, charge (peak), area, peak area, and the limits (start and end) of the measurement for electrochemical curves. Information extracted from optical bands is exactly the same but without the charge of the peak because has not sense for UV-VIS, Raman nor NIR bands.

However, "Automeasurement" configuration can be modified in order to optimize this tool according to the shape of the selected curve. This configuration can be changed in DropView SPELEC following the route: Menu bar > Measurements > Config automeasurement > Select the type of curve that will be measured. Figure 2 shows the configuration menu:

b)

a)

b)
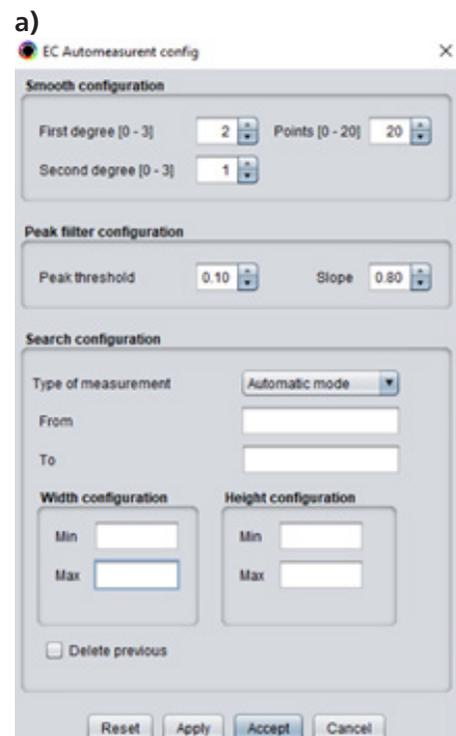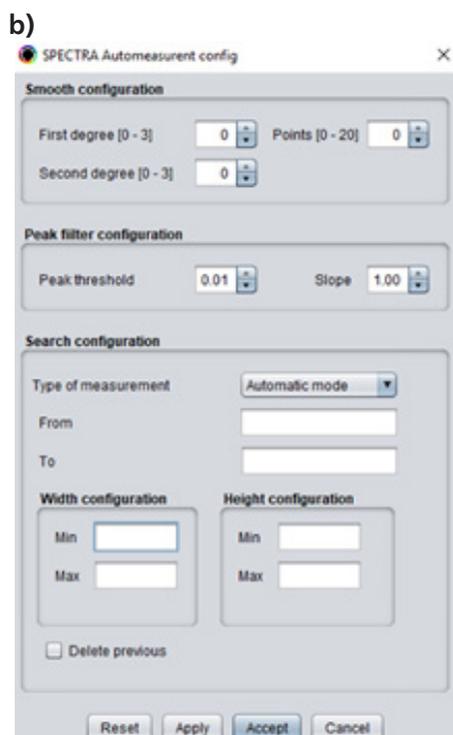
Figure 2. "Automeasurement" default configuration for (a) electrochemical, UV/VIS, NIR and ECL measurements and for (b) Raman measurements.

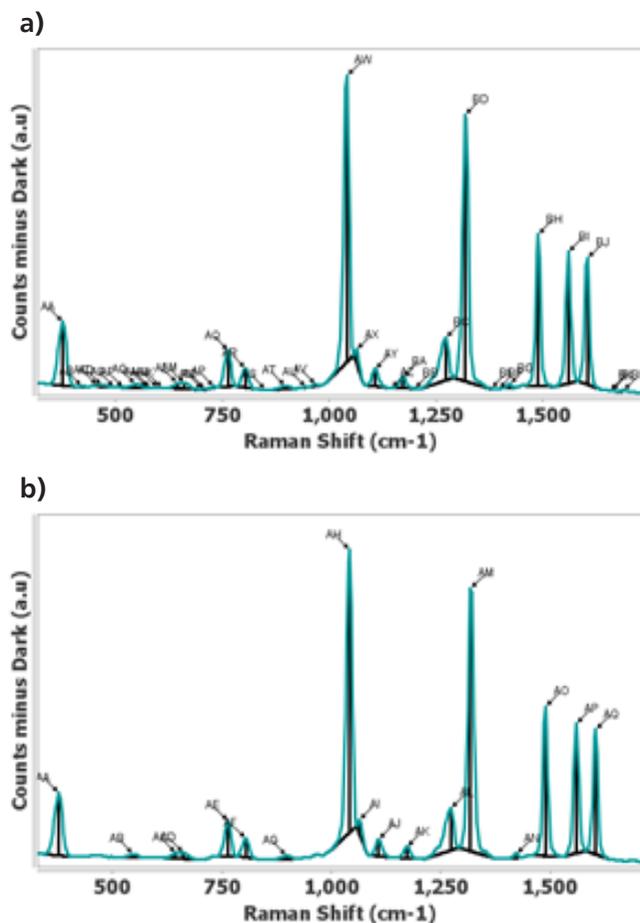**Figure 3.** "Automeasurement" of Raman spectra using (a) 0.00 and (b) 0.01 peak threshold.

"Automeasurement" parameters allows us to define:

• Smooth configuration: allows smoothing the curve, once or twice, by Savitzky-Golay algorithm before "Automeasurement" is applied. First and second degree values correspond to the degree used in the first and second smoothing, respectively. Points parameter defines the number of neighboring points to use in both smoothing execution.

• Peak filter configuration: allows the software to consider if the signal will be accepted or rejected as a peak. It depends on two parameters:

- Peak threshold defines the minimum value of height that will be accepted as real peak. The value is defined using a relative value that depends on the height of the greatest peak found. For example, peak threshold of 0.10 means that peaks will be differentiated when their height is higher than 10% of the height of the greatest peak. As can be observed in Figure 3, this parameter is useful to discard the noise signal and only differentiate the real peaks. Figure 3a shows that "Automeasurement" of this Raman spectrum, using 0.00 peak threshold, does not differentiate between real Raman bands and noise.

However, a higher value of peak threshold, 0.01 in this example, allows the "Automeasurement" tool to discard noise and only Raman bands are considered (Figure 3b).

- Slope: defines the minimum value of the slope of the partial curve where the peak is located. In order to accept peaks with high slope, a value near 1.0 must be selected. If the elimination of noise signal is required, it is a good choice to decrease this value. Figure 4 shows the same Raman spectrum measured with different slope values. As can be noticed in Figure 4a, only one Raman band is taken into account with 0.65 slope value. On the other hand, Figure 4b shows that all Raman bands are differentiated when selected slope value is 1.00.
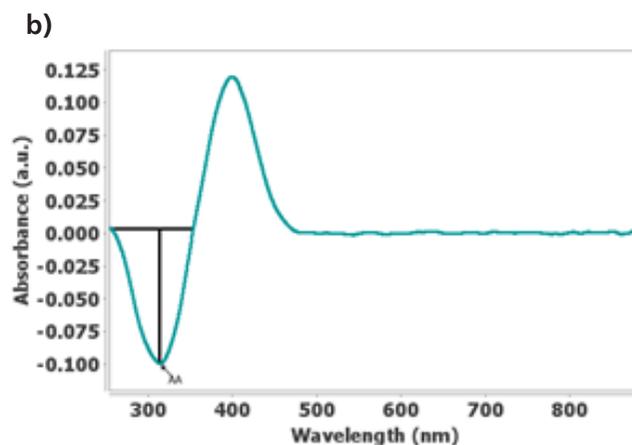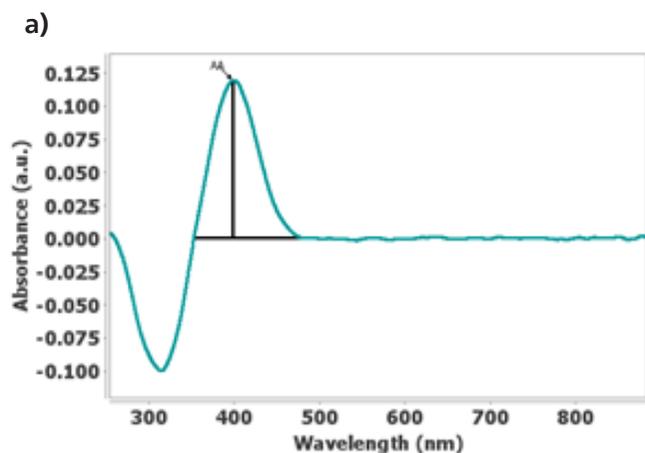
a)

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b)

b)
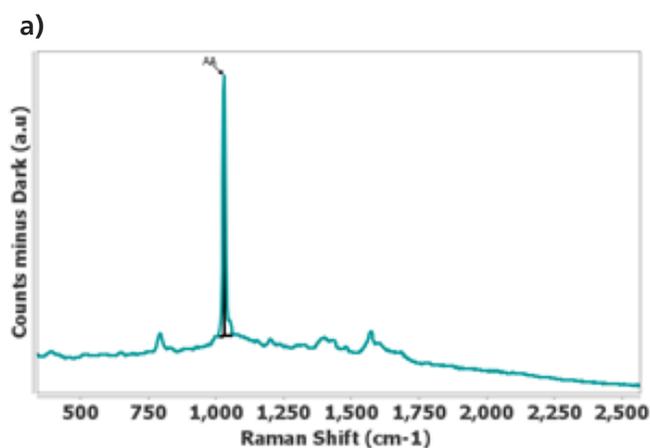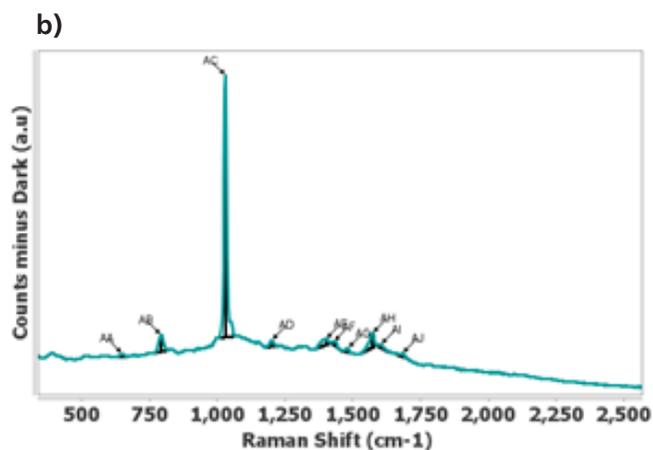
Figure 4. "Automeasurement" of the same Raman spectrum using (a) 0.65 and (b) 1.00 slope values.

Figure 5. "Automeasurement" of the UV-VIS signal using (a) maximum mode between 350 and 500 nm and (b) minimum mode between 250 and 350 nm.

- Search configuration: defines the type of measurement (automatic, maximum and minimum mode), the limits of the region where the "Automeasurement" will be applied and also width and height that the peaks must have to be measured. Maximum mode only considers positive peaks while minimum mode only recognizes negative signals. Figure 5 shows an example of a UV-VIS spectrum measured using these configurations in specific regions.

As can be observed in Figure 5a, "Automeasurement" using maximum mode between 350 and 500 nm shows the accurate measurement of UV-VIS band at 400 nm. In addition, minimum mode between 250 and 350 nm demonstrates a useful measurement of 315 nm band (Figure 5b).

CONCLUSIONS

DropView SPELEC is a dedicated software to perform electrochemical, optical and spectroelectrochemical measurements, but a wide variety of tools for data treatment and analysis are also included. One of these interesting tools in the "Automeasurement" of electrochemical peaks and spectroscopic bands, when the software obtains the information associated with each of these signals. However, if the default configuration does not provide as accurate measurements as are expected DropView SPELEC allows us to configure its parameters.

a)

Method:	Electrochemistry, Spectroelectrochemistry
Industry:	R&D

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