

SUPPLEMENT A

AUTOMATED DATA ACQUISITION

To take a large amount of data, an automation was carried out in the way of acquiring the experimental measurements.

Two M-403 Physic Instruments motors are used, aligned with each other in such a way that they can move in the XY plane. These engines are controlled through their respective C-863 controllers.

A QE-Pro spectrometer from Ocean Optics is used for the acquisition of spectra, for the activation of the sensor a red laser at 785 nm is used, from the same Ocean Optics.

All SERS acquisition is controlled by a series of programs developed in MATLAB.

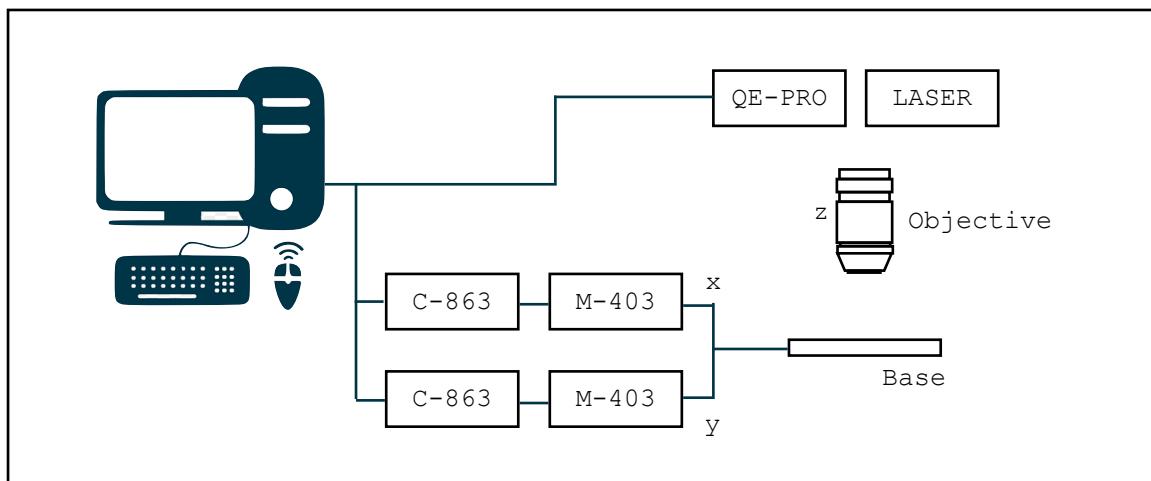


Fig 1-A. Scheme of the optical setup for automated acquisition

A compromise is sought between the sensor and the acquisition time. It depends on the sensor. In our case a silicon sensor and a silicon sensor with gold nanoparticles on its surface.

For which we wax the spectrometer with an integration time equal to 10s with the acquisition of 1 spectrum, this sensor is illuminated with the laser source with a power of 350 (laser units).

The sensors to be analyzed have a measure of 5mm x 5mm so a mapping of the sensor is made to cover the largest possible area; in this case we perform a mapping of the sensor and perform the characterization of 16mm² which is similar to 64% of the entire area of the sensor.

For the sensor, the Cartesian coordinates are used to determine the initial positions starting at a $P(0,0)$ and ending them at $P(4.4)$ in steps of 0.5mm as shown in figure 2-A.

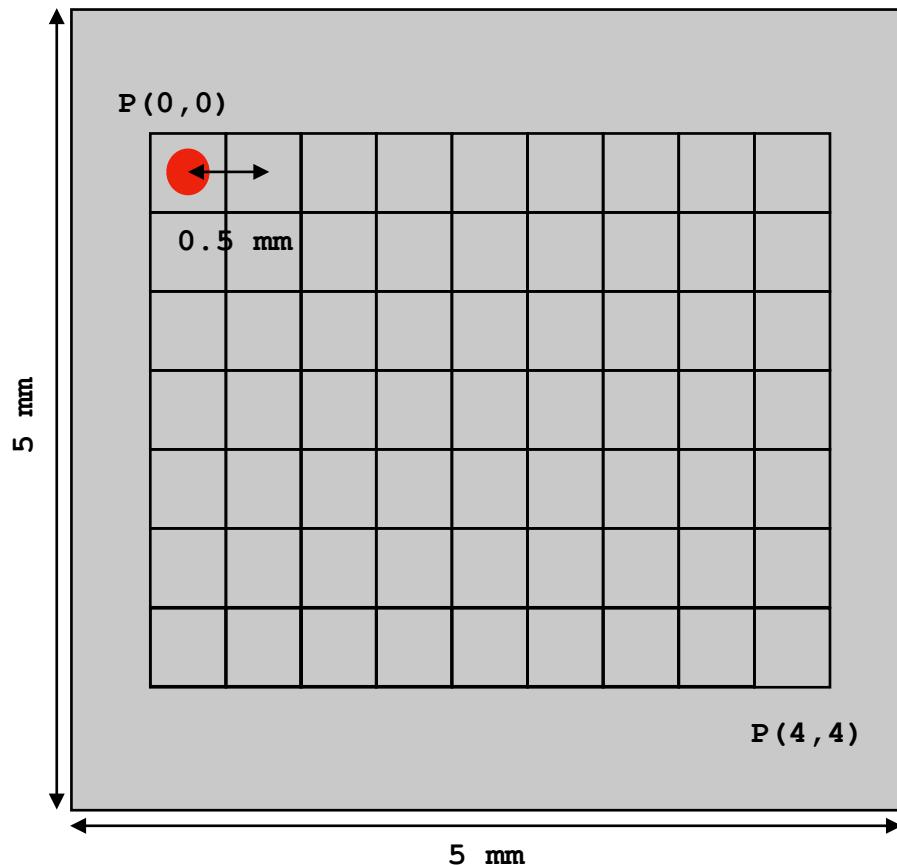


Fig 2-A. Scheme of the sensor and mapping measurement

When performing this type of measurement, the operator only has to check that they are correct in the first image, the operator will observe the mapping of spectra as shown in figure 3-A.

Each subplot will appear in real time of acquisition of the measure, for this study by having a movement of 0.5 mm of passage in both X and Y.

In this case we have 81 points, in each point 3 measurements are made, for this reason each point takes 30 seconds, giving us a total of 45 minutes for each sensor.

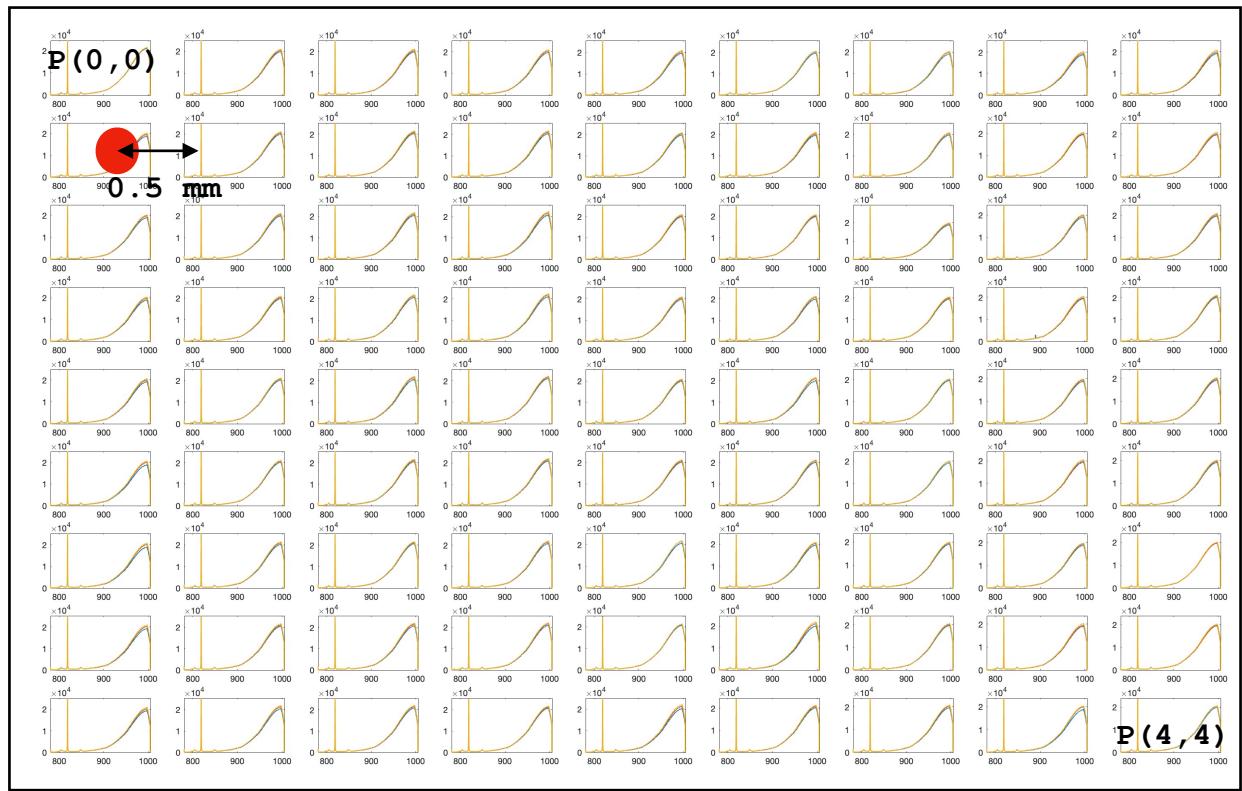


Fig 3-A. Window that observes the operator for the visualization of data in the laboratory

Once the data has been regrouped, the operator will observe the number of acquired spectra and their average in black linearity through mathematical methods and functions applied in Matlab, as seen in figure 4-A.

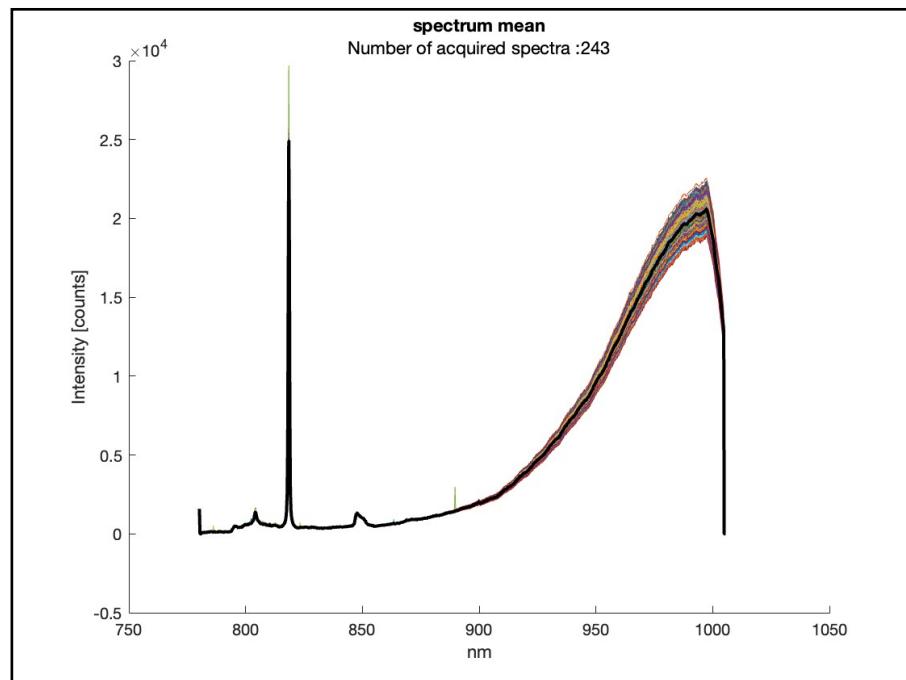


Fig 4-A. Mean spectrum in one acquisition

In the same way, the average of the DARK was calculated to eliminate any rumor that could have been caused by any interference. A measurement of 100 spectra is made to determine the residual noise, as shown in Figure 5-A.

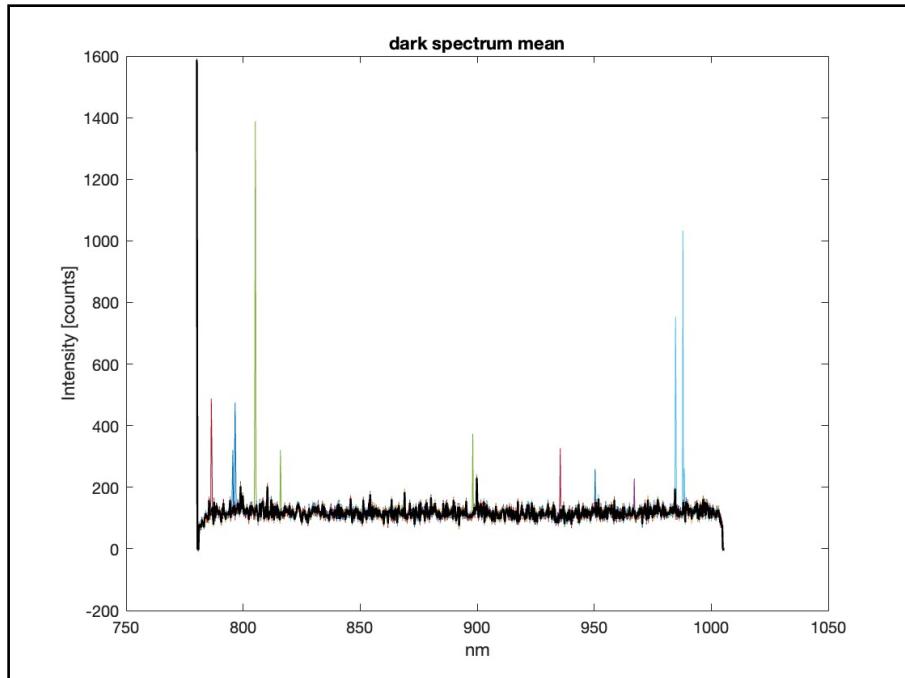


Fig 5-A. Mean dark noise spectrum, 100 acquisition

When we have these means we perform the conversion the wavelengths in [nm] to Raman shift [cm^{-1}] with the next equation.

$$\text{Raman shift}[\text{cm}^{-1}] = \frac{10^7}{\lambda_{ex}[\text{nm}]} - \frac{10^7}{\lambda[\text{nm}]}$$

Then we subtract the average of the sensor with respect to the average of the dark noise, which will give us a final graph of the characteristic of the sensor as shown in figure 6-A. It should be emphasized that the images are identifying and allow to determine errors in the data acquisition process, which allows the operator to realize if his sensor works correctly or has some imperfections, or simply has to align his system. It should be emphasized that none of this data is deleted and is saved in matrices that will allow the analysis to continue in the future. (Supplement B)

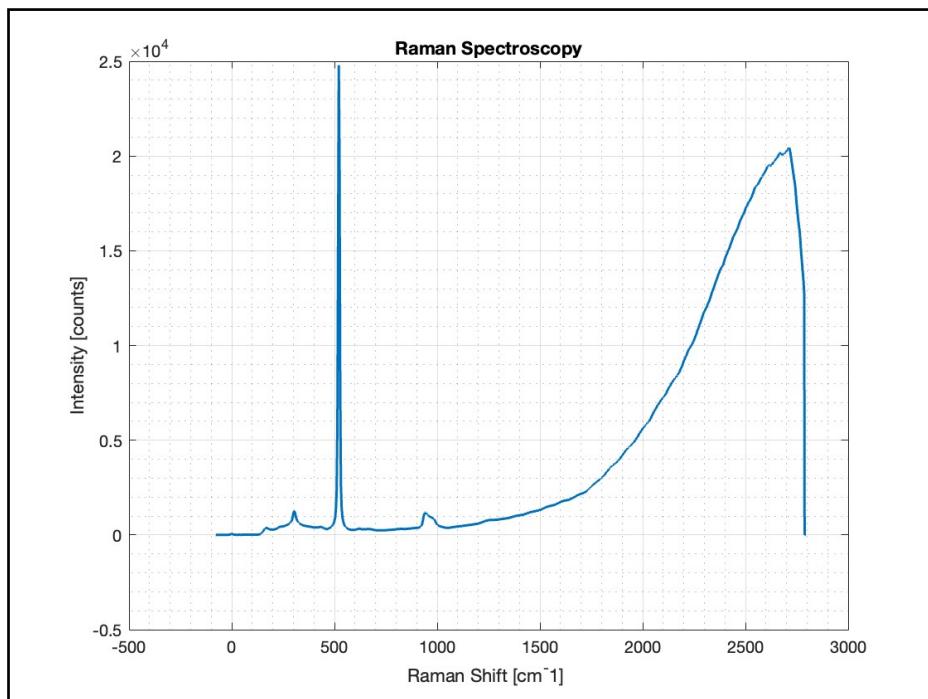


Fig 6-A. Mean spectrum experiment subtract dark mean spectrum