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Raman spectra processing algorithms and database for RLS-ExoMars

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Abstract

Here the authors present both a set of algorithms and a Raman spectra database that are being developed in the framework of the development of the Raman Laser Spectrometer (RLS) instrument for the 2018 ExoMars mission. These algorithms will be integrated in the ground segment tool for scientific data exploitation but also adapted for implementation as on-board operation software.

1. Introduction

For the operation of an autonomous instrument such as RLS, the development of a set of algorithms for the automatic optimization of the operation parameters is of paramount importance. The algorithms and Raman spectra database presented in this abstract provide the means for achieving the following objectives:

- Optimum automatic spectral acquisition on Mars.

- Efficient scientific data exploitation on Earth.

The instrument must optimize the acquisition parameters on-board for each spectrum acquisition in order to maximize the final SNR and minimize the time consumption. It is also expected to detect spectral traces of interest in the acquired spectra, these spots requiring enhanced quality acquisitions. This calls for a background signal (or baseline) extraction and elimination method, a peak detection mechanism and a material identification based on the detected Raman peaks.

Once the raw scientific data has been correctly received on Earth, these have to receive spectral data treatment to extract scientific information that help the scientists to interpret the findings of the instrument. This data treatment comprises spectrum extraction, a more exhaustive peak detection and a compound identification based on identification algorithms fed by a complete Raman spectral database that is being constructed.

2. Baseline detection

The background of a Raman spectrum is a wide band signal that adds up to the Raman spectrum and has its origin in fluorescence derived from the nature of the samples under study, the grain size distribution of the powdered sample and stray light effects, among others. This is, therefore, an undesired phenomenon that provides no useful information and must be somewhat filtered or extracted from the spectra.

The algorithms developed by our team provide satisfactory smoothing and filtering approaches that result in the consecution of this objective, as it can be appreciated in Fig. 1. Several methods of baseline determination can be found in the literature, one of them being [1].
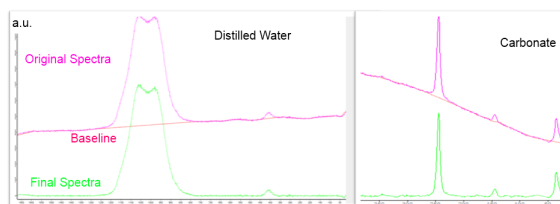

Figure 1: Example of automatic baseline detection and correction for two different materials

3. Automatic peak detection

Once the background has been removed, the next step is the automatic location of the Raman peaks, which contain the molecular information related to the sample under analysis. This identification is currently made by detection of peaks by means of the finding of relative maxima and minima within the baseline corrected spectrum, and by its subsequent comparison

with the noise level of the spectrum. The end product of this process is a list of peak positions and amplitudes that will be used to uniquely identify the materials the sample is comprised of.

This operation is performed both on-board for the detection of traces of interest, and on-ground for the precise material identification.

4. Material identification

Our proposal of identification of constituent compounds of the sample from its Raman spectral signature is based on peak comparison, such as the one developed by [2]. This algorithm has two main phases, an initial search and matching of the highest intensity peaks for identifying pure compounds and a recursive search that matches the secondary peaks for mixtures determination. The aim is to create a *tree of solutions* capable of identifying both pure materials and mixtures.

5. Raman spectra database

For the on-ground identification of Raman spectra a standard database of Raman spectra is being developed which, at the present time, contains 224 spectra. All of these spectra contain detailed information about how they were acquired. This is an online database designed to be used with a web browser that has functionalities such as identification, visualization, downloading, searching...

This not only is a powerful spectra management tool, it also sets the starting step in the interpretation of the origin of the compounds found in the analyzed materials, which begins with their identification.

6. Summary and Conclusions

The algorithmic spectral processing in the framework of the RLS instrument, with results summarized in Fig. 3, is planned to be performed both in Mars and on earth, and comprises baseline detection and subtraction, raman peak detection and mineral identification.

References

[1] Schulze, H. G., et al.: A Model-Free, Fully Automated Baseline-Removal Method for Raman Spectra, Applied Spectroscopy, vol. 65, no. 1, pp. 75-84, 2011.

[2] Vandenabeele, P.: Evaluation of a spectral searching algorithm for the comparison of raman band positions, Spectrochimica Acta Part A 80, 2011.
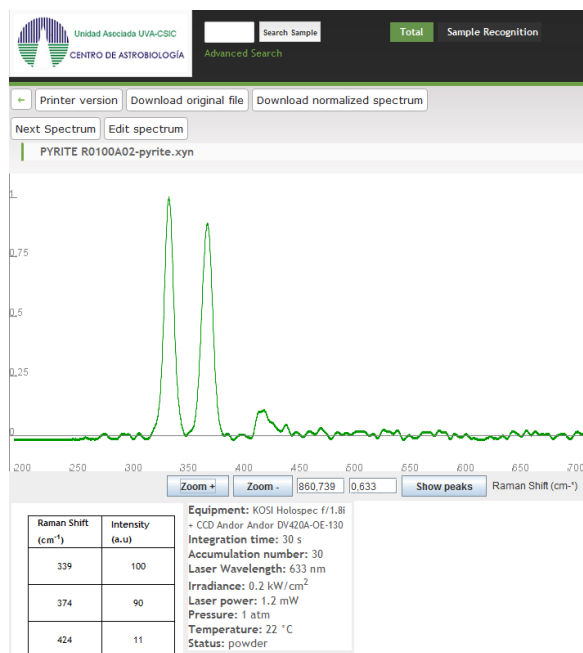
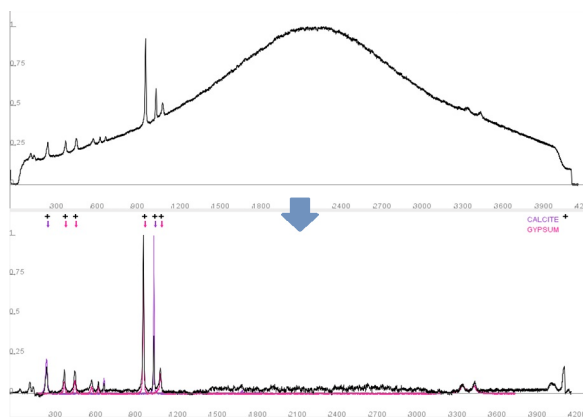Figure 2: Screen capture of the Raman spectra database

Figure 3: Example of baseline detection and correction, peak detection and material identification