AUTOMATIC MINERAL IDENTIFICATION USING RAMAN SPECTROSCOPY FOR PLANETARY EXPLORATION: IMPLICATIONS FOR RLS AND SUPERCAM INSTRUMENTS

Pascual-Sanchez, Elena[1,2], Khadmaoui-Bichouna, M.[3], Prieto-Garcia, C.[1], Veneranda, M.[1], Sanz-Arranz A.[1], Manrique, J. A.[1,4], Reyes-Rodriguez, I.[1], Julve-Gonzalez, S.[1], Rull-Perez, F.[1], Lopez-Reyes, G[1].

[1] ERICA Research Group. Universidad de Valladolid (Spain); [2] Universidad Complutense de Madrid (Spain) ; [3] University of West Scotland (Scotland); [4] Institut de Recherche en Astrophysique et Planétologie, Toulouse (France)

INTRODUCTION

Automatic identification of minerals allows a better classification of data. Raman spectroscopy can identify mineral phases in rock samples. The accumulation of Raman spectra improves the Signal-to-Noise Ratio (SNR) of a sample. Spectra multiplication appears as an innovative signal-processing technique that improves the detection capability of autonomous algorithms.

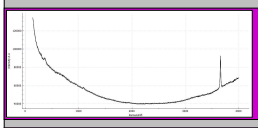
algorithm structure: SPECTRAL PROCESSING → PEAK DETECTION → AUTOMATIC IDENTIFICATION OF MINERALS

The identified advantages of the spectra multiplication are the highlighting of the main peaks of the spectra, the improvement of the SNR and the self-definition of the Raman peaks. These advantages have been exploited to provide a fully automated method for classifying a mineral sample. Combined with automated sample acquisition routines, this method would enable greater efficiency and scientific return from space missions such as ExoMars or Mars2020.

METHODOLOGY

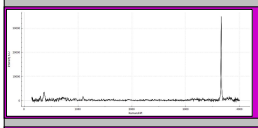
SPECTRAL PROCESSING

A new spectral processing sequence is required to take advantage of spectra multiplication.



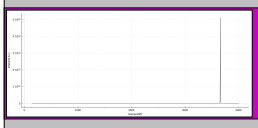
INTENSITY CORRECTION

The spectra are divided between the normalised amorphous Zinc borate signal[1].



BASELINE REMOVAL

The baseline is eliminated by a noble curve

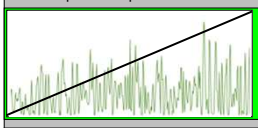


ACCUMULATION BY MULTIPLICATION

Raman spectra of different points corresponding to the same sample are multiplied.

PEAK DETECTION

Taking advantage of the increase in SNR and preventing the risk of over-detection, stop and improvement criteria are established to detect Raman peaks automatically:



STOP CRITERIA

- Intensity > 3 std
- Maximum peaks per iteration (11)

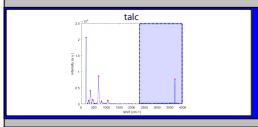
down-part	up-part
3	6
20	15

IMPROVEMENT CRITERIA

- Split of the spectrum (at 2300 cm^{-1})
- Width filter
- Maximum number of iterations

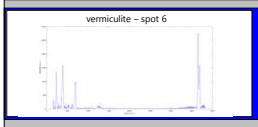
AUTOMATIC IDENTIFICATION OF MINERALS

Search for candidates based on a match factor [2]. The ADAMM database is used [3].



HYDRATATION CRITERIA

If the sample is moisturized, all compounds in the database with peaks in the region of the OH vibrations are included as candidates.



INTENSITY VARIABILITY

Certain samples alternate their main peak depending on the analysed point (e.g. main peak of vermiculite).

some samples belong to the olivine solid solution or vermiculite group

MINERAL GROUPS

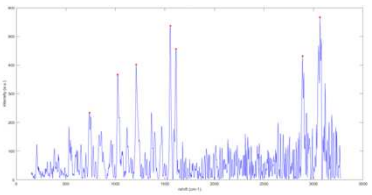
All phases of the group are considered when a sample is part of a mineral group.

RESULTS

PEAK DETECTION

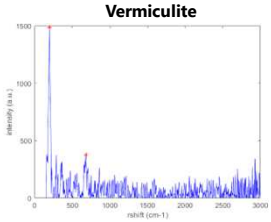
Automatic detection based on spectrum multiplication can detect more peaks than the arithmetic average. The method has been shown to be effective even in noisy spectra.

Indene



The indene exemplifies how the automatic peak detection algorithm avoids noise detection. All Raman peaks correspond to molecular vibrations.

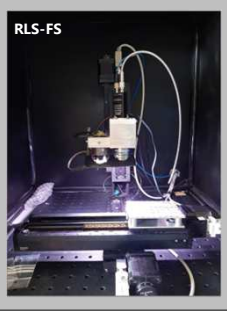
Vermiculite



The arithmetic average detects the main peak of vermiculite. The multiplication method detects the secondary peak in a noisy region.

MINERAL IDENTIFICATION

Test samples acquired with the RLS-FS (Flight Spare) instrument were used. Comparison is made with spectra from the ADAMM database and the standards database.



PROBLEM SAMPLES

- Olivine 100%
- Serpentine 100%
- Vermiculite 100%
- Kaolinite 100%
- Serpentine – Olivine 47,5%
- Vermiculite – Kaolinite 50%

The samples have been selected for their relevance to the study of Mars.

IDENTIFICATION

- Fosterite
- Serpentine (antigorite/lizardite)
- Vermiculite
- Kaolinite
- Serpentine (lizardite) + fosterite
- Kaolinite

A 36% false positive rate has been detected in the second iteration. This represents an outstanding improvement of the method.

CONCLUSIONS

- The multiplication of spectra improves the detection capability compared to the arithmetic average.
- The contribution of all the characteristics of the spectra (baseline, relative peak intensity, intensity variability, etc.) must be considered to achieve a robust automatic identification method.
- It is advantageous to split the spectrum into two parts to deal with OH vibration separately.
- Grouping the identification by mineral group helps to improve the results.

REFERENCES

[1] Sanz-Arranz, A., Manrique-Martinez, J.A., Medina-Garcia, J. & Rull-Perez, F. (2017). Amorphous zinc borate as a simple standard for baseline correction in Raman spectra, Journal of Raman Spectroscopy, 48(1), 1644-1653.
[2] Khadmaoui Bichouna, K. (2020). Desarrollo de algoritmia para la identificación automática de espectros Raman de la mision ExoMars, Final degree Project. University of Valladolid, degree in telecommunications engineering. Valladolid (Spain).
[3] Veneranda, M., Sanz-Arranz, A., Manrique, J. A., Saiz, J., Garcia-Prieto, C., Pascual-Sánchez, E., ... & Lopez-Reyes, G. (2022). Analytical database of Martian minerals (ADaMM): Project synopsis and Raman data overview. Journal of Raman Spectroscopy, 53(3), 364-381.

ACKNOWLEDGEMENTS

The authors thank the Agencia Estatal de Investigación (Spain, grant PID2019-107442RB-C31/AEI/10.13039/501100011033) E. Pascual-Sánchez thanks the funding support from a Programa Investigo of Madrid council as part of the Recovery, Transformation and Resilience Plan for the development of the Next Gen recovery funds; I. Reyes Rodríguez thanks the European Social Fund and the Consejería de Educación de Castilla y León for his predoctoral scholarship. Additional thanks to be given to the Universities Ministry of Spain.

Universidad de Valladolid

Erica

European Union
European Social Fund