INTERNSHIP PROPOSAL

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Deformulation of complex glass-like materials through statistical analysis of Raman spectra

The characterization of complex materials, in particular obtaining a three-dimensional map of their chemical composition and phases, represents a major challenge with important applications in industry. In the field of glasses, the analysis of Raman spectra is commonly used to identify the molecules present from individual peaks [1]. However, this approach does not take into account the correlations between peaks, which contain essential information on collective effects.

Advances in machine learning now enable more sophisticated data analysis. These approaches open up new possibilities in analytical chemistry, which are only just beginning to be explored [2]. In the field of glasses, the application of classic data projection tools has enabled the reconstruction of cutting profiles [3]. However, the interpretation of these profiles is still based on visual inspection, which limits the automation and quantification of the analysis.

In collaboration with the Surface Verre Interface (SVI) laboratory associated with Saint-Gobain, we propose to develop a more in-depth approach to the analysis of Raman spectra. The aim is to automate data interpretation and assign a confidence score, enabling more robust and quantitative analysis of complex materials.

For this, we will use the rruff database [4] and spectra associated with model sands of known composition synthesized by our collaborators at Saint-Gobain. These data will enable us to implement a supervised learning approach based on numerical tools developed for deep learning.

The aim of this internship is to lay the foundations for a supervised method of analyzing Raman spectra for glasses. Eventually, this method will be extended to other types of analysis used by Saint-Gobain (SIM, IR spectra, etc.).

References:

[1] Ben Khemis, S., Burov E., Montigaud H., Skrelic D., Gouillart E., Cormier L., (2021). Structural analysis of sputtered amorphous silica thin films: A Raman spectroscopy investigation . *Thin solid films*, *733*, 138811.

[2] Debus, B., Parastar, H., Harrington, P., & Kirsanov, D. (2021). Deep learning in analytical chemistry. *Trends in Analytical Chemistry*, *145*, 116459.

[3] Analyzing 3D hyperspectral TOF-SIMS depth profile data using self-organizing map-relational perspective mapping, Gardner et al. *Biointerphases*, 15 (2020).

[4] *https://rruff.info/*