Archeology and Chemometrics: Raman imaging to characterize specific spectral sources without prior knowledge.

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1 Introduction

The application of analytical chemistry to archeological material has become an essential part of modern archeological investigations and the instrumental progress in it, has made possible to generate more and more data in a very short time. In particular, Raman spectral imaging can be successfully applied in Archeological research by its simplicity of implementation to study past human societies through the analysis of materials remains. This technique makes it possible to simultaneously obtain spatial and spectral information without damaging the sample. However, their complexity may make its chemical interpretation complex at first glance (e.g. specific problem of selectivity in spectroscopy for unexpected chemical compounds). Mathematical approaches from chemometrics are therefore important to overcome this drawback. As a part of this continuity in the development of high-performance mathematical tools, we present here a chemometric strategy to characterize specific spectral sources in Raman spectral imaging on an archeological sample: a piece of mosaic. In Archeology, efficient exploratory analysis of spectroscopic images are an important part to resolve the chemical information. Therefore, the objective is to present a spectral analysis with Orthogonal Projection Approach (OPA) [1] to improve the initial estimate step in the Multivariate Curve Resolution and Alternating Least-Squares (MCR-ALS) [2,3] optimization to characterize the chemical constituents in the mortar of the mosaic sample.

2 Material and methods

The sample come from a ditch filling found in the *Ruscino* archaeological excavation (periphery of Perpignan, France). The site was occupied by Roman from the second half 1nd century BC to the end of the 1st century AD (i.e. oppidum period). The area on the archeological sample was specifically chosen with the aim of including both, the adhesive mortar at the junction between the stone and the tesserae, and the original bedding mortar present between the tesserae. The experimental conditions of acquisition for this area of $905 \times 395\ \mu m^2$ are optimized in Raman imaging to obtain the best signal-to-noise ratio representing a 3D data matrix to be analyzed of size $181 \times 79 \times 1009$ (i.e. pixels by pixels by wavelengths). Then, after preprocessing the raw data, the OPA was used for the initial spectra in the MCR-ALS optimization in order to identify pure components (results are also confirmed by other techniques including SEM).

3 Results and discussion

The chemometrics strategy presented, demonstrates the possibility of characterizing an archeological sample in Raman imaging without prior knowledge. The archeological outstanding result of this study is the use of biogenic materials (magnesium calcites or the amino-acid) of animal origin, in particular fish or shellfish. The local origin of the materials seems difficult to ascertain but could nevertheless well come from supplies of various materials by a trade covering the whole of the Roman Empire. Nevertheless, the historical dating and the exact role of the glue between the mosaic and the stone is still in discussion from an archaeological point of view.

4 References

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