



B84 Chemical Pattern Recognition: What Can Be Extracted From Geo-Located Spectroscopic Data Sets?

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After attending this presentation, attendees will understand the usage of X-Ray Fluorescence (XRF) and Raman microscopy in applications of sand analysis, an important element in forensic identification of these materials.

This presentation will impact the forensic science community by serving as a key aspect of sand/soil analysis and as an example of a practical application of XRF and Raman spectroscopy to materials identification.

XRF and Raman spectroscopies are useful tools for analyzing substances and confirming their identity with little or no sample preparation. XRF provides information about the elemental composition of the material whereas Raman spectroscopy gives molecular information. Both techniques enable the recording of not only spectra of small sand particles (as small as 50-100 microns) but also hyper-spectral imaging and collection of average spectra over a given area. Multivariate Analysis (MVA) can produce chemical distributions of elements and/or material classification based on Principal Component Analysis (PCA) and Partial Least Square Discriminative Analysis (PLSDA) in particular with association between elements that can aid in the identification of bonded phases. The analysis of micro-XRF data and Raman data of sand taken from different areas can be used to identify geographic locations.

XRF and Raman analytical microscopes were used in this study. XRF spectra of the materials were collected using a 50keV acceleration voltage with an X-ray spot size of 1.2mm. Two excitation wavelengths (532nm and 633nm) were used to collect Raman spectra with a spot size of 10-100 microns, depending on the material. Samples of sand (10g in weight) were ground and the resulting powder was used for XRF and Raman measurements.

The spectra of sand from different locations (the United States, Europe, and the Middle East) were collected and analyzed by micro-XRF and Raman spectroscopy. XRF analysis was performed in the range of 1.00keV-40.96keV (<400 spectra). Because only few spectra have additional features in the energy range above 15keV, spectra were truncated and analysis was performed in the spectral range of 1.00keV-15keV. A standard Fixed Point Multiplication (FPM) algorithm was used to calculate the concentration of oxides in all samples. This concentration set was used to build a data set for PCA and PLSDA. Correlation between classifications based on spectral analysis and concentration analysis will be shown. Raman spectra were collected in the range of 100cm⁻¹-3500cm⁻¹ and MVA was applied to these spectra to extract differences in connection with geolocation. The data show that MVA allows clear differentiation of samples; for example, from the east or west coasts of the United States or from the United States, Europe, or the Middle East. PCA and PLSDA models for the east and west coast data sets were created and show significant separation between the sand originating from different geolocations. Raman spectra of the materials show that the main feature is SiO₂, but other spectral features originating from different oxides allow the differentiation of samples collected from the different locations. Data fusion technology was applied to the set of XRF and Raman data to create PCA and PLSDA models. Misclassification in PLSDA models was studied using randomly selected samples from available data. The results of standard and data-fused analysis are compared and discussed. In conclusion, this study provides methods that allow the differentiation of samples without knowing the actual concentration of elements/oxides and, therefore, this approach does not require any calibration for material identification.

Sand, Glass, XRF