B90 Chemical Pattern Recognition in Glasses: What Can Be Extracted From Spectroscopic Data Sets?

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After attending this presentation, attendees will understand X-Ray Fluorescence (XRF) microscopy in applications to glass analysis, which is an important element in forensic identification of these materials.

This presentation will impact the forensic science community by providing key aspects of glass analysis and an example of a practical application of XRF spectroscopy to materials identification.

XRF spectroscopy is a useful tool in the identification of substances and in confirming their identity with little or no sample preparation. New capabilities of the energy-dispersive XRF analytical microscope (micro-XRF) enable recording not only spectra of small glass particles (as small as 50-100 microns) but also hyper-spectral images of any object with high spatial resolution (<10 micrometers). Hyper-spectral image is a set of the data which contain information about position of the point along with a full XRF spectrum at this point. This means the data can be mined for unsuspected elements after the measurements have been made, and that statistical methods can produce chemical distributions of the elements and/or material classification based on Principal Component Analysis (PCA), in particular, with association between elements that can aid in the identification of bonded phases. For example, statistical analysis of micro-XRF data for glass can be used to locate the make, model, and year of cars by analyzing a glass chip. This presentation will provide practical insights into the application of the micro-XRF to the analysis of glass and soil.

The XRF analytical microscope was used in this study. XRF spectra of the glass were collected using 30keV acceleration voltage and with an X-ray spot size of 50 microns. XRF spectra of the glass strongly depend on X-ray optics, sensitivity of the detector, and accelerating voltage. In addition, background from the substrate will contribute to the spectrum of the small glass pieces because excitation X-ray penetrates through the glass and interacts with the substrate. This effect becomes very importance for the particle size of 300 microns (or less) or powder. The change in the spectrum due to the shape or size will lead to the different quantification of the sample (different composition). A method that allows one to minimize this effect or take it into consideration was developed. In this presentation, examples of the spectra from bulk material, small glass pieces, and powder will be shown.

The spectra of glass from several car manufactures and commercial glass (microscope slides, window glass, fuse glass) in the range of 1.00keV–40.96keV (<400 spectra) were collected. The spectra were truncated and analyzed in the spectral range of 1.00keV–15keV because major X-ray lines are in this range. A standard Fixed Point Multiplication (FPM) algorithm without any correction and/or calibration was used to calculate concentration of Na_2O, MgO, Al_2O_3, SiO_2, K_2O, CaO, TiO_2, MnO_2, Fe_2O_3, As_2O_5, and CeO_2 in all samples. All spectra and concentration data sets were scaled before PCA was applied. The correlation between classification based on spectral analysis and concentration analysis was found.

Glasses, XRF, PCA

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