Industrial and Forensic application of micro-XRF: glass analysis.

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X-Ray Fluorescence (XRF) spectroscopy is a useful tool for identification substances and confirming their identity with little or no sample preparation. New capabilities of the energy dispersive XRF analytical microscope (micro-XRF) enable the recording not only spectra of small glass particles (as small as 50-100 microns), but also hyper-spectral image of any object with high spatial resolution. Hyper-spectral image is a set of the data, which contain information about position of the point along with full XRF spectrum at this point. This means that after the measurements have been made, the data can be mined for unsuspected features. Multivariate analysis (MVA) can produce chemical distributions of elements and/or material classification based on Principal Component Analysis (PCA), particularly with association between elements that can aid in identification of bonded phases. For example, analysis of micro-XRF data of glasses treated in ionic melt can be used to determinate concentration profile of diffused ions; it can likewise identify the make, the model, and the year of a car, based on analysis of similarly/differences in spectra of window glass for different vehicles. This presentation will provide practical insights into the application of the micro-XRF to the analysis of glasses and application of PCA to data analysis.

The XGT-7200V XRF analytical microscope was used in this study. This desktop unit utilizes a portable 50W X-ray source, two switchable monocapillaries, and the capability to work in vacuum, in partial vacuum, and under ambient conditions.

X-ray fluorescence spectrum of the materials strongly depends on X-ray optical system, sensitivity of the detector, and accelerating voltage. In addition, background from the substrate will contribute to the spectrum of the small pieces because excitation X-ray penetrates through the material and interacts with substrate. This effect becomes very importance for the particle size of 300 microns or less. The change in the spectrum due to the shape or size will lead to the different concentration profile of the sample when FPM is in use. Application of MVA will allow one to minimize this effect or take it into consideration. In this presentation, we will show examples of the spectra from bulk material, small pieces, and powder.

Hyperspectral images/spectra of commercial glasses and glasses from several cars manufactures were collected and analyzed in the range of 1.00-40.96 keV. Chemical images produced by CLS deconvolution of hyperspectral data set will be presented. Spectra of the glasses from different car manufactures were analyzed in spectral range of 1.00—15 keV. Standard FPM algorithm was used to calculate concentration of oxides in all samples. Correlation between classification based on spectral analysis and concentration analysis will be shown. The data shows that MVA allows differentiate samples, which have very similar spectra features (concentration profiles) and this approach may be useful for forensic investigation.