MULTIVARIATE STATISTICAL ANALYSIS of MICRO-XRF SPECTRAL IMAGES FROM A BRUKER M4 TORNADO SYSTEM

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We employ multivariate statistical analysis (MSA) to the extraction of chemically relevant signals acquired with a Bruker M4 Tornado micro-XRF mapping (full-spectral imaging) system. This instrument is equipped with a micro-focused Rh source with a poly-capillary optic for concentrating the beam to a small (~30 μm) spot-size, thereby generating a high-intensity beam with spatial-resolution sufficient for excellent chemical mapping of materials. The detector system employs two silicon-drift detectors (SDD) which can be used individually, or in-tandem, to collect fluorescence spectra from the specimen. Mapping datasets are collected as a large data-cube with full X-ray spectra collected at each pixel in a 2D array. While elemental mapping is possible based on plotting of spectral regions of interest specific to the atomic species, we have developed MSA methods, to extract individual "component" spectral shapes and their corresponding spatial distributions, which are physically intuitive (e.g., no negative intensities). The benefits of employing MSA are numerable. First, the procedure can help in the identification of spatially-correlated spectra, which in-turn allows for quick diagnosis of chemical phase and distribution. Secondly, it is possible to detect trace atomic species that may be difficult to discern with conventional micro-XRF analysis. This is because MSA interrogates (with no *a priori* information) the entire data-cube with the added advantage of removing Poisson noise. Thirdly, because the two SDD detectors are positioned in different locations relative to the specimen and beam, the dual-detector configuration is convenient for assessing and removing the presence of artifacts such as diffraction peaks. Finally, the separation of components into individual histograms enables separation of overlapping peaks, which is of great help when trying to qualitatively determine the presence of atomic species that have overlapping emission lines. We demonstrate the usefulness of MSA for micro-XRF analysis through the application of this technique to a geological sample (core-drill cross-section).

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