Abstract

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COSIMA data analysis using multivariate techniques.

We describe how to use multivariate analysis of complex TOF-SIMS (time-of-flight secondary ion mass spectrometry) spectra by introducing the method of random projections. The technique allows us to do full clustering and classification of the measured mass spectra.

In this paper we use the tool for classification purposes. The presentation describes calibration experiments of 19 minerals on Ag and Au substrates using positive mode ion spectra. The discrimination between individual minerals gives a cross-validation Cohen κ for classification of typically about 80 %. We intend to use the method as a fast tool to deduce a qualitative similarity of measurements.