Spectromicroscopy analysis: clustering, error-finding, and interpreting

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Soft x-ray spectromicroscopy provides the means for studying chemical speciation at the 30-50 nm resolution scale, and it is finding wide use in studies in biology, environmental science, astrobiology, polymer research, and other fields. For a specimen that can be characterized in terms of a set of known spectra, a variety of approaches[1,2] can be used for compositional mapping. However, this is rarely the case in biology or environmental science where the complexity of the specimen and reactivity of components precludes advance knowledge of all signature spectra.

Cluster analysis provides a way to find the signature spectra that exist in a specimen, and form compositional maps based on these "discovered" spectra. Following preliminary work[3], we have carried out a systematic development[4] of this approach to soft x-ray spectromicroscopy analysis, and have extended it with methodologies aimed at classifying only on compositional variations rather than specimen thickness[5]. New developments include the recovery of the "true" incident flux spectrum from a dataset, and new methods for the analysis of mixtures such as non-negative matrix factorization. These and other developments will be reviewed and illustrated with examples from studies in biology and environmental science.

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