Multi-dimensional classification and correlation of water and trace element maps in a magmatic clinopyroxene using SpecXY.

Nils B. Gies[a], Jörg Hermann[a], Pierre Lanari[a]

[a] Institut für Geologie, Baltzerstrasse 1+3, 3012 Bern, Switzerland

Spectroscopic techniques such as Fourier Transform Infrared Spectroscopy (FTIR), Raman or hyperspectral imaging are important in modern geoscience. In recent years there has been a shift away from using exclusively single-spot analysis towards 2-dimensional maps. Maps help to reveal patterns in a sample that would not be revealed by single point measurements. Filtering and extracting signal information from multiple combined pixels can help improve the signal-to-noise ratio and therefore the accuracy of the data. However, the amount of data and information in the dataset increases significantly when maps are used instead of single spot analysis. Combining multi-layered numerical datasets - bringing together different types of information (e.g., obtained using different instruments or measurement settings) - expands the ability to explore and investigate individual datasets in much greater detail.

To explore these large datasets, we have developed SpecXY, a user-friendly software solution for preparing, manipulating, exploring, extracting, and comparing spatially resolved spectral datasets. SpecXY can be used to visualise and classify spectra, perform peak deconvolution, and correlate spectral data with chemical data (e.g., from EMPA, LA-ICP-MS) or other numerical data of the same area.

In this contribution, an application example is used to demonstrate the workflow implemented in SpecXY. Spatially resolved data sets are used to investigate the magmatic history of a single augite crystal. By combining spatially referenced FTIR imaging of clinopyroxene water content with spatially resolved quantitative chemical data (EPMA), it is possible to investigate the correlation between the components of these independent datasets, which can be used as a proxy to monitor the effects of fluid in magmatic processes. In the studied augite from Aetna, Italy, oscillatory zoning, and sector zoning in major and trace elements and preserved zoning in water content can be observed. A dominant correlation of water content with Al is present, supporting the role of Al as a key element facilitating the incorporation of H^+ cations. A secondary correlation of the water signal with other elements (e.g., Ti, Fe and Cr) can be observed.