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

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Spectroscopic analytical techniques such as Fourier Transform Infrared Spectroscopy (FTIR) are important in modern geosciences. In recent years there has been a shift from using exclusively single-spot analyses to 2-dimensional maps. The ability to combine multi-layer numerical datasets—bringing together different types of information (e.g., acquisition using different instruments or measurement settings)—opens up the possibility of exploring and investigating individual datasets in much greater detail. This approach also allows a better understanding of unknown systems by finding out correlations in the dataset with known references. However, when working with spatially resolved high resolution data, the amount of data increases significantly compared to single point measurements, making the data examination and data validation more challenging and time consuming.

In this contribution, two application examples are used to demonstrate the new workflow implemented in the SpecXY software. Spatially resolved datasets are used to investigate the metamorphic history of a multi-phase eclogite sample and the magmatic history of a single augite crystal. By combining spatially referenced FTIR imaging of clinopyroxene water content with spatially resolved quantitative chemical data (LA-ICP-MS), 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 various metamorphic and magmatic processes.

Metamorphic samples often show a diffusion profile in the water signal. However, samples from Cima di Gagnone (Central Alps, Switzerland) show preserved water zonation with a sharp contact. In the magmatic augite, oscillatory zoning, and sector zoning in major and trace elements and preserved zonation in water contents can be observed. A dominant correlation of water content with Al is present in both examples, supporting the role of Al as key element facilitating the incorporation of H+ cations. In the magmatic sample, a secondary correlation of the water signal with other elements (e.g., Ti, Fe and Cr) can be observed.

Finally, visualisation of the generated results for both examples is further demonstrated using classified multidimensional correlation matrices of these complex numerical data sets, allowing visualisation of the spatial distribution of gradients and correlations within the sample.