Evaluating detection limits, reconstruction algorithms, and self-absorption in X-ray fluorescence tomography of minerals

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In the geosciences, low detection limits for many elements, non-destructiveness, and possibility to combine the results with other X-ray modalities [1], make X-ray fluorescence computed tomography (XRF-CT) an attractive characterization technique especially for rare samples, e.g. extraterrestrial matter [2] or shocked or Hadean zircons.

However, XRF-CT reconstructions of minerals are influenced by self-absorption of the fluorescence X-rays, limiting the size of sample in which a given element can be reliably quantified. Since self-absorption is a function of both the energy of fluorescence X-rays, and the X-ray attenuation properties of the sample, also detection limits vary from one experiment to the next. We will evaluate strategies of correcting for self absorption and determining absolute trace element concentrations from synchrotron nanobeam XRF-CT data. In the case of zircon, the spectrum from the sample can be compared to a known standard (figure) in order to estimate the overall trace element concentrations, and a priori knowledge of the sample composition utilized in order to correct for absorption effects. In terms of reconstruction strategy, both channel-wise reconstruction (i.e. hyperspectral imaging), and fitting of XRF spectra prior to algebraic reconstruction offer advantages as well as drawbacks.

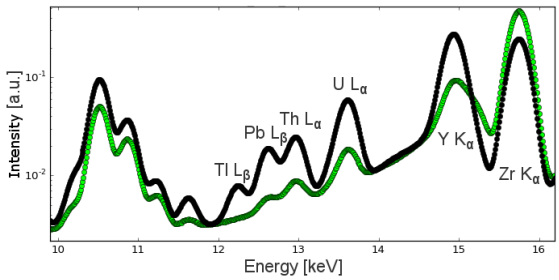

Figure 1: XRF spectra showing trace element enrichment in a Paleoproterozoic zircon (black) compared to the zircon 91500 standard (green).

[1] Suuronen & Sayab (2018), *Sci. Rep.* **8**, 4747. [2] Hanna & Ketcham (2017), *Chem. Erde* **77**, 547-572.