Interrogating LA-ICP-TOF-MS Mineral Maps: Methods and Applications to Critical Metal Research

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Efficient and sustainable extraction of critical metals as by-products or from legacy mine waste requires a thorough understanding of the deportment of the metals of interest and penalty elements. LA-ICP-MS mapping is well suited for deportment studies, and time-of-flight (TOF) LA-ICP-MS systems make it possible to measure nearly all elements from single laser pulses at speeds up to 100 times faster than possible with quadrupole systems. Because nearly all elements are measured, each pixel can be grouped into prospective mineralogical classifications. Interpreting these large high-dimensional data sets benefits from novel data science approaches, such as machine learning algorithms.

We present an app (LazAbMapper) written in Python with a Shiny user interface, implementing some of the vast number of algorithms available in the Python ecosystem. Highlights of LazAbMappers's functionality include: 1) displaying and exporting single maps, composite RGB maps, maps calculated from multiple elements, and multi-map panels; 2) classifying minerals using library matching, compositional criteria, or K-means clustering; 4) selecting regions of interest and extracting their compositions; 5) performing statistical analyses of the data using a variety of algorithms.

We demonstrate LazAbMapper's capabilities using a map of a magnetite crystal with silicate inclusions from the Kara deposit in Tasmania. Data were collected at CODES Analytical Laboratories with a Tofwerk icpTOF R and RESOlution-SE laser ablation system using a 12 µm square beam scanning at 360 µm/s, firing at 30 Hz. Spectral baseline subtraction was performed with Tofware software, and data were reduced using LADR's new imaging capabilities. Nearly all pixels were classified as either magnetite or silicates. Sn, V, and Ti are hosted primarily in magnetite, with Sn exceeding 1200 ppm in some zones. Cu and Zn occur primarily in the silicate phases and in some magnetite domains. Small inclusions of calcite were identified.