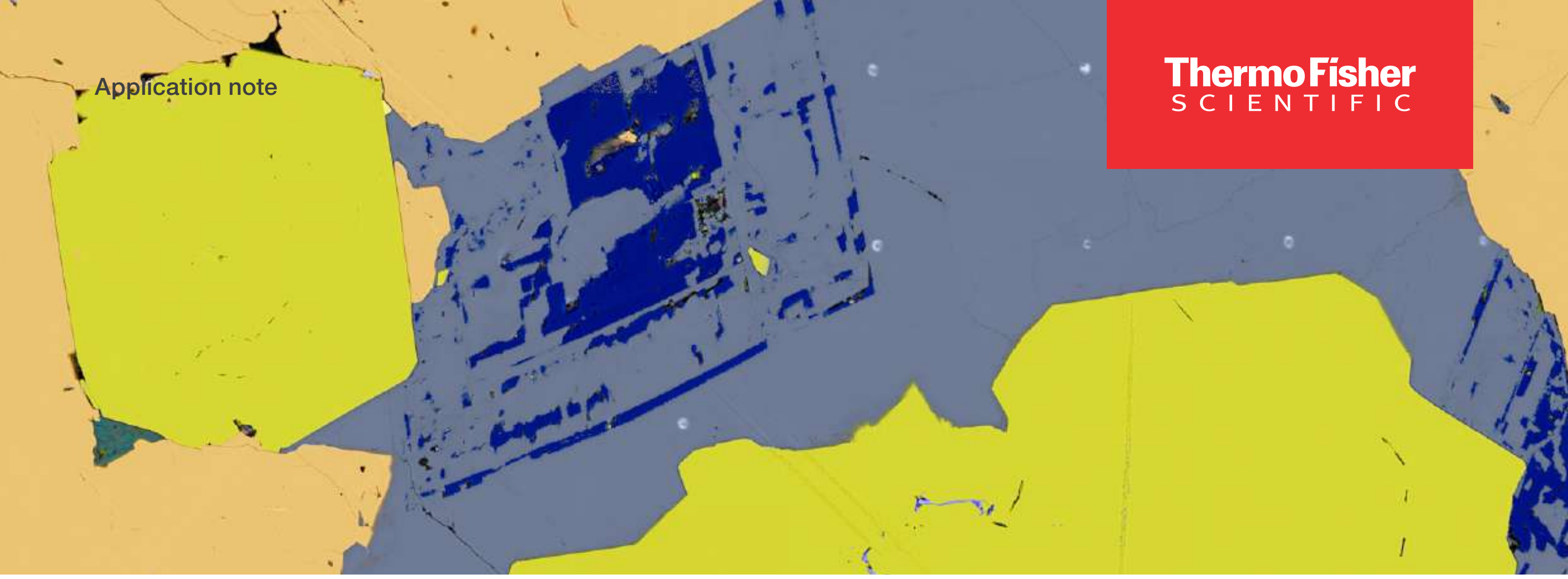
Application note



Enhancing mineralogical analysis of critical minerals with Maps Min Software

Case studies and technological innovations

The importance of critical minerals in the current economy and energy transition

The term “critical minerals” encompasses any minerals and metals that are considered essential to a nation’s economy and security, whether they are used for the manufacturing of high-tech devices and renewable energy technologies, or are leveraged for defense applications and various industrial processes. The “critical” designation is typically based on a mineral’s importance to the economy, the risk of supply disruption, and the lack of substitutes. Many countries define their own lists of critical minerals and elements, which commonly include the rare earth elements (REEs) along with cobalt, lithium, graphite, and nickel.

Examples of critical minerals

Rare earth elements are essential for the production of high-tech devices, renewable energy technologies, and advanced defense systems. For example, REEs are critical components in the permanent magnets that are used in wind turbines and electric vehicle motors, as well as in the phosphors of light sources and displays, and in the catalysts used for petroleum refining. The demand for REEs is expected to continue to grow significantly as the world transitions to a low-carbon economy, making the security of their supply chains a strategic priority for many nations.

Cobalt plays a crucial role in the production of rechargeable batteries due to its uniquely high energy density and thermal stability. In particular, it is used in lithium-ion batteries, which are pivotal for transportation and renewable energy applications. The increasing adoption of electric vehicles and the expansion of renewable energy infrastructure are driving higher demand for cobalt, highlighting the need for sustainable and ethical sourcing practices.

Columbite-tantalite, commonly known as coltan, is a vital source of niobium and tantalum, which are utilized in the production of electronic components, such as capacitors and high-power resistors. Additionally, tantalum’s high melting point and corrosion resistance make it valuable in aerospace and medical applications.

The strategic importance of these minerals underscores the need for advanced mineralogical techniques that help ensure efficient and responsible resource utilization. Thermo Scientific™ Maps Min Software is an automated mineralogy solution that pairs with scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDS) technology. It provides highly accurate and detailed mineralogical and textural characterization through fast automated acquisition, intuitive data validation and visualization, along with an easy-to-use UI for reporting and data interrogation. This application note explores some of the ways in which Maps Min Software can provide invaluable insights for the mineralogical characterization of complex, critical mineral ores.

Case study 1: Coltan solid solution

Maps Min Software is well-suited for the analysis of complex solid solutions, as it can synthetically predict the spectrum of any intermediate composition using its Mixel spectrum deconvolution algorithm and solid solution support. This allows the software to automatically determine which proportions of the end members give the best spectral match for the measured spectrum and, as a result, you do not have to create separate definitions that cover the entire solid solution range, which simplifies mineral library creation and management.

In this example, the advanced spectrum deconvolution of Maps Min Software was used to accurately identify and quantify the compositions of different columbite-tantalite species within its four end-member solid solution (Figure 1). This approach is essential for understanding a deposit's economic potential and processing behavior. The ability of Maps Min Software to handle complex chemistries and mixed spectra is particularly beneficial for the analysis of solid solutions, such as the coltan sample shown here.

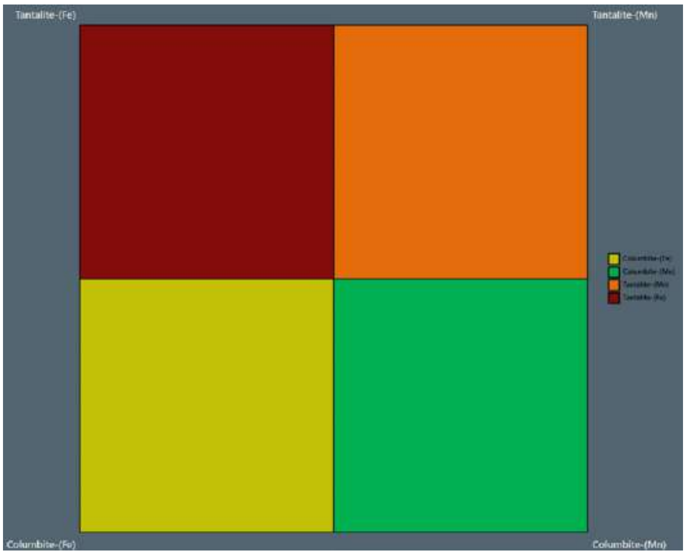


Figure 1. Visualization of the columbite-tantalite solid solution in the Mineral Reference Editor of Maps Min Software.

To demonstrate the accuracy of this approach, a synthetic test sample was created from a blend of different intermediate members of the coltan solid solution. These were mixed, in known weight percentages, together with spodumene and river sand to introduce variability. For data validation, the chemical composition of the sample was determined by ICP-OES bulk quantification and compared to the Maps Min results. A cross-section of the particle mount was used to help ensure that results were representative, accounting for any density or particle-size segregation that may have occurred during preparation. A total of 177,812 particles were acquired using a grid map with 4 µm point spacing; at least 4,000 X-ray counts were obtained at each EDS acquisition point (Figure 2).

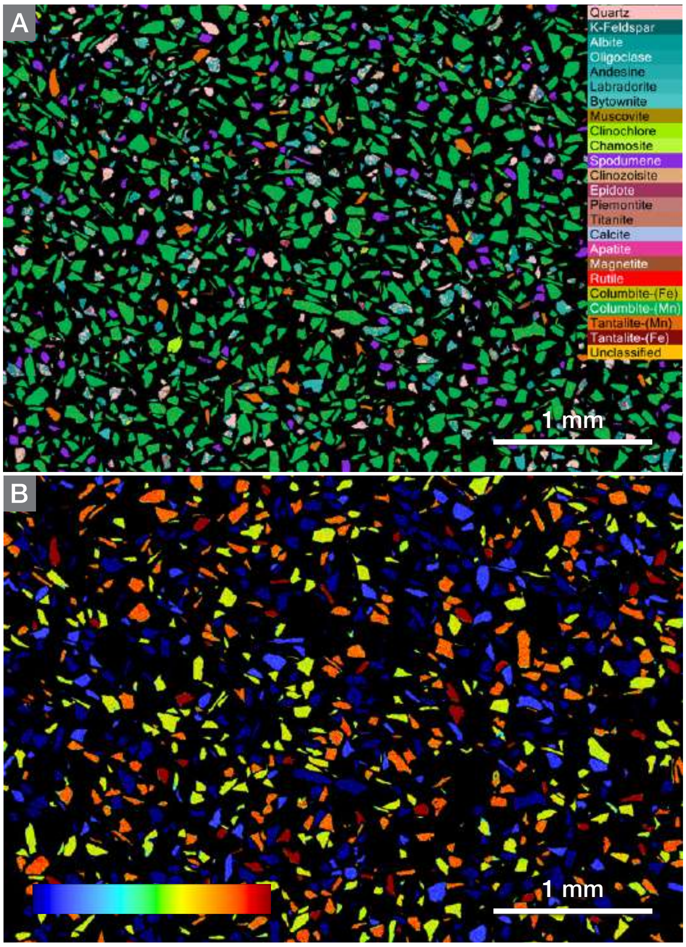


Figure 3. A close up of the mineral map shown in Figure 2. A) Mineralogy map. B) Tantalum elemental map, where blue is low concentration and red is high concentration. The tantalum distribution map highlights the presence of multiple compositions within the columbite-tantalite solid solution.

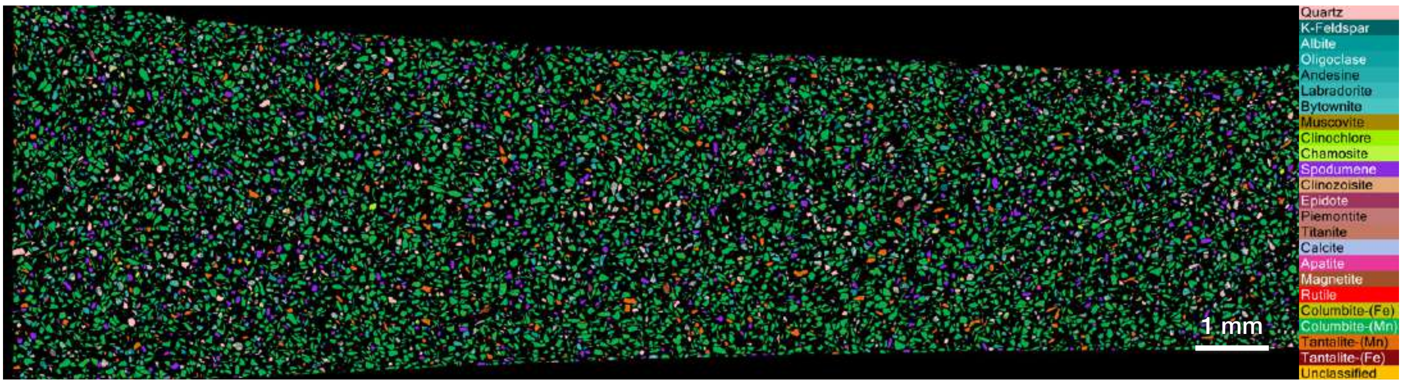


Figure 2. Mineral map obtained in Maps Min Software, showing 177,812 particles in a synthetic coltan sample. The different columbite-tantalite compositions can be seen throughout the specimen.

Resolution of complex solid solutions

The accurate characterization of this columbite-tantalite sample highlights how Maps Min Software can resolve solid solutions with up to four end members. This capability is crucial for distinguishing between the various compositions within a solid solution series and, ultimately, for understanding the economic value of a given deposit (Figure 3).

True bulk elemental assay

After classification, all spectra from the same mineral are added together to create a sum spectrum. Maps Min Software then performs a proprietary standards-based element quantification on each sum spectrum to calculate the true elemental composition of the sample. This helps ensure that the elemental assay and deportment results are accurate and can be used confidently to make decisions (Figure 4).

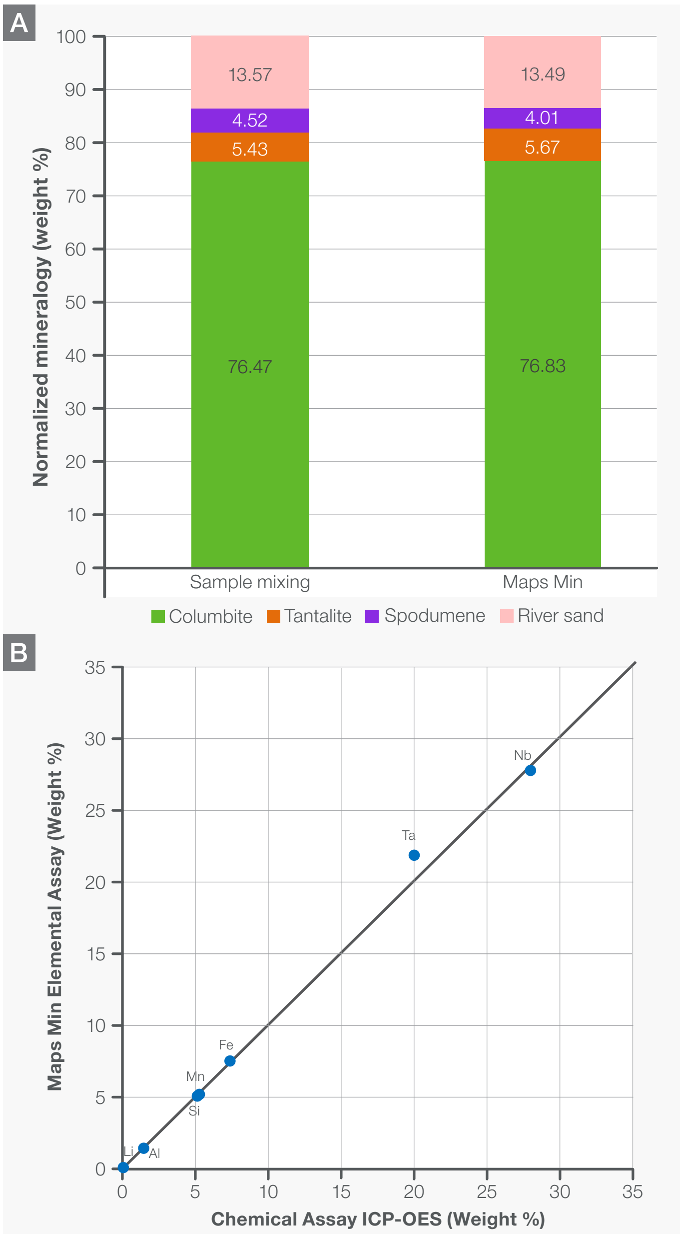


Figure 4. A) Mineral proportion comparison for the synthetic coltan sample, showing the known mixture components and the modal mineralogy obtained with Maps Min Software. B) Assay reconciliation of the ICP-OES chemical assay and Maps Min elemental assay results.

Spodumene classification and lithium quantification

Spodumene, a primary lithium ore mineral, can be detected with Maps Min Software, even though EDS can only directly identify elements with an atomic number higher than boron, and therefore cannot obtain a lithium peak. Despite this limitation, Maps Min Software can still correctly classify Li-bearing phases by matching the portion of the spectrum that can be seen (i.e., without the Li peak or any other light element peaks). The lithium concentration in spodumene is inferred based on the mineral's stoichiometric Li content, while all elements above oxygen are directly quantified from the sum spectrum (Figure 5). This comprehensive analysis can provide accurate assessment of lithium-bearing minerals together with any other minerals in a sample.

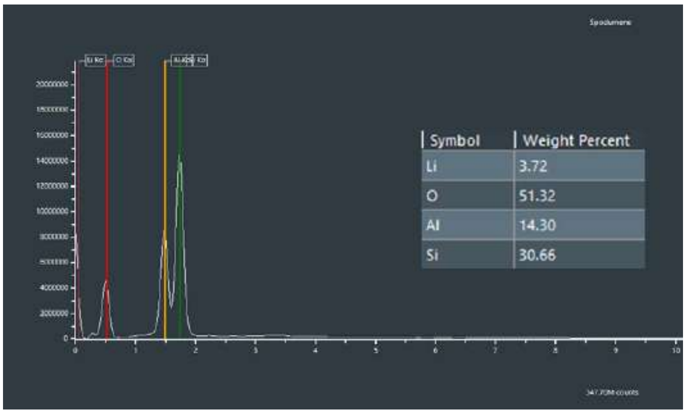


Figure 5. Sum spectrum and elemental quantification of spodumene in the coltan sample.

Case study 2: Characterization of an REE ore

In this example, an ore sample containing two REE-bearing minerals, bastnasite and monazite, was analyzed (Figure 6). Such ore samples are challenging mineralogical specimens as REE-bearing minerals are chemically complex, resulting from the tendency of rare earth elements to replace each other in a mineral's crystal structure. For example, monazite can have variable amounts of multiple REEs, as well as thorium (Th) and uranium (U). Monazite rich in cerium (Ce) is most common; lanthanum (La) and neodymium (Nd) are generally also more abundant in monazite than the other REEs. As a result, a simplified solid solution with monazite-(Ce), monazite-(La), and monazite-(Nd) end members is generally used by Maps Min Software (Figure 7) to classify the chemical variations in this mineral (Figure 8). Additional rare earth elements, as well as Th and U, are also accounted for as potential substitutions or trace elements within this solid solution.

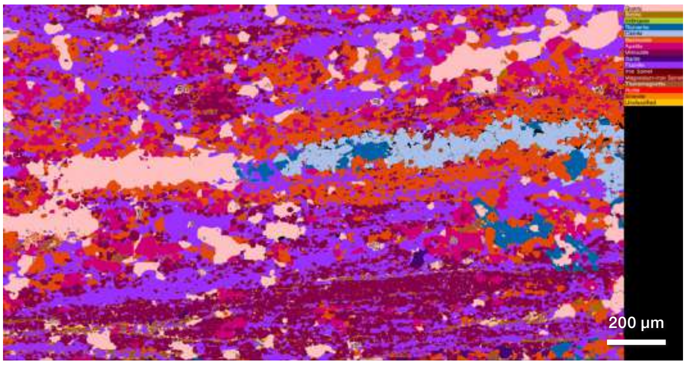


Figure 6. Mineralogy map of an REE ore sample containing bastnasite (orange) and monazite (dark magenta), obtained with Maps Min Software.

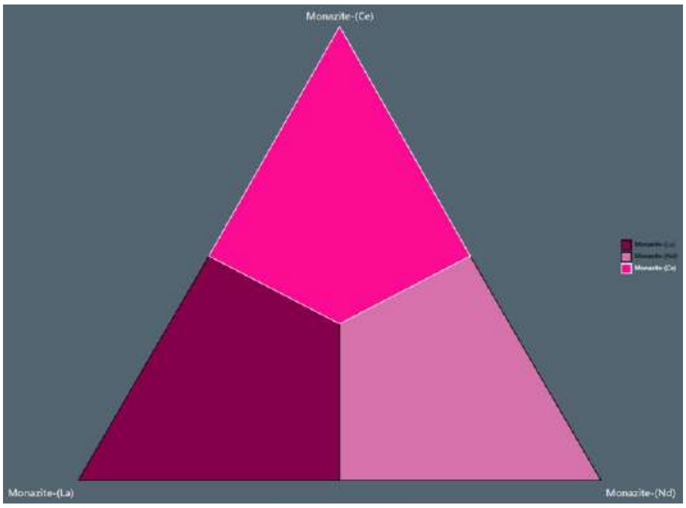


Figure 7. Monazite solid solution with Ce-rich, La-rich, and Nd-rich end members. Only the end members of a solid solution series need to be included in a mineral recipe; Maps Min Software automatically interpolates any other compositions within this space.

Elemental deportment and spatial distribution

Maps Min Software reports not only the deportment of elements of interest (i.e., particular REEs, as shown for neodymium in Figure 9), but also high-resolution textural information for the REE minerals, including grain size distributions and associations with other minerals. Such detailed information can be obtained from rock sections (e.g., core samples), polished thin sections, or particulate material.

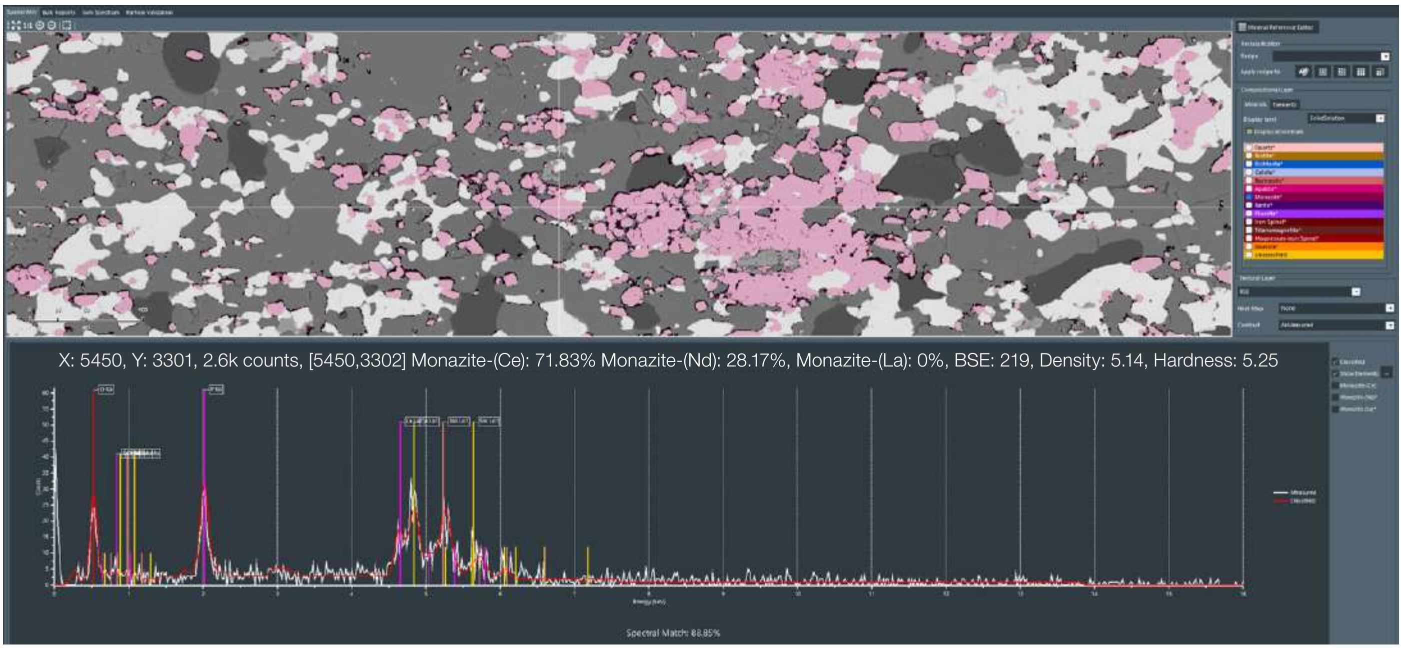


Figure 8. Data validation in the interactive Nanomin interface of Maps Min Software. The monazite map (pink) is superimposed on the BSE layer. A measured spectrum, obtained at a point within a Ce-rich monazite grain, is shown along with its interpolated classification within the monazite solid solution.

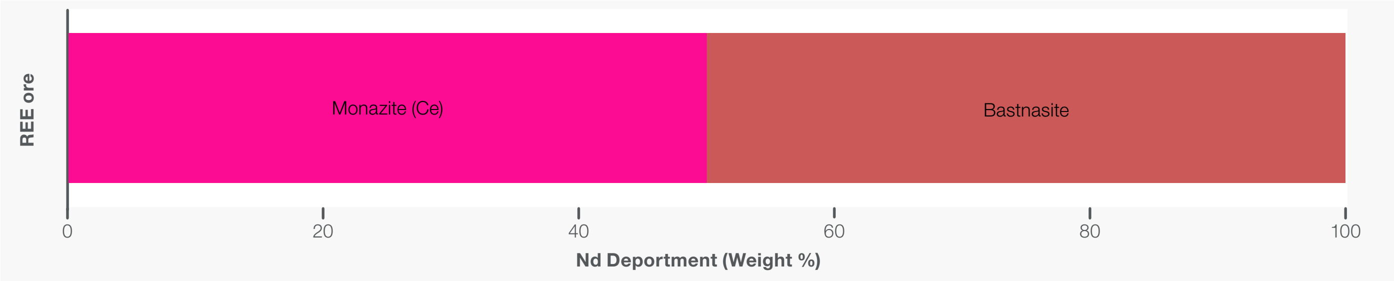


Figure 9. Deportment of neodymium between bastnasite and monazite in the REE ore sample.

Grain chemistry quantification

The Grain Chemistry Quant feature in Maps Min Software can quantify the composition of each monazite grain by creating a sum spectrum from the individual low-count spectra in each mineral grain. The proprietary standards-based quantification is then applied to these grain sum spectra, providing valuable insights into the compositional variations within a sample, or across samples (Figure 10).

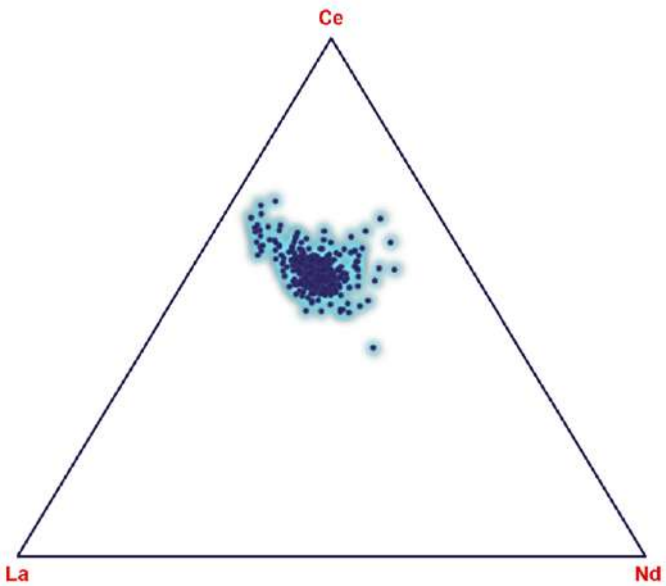


Figure 10. Ternary diagram visualizing the relative proportions of Ce, La, and Nd in the monazite grains of the REE ore sample. Data was obtained with the Grain Chemistry Quant feature in Maps Min Software; only grains with a sum spectrum of at least 10,000 X-ray counts are included.

Case study 3:
Cobalt-bearing pyrite

Cobalt (Co) is typically a by-product of mining copper, nickel, or other metallic sulfide ores. Common cobalt ore minerals include carrollite, cattierite, linnaeite, cobaltite, skutterudite, smaltite, and erythrite. Cobalt-bearing pyrite is also a potential source, but understanding the distribution and concentration of cobalt within the pyrite grains is essential for optimizing extraction processes and cobalt recovery.

Long count trigger for improved elemental detection

A long count trigger can be set for specific minerals or solid solutions in Maps Min Software in order to improve the detection of low elemental concentrations. This features facilitates the acquisition of more X-ray counts for those target phases, reducing spectrum noise and improving the accuracy of classification and elemental quantification. For all other phases, fewer X-ray counts are collected at each EDS acquisition point. This approach optimizes spectral sensitivity only where it is needed, with minimal impact on overall measurement times (Figure 11).

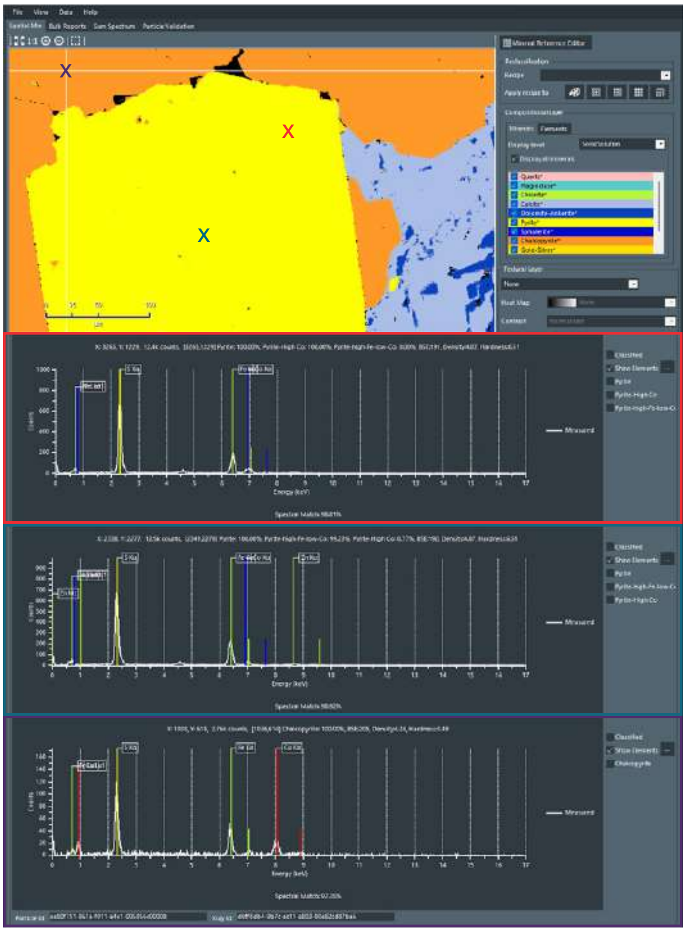


Figure 11. 12,000-count spectra of pyrite, which allows for the differentiation of cobalt-bearing pyrite (marked with a red X) and pyrite with little or no cobalt (blue X). For all other minerals, spectra with lower X-ray counts were acquired; for example, only 2,800 counts were obtained for chalcopyrite (purple X).

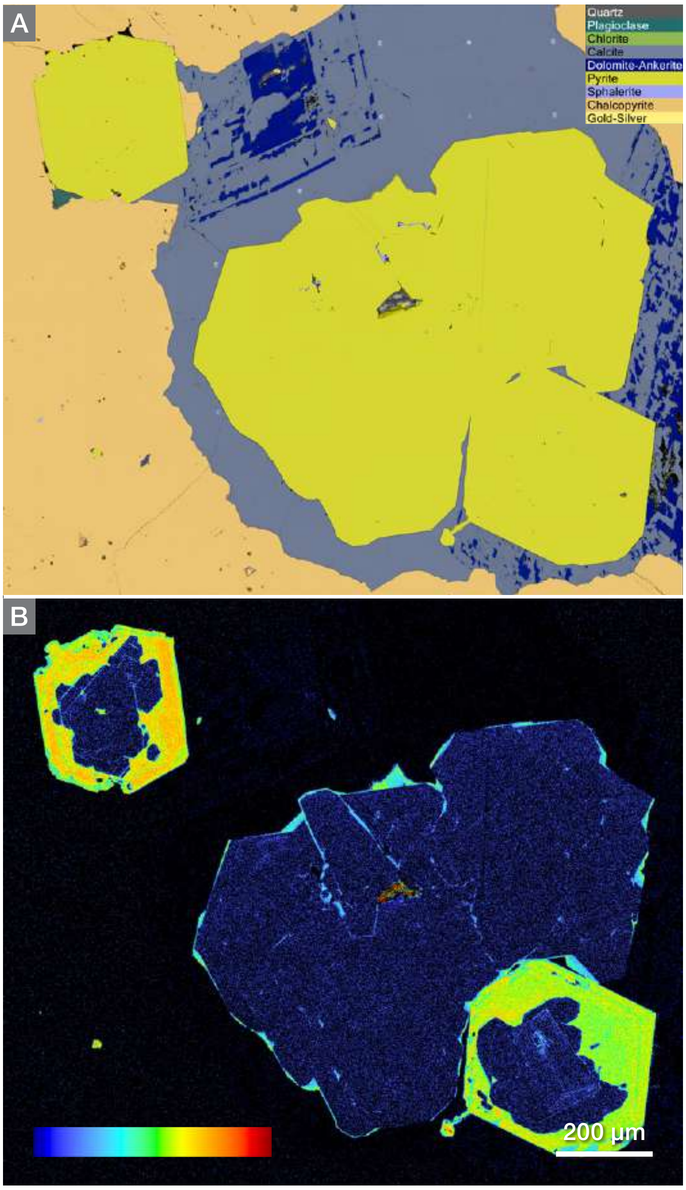


Figure 12. A) High-resolution mineral map of several Co-bearing pyrite grains (yellow) with BSE overlay. B) Cobalt elemental map showing the heterogeneous distribution between, and within, the pyrite grains.

Quantification and visualization of cobalt

Maps Min Software can quantify cobalt concentrations down to approximately 0.3 wt%, providing accurate measurements, even in complex matrices. The software can also visualize the spatial distribution of cobalt across the sample or within a mineral. In this case, areas of higher and lower concentration could be highlighted in the pyrite grains, revealing the heterogeneous nature of the cobalt distribution (Figure 12).

Enhanced analysis with ICP-MS

For cases where cobalt concentrations are below the detection limit of EDS analysis, a workflow incorporating laser-ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) can be applied. This technique enables highly sensitive and accurate measurement of trace elements, providing comprehensive characterization of samples such as cobalt-bearing pyrite. Here, the pyrite grain coordinates and their compositions were extracted from the dataset with the Grain Chemistry Quant feature in Maps Min Software. Fiducial marks on the holder or sample surface can be used to easily transfer the coordinates obtained in Maps Min Software to the LA-ICP-MS coordinate system. This allows for automated point analysis of the same grains. It is also possible to export the coordinates and quantify the composition of a circular area in the grains based on a user-defined diameter that matches the size of the laser, thereby correlating the data to the exact location where the LA-ICP-MS analysis is acquired.

The ability of Maps Min Software to handle variable chemistries is crucial for the accurate analysis of cobalt-bearing pyrite. The software can differentiate between pyrite with varying cobalt contents, providing detailed insights into the mineral's composition and distribution. This capability is essential for understanding the economic viability of cobalt extraction and for the optimization of processing techniques.

Conclusion

Thermo Scientific Maps Min Software builds on previous QEMSCAN and MLA Software from Thermo Fisher Scientific, providing an innovative solution for both research and industrial applications that features enhanced mineral characterization, automation, and data analysis.

Maps Min Software supports advancements in mining, resource exploration, and environmental monitoring, helping you meet the challenges of the increasingly complex ore deposits that are being discovered and developed today. The integration of Maps Min Software in geological analysis not only enhances the accuracy of mineral characterization but also supports the sustainable development of critical mineral resources. This is essential for meeting current, growing mineral demands and facilitating the global energy transition.

Learn more at **thermofisher.com/maps-min**