Maps Mineralogy Software for QEMSCAN Software users

Thermo Scientific™ Maps Mineralogy Software is a new data processing suite tailored for mineralogy applications and built on the widely used Maps Software platform from Thermo Fisher Scientific.

Maps Mineralogy Software features novel mixel technology that works differently from the spectral engine algorithm of QEMSCAN Software, formerly produced by FEI. One of the most significant differences is the best-match principle used in Maps Mineralogy Software, compared to the first-match principle used by QEMSCAN Software. The first-match principle increases the risk of misclassifications, as a better fit may be lower down the list of entries, making results highly dependent on how you organize the QEMSCAN SIP entries.

QEMSCAN SIP entries use elemental ranges that encompass all elements that must be (or may be) present in the spectrum for classification. These ranges are rectangular regions in n-dimensional compositional space, while the true variation in the photon count of the elements tends to have a cloud/ ellipse-shaped distribution (Figure 1). This is mainly caused by statistical variations in the photon counts that result from the low-count energy-dispersive spectroscopy (EDS) spectra that are used for automated mineralogy analysis. Minerals of similar chemistry tend to have an overlap of these distribution clouds, and consequently so do the specified elemental ranges in the SIP entries (Figure 2). In such cases, the sequence in which the SIP entries are placed can significantly influence the accuracy of the classification.

In QEMSCAN Software, the peak heights (or peak height ratios) in the spectrum are compared to the elements and their ranges within the SIP definitions. However, Maps Mineralogy Software compares the entire spectrum to the spectra of the minerals in the recipe, and all the spectra in the list, independent of sequence, leading to fewer misclassifications.
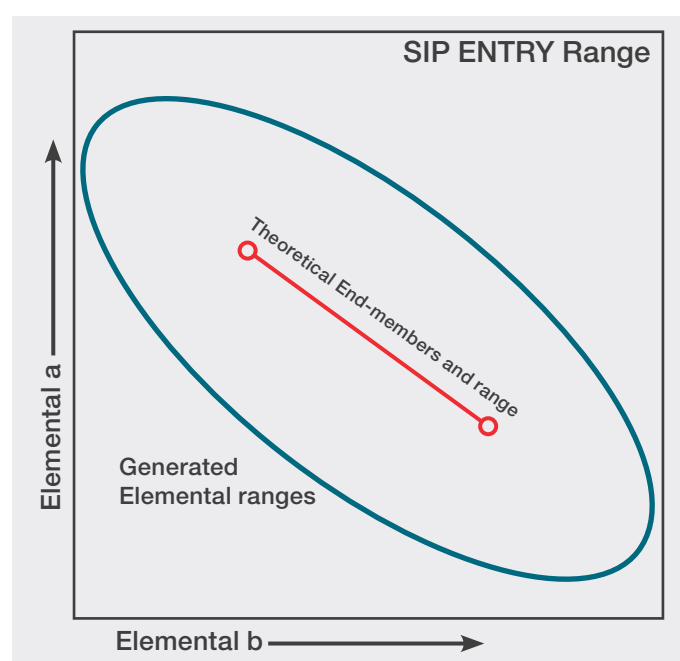

Figure 1. Schematic representation of a mineral in 2D composition space. The theoretical and observed compositional ranges differ due to the variation in elemental ranges at low X-ray counts during a classical, automated mineralogy acquisition.

QEMSCAN Software users have the option to minimize elemental ranges in SIP entries by dividing large ranges into multiple SIP entries, each with a smaller sub-range. However, this can be a time-consuming process, and will not capture all measured spectra. (E.g. when element A falls in the small range of SIP entry 1, while element B falls in the small range of SIP entry 2 for the same mineral, as demonstrated in Figure 2.) Creation of such narrow SIP entries becomes more complex with more than two element interactions/substitutions (e.g. spinel, pyroxenes, or garnets). The actual overlaps between SIP entries are always user dependent.
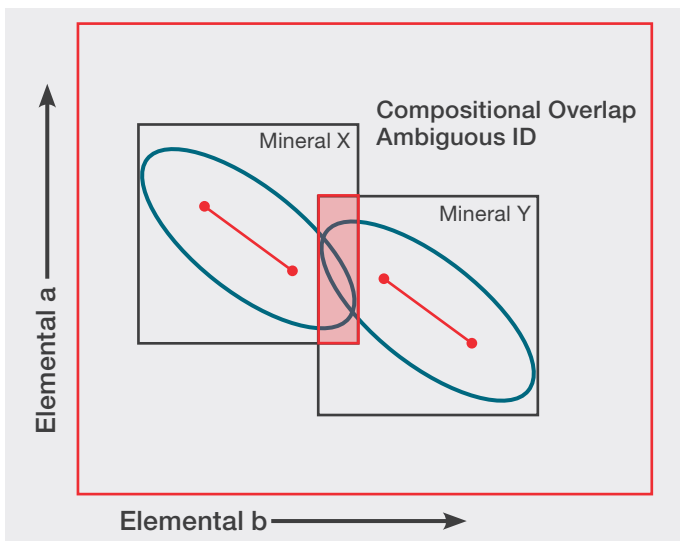
Figure 2. Schematic representation of two SIP entries in binary compositional space. It is common for SIP entries to overlap, making accurate mineral ID strongly dependent on the ordering of mineral entries in the SIP list. Overlaps become more common and complicated as the number of compositional dimensions increases.

Maps Mineralogy Software uses a modern algorithm that makes the most of current computing capabilities as well as high-quality EDS signal and throughput. This allows for a unique, next-level AM mineral classification system, that is ahead of most commercially available technologies.

During spectrum matching, the algorithm automatically deconvolutes each measured spectrum to determine whether it was collected on a single phase or is the result of the electron-beam interaction volume spreading across multiple phases. For the latter, Maps Mineralogy Software matches the deconvoluted spectrum to the phases that are present and reports their relative proportions within the spectrum. This results in highly accurate classification for each measurement point, adding a layer of detail that would otherwise be unavailable.
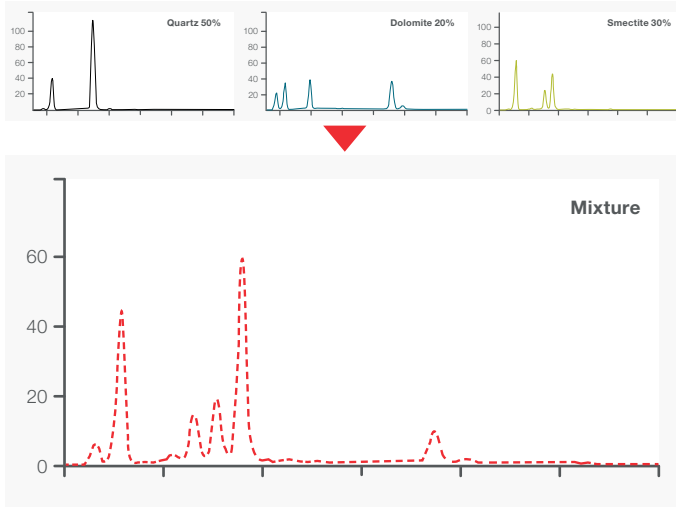

Figure 3. Simplified example of the mixel algorithm at work. At grain boundaries, within fine-grained samples, and within complicated mineral textures, mixed spectra are common due to the generated X-rays sampling multiple phases within the electron beam-sample interaction volume. The mixel approach accurately identifies the phases that make up a mixture and generates a relative proportion of each phase identified.

Mixel technology is especially powerful and valuable for samples that contain fine-grained sub-pixel phases and boundary textures, such as: shales and mudstones, microcrystalline groundmasses in volcanic rocks, cryptocrystalline rocks, and small inclusions.

The deconvolution also allows for the accurate identification and quantification of sub-species in solid-solution series, including compositional zonation (e.g. plagioclase, chromite-spinel), and trace or minor element substitutions (such as arsenic in pyrite or iron in sphalerite).

Within QEMSCAN Software, individual phase composition ranges must be defined for the various sub-species (e.g. plagioclase). Mixtures would then have to be manually built out of additional phases until a sufficient quantity has been defined, as determined by the user. Finally, the phases and mixtures have to be ordered properly to capture the correct analysis. As with general mineral ID, the ordering of the mineral list is perhaps the most objective and error-prone step for this kind of phase ID methodology.

Maps Mineralogy Software, meanwhile, automatically detects which sub-species of a solid-solution are present in the sample; you are only required to add the solid-solution end members to the mineral library and to link them as a solid-solution series. There is no need for you to add intermediate compositions as separate mineral definitions, as the software will automatically determine the composition of the sample using its mixel spectrum deconvolution.
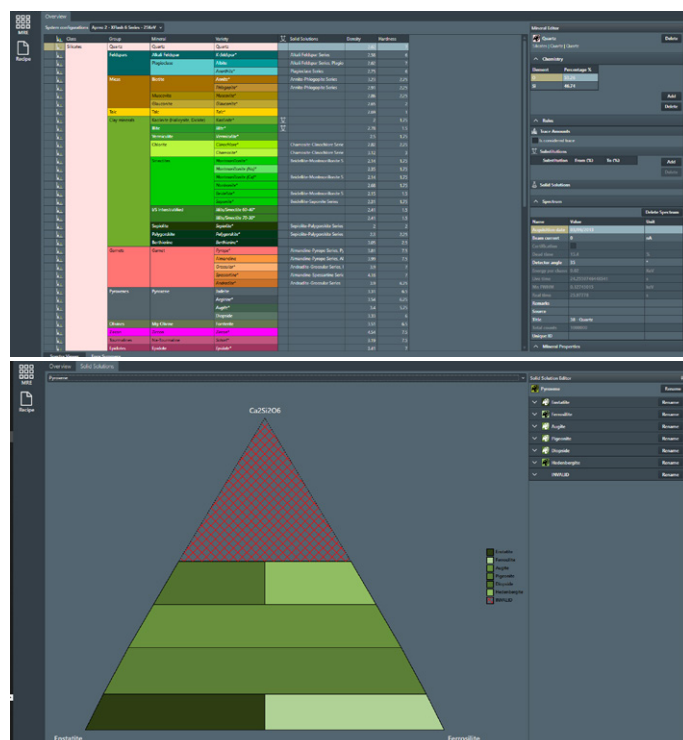

Figure 4. Top: Screen capture of the Mineral Reference Editor (MRE). The UI can be used to generate new recipes for specific samples/ore types and to customize mineral entries based on color, physical properties, etc. The MRE can also be used to hone specifics around trace elements, solid solution definitions, and to create new mineral species. Bottom: Intermediate solid solution species identification including "impossible" regions for a partial solid solution.

For mixed spectra (e.g. at grain boundaries or in fine-grained materials), the deconvolution process automatically identifies and quantifies the separate mineral species contributing to the mixed spectrum, without the need for you to add infinite mixed spectra or boundary texture definitions.

Because of the way that the spectral matching works, mineral phase ID becomes increasingly accurate with longer EDS dwell times, without any changes/input required. This differs from QEMSCAN Software, in which running a SIP designed for 1000-count analysis at 2000 counts does not automatically improve accuracy.

In the example shown in Figure 5, the user only needed to add the end members of the series (albite and anorthite) to the MRE (if they are not already in the overview list of mineral species) and then indicate that these two minerals form a solid-solution series.

Once the series is available in the overview list of mineral species, it can be added to any recipe (with any system configuration) for classification/analysis. During classification, Maps Mineralogy Software will identify when a spectrum belongs to this solid solution series and allocate the appropriate sub-species to the classification.
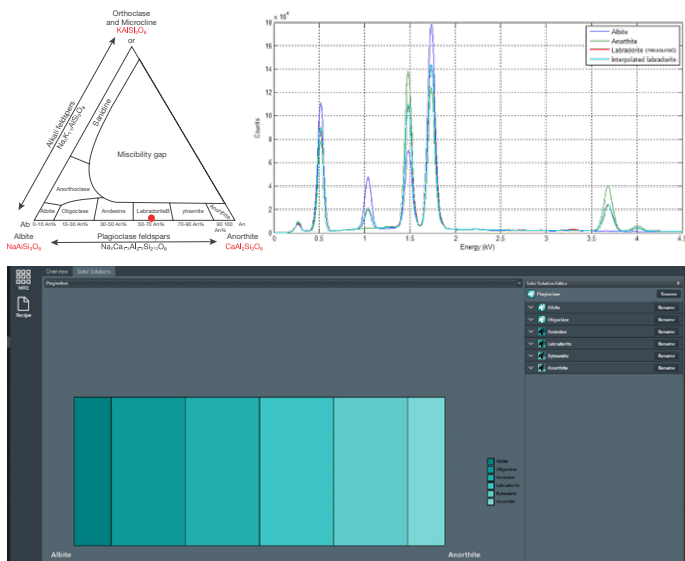

Figure 5. Top: Example of the intermediate solid-solution fitting process applied to an unknown phase. Only the end members of a solid solution definition are needed to correctly identify all intermediate species. The mixel algorithm automatically identifies the intermediate species by mixing proportions of the end member phases. Labradorite is correctly identified and automatically added to the mineral list. Bottom: Plagioclase feldspar.

By contrast, QEMSCAN Software users would need to create separate SIP entries for the end members as well as the intermediate compositions of a solid-solution series, and also adjust these definitions to work on real, measured data. It would be up to you to decide how many intermediate SIP entries to create; the more sub-species definitions, the narrower the elemental ranges can be and the lower the chance for potential misclassifications of similar phases. This would, however, require more work and testing. If only a limited number of subspecies are defined, the risk increases that entries with broader ranges may capture measurement points of different minerals containing the same elements.
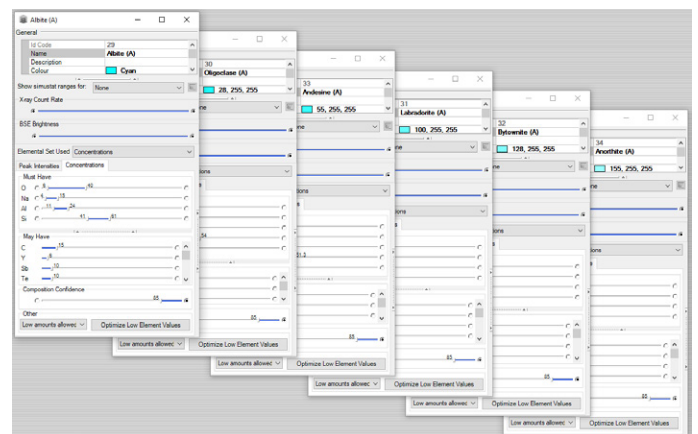

Figure 6. Example of the number of individual species that must be generated in QEMSCAN Software to cover the albite-anorthite solid solution. Each of these entries must then be used to generate common mixed spectra that may be encountered during the analysis.

The approach for classifying boundary textures or mixed spectra of any kind (e.g. fine-grained intergrown phases, grain boundaries, small inclusions) is similar to the solid-solution approach in QEMSCAN Software: you need to define SIP entries for intermediate "compositions" of the two (or more) phases (generally creating two intermediate definitions works well), and adjust these to work with real measured data.

This process can be time consuming, as there are nearly unlimited possibilities for such boundary textures in rock samples. The adjustment and testing process also needs to be carried out conscientiously to ensure the SIP entries correctly classify the intended boundary textures and that they are not capturing any pure mineral spectra. The sequence of these boundary texture definitions is therefore very important.

QEMSCAN Software also offers the Boundary Phase Preprocessor to filter out any boundary texture definitions or misclassifications on boundary textures after analysis.

In Maps Mineralogy Software, this process is all done automatically by the mixel algorithm, and no input is needed in the mineral recipe. The only requirement is a quality control check of the data to ensure that no real mineral phases are being misclassified as mixed spectra. (Several settings in the recipe can be adjusted to avoid/reduce this.) You could also remove a mineral definition of the incorrect mixed spectrum from the recipe altogether, if the phase does not occur in the samples analyzed.
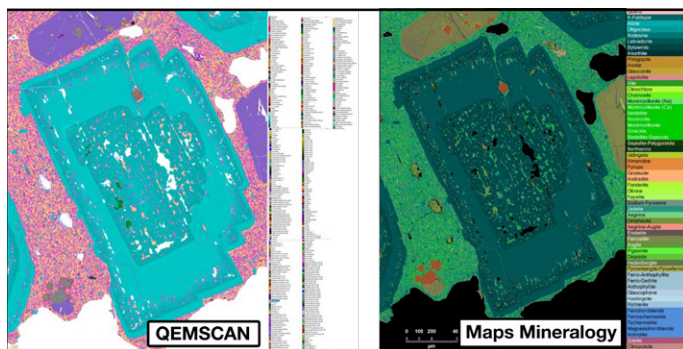

Figure 8. Comparison of the same plagioclase porphyroclast within a fine-grained volcanic matrix. The QEMSCAN mineral list (left) is extremely long due to the number of mixed spectra and subspecies necessary to limit the number of unclassified spectra in the sample. Maps Mineralogy Software (right) derives a much more straightforward mineral list that is easy to interpret, even if you are not an expert in the software. While quality control of data is still required in Maps Mineralogy Software, the focus is more constrained and takes less effort than QEMSCAN Software.

In addition to improved phase ID accuracy and objectivity, elemental output is more robust within Maps Mineralogy Software. In QEMSCAN Software, an elemental based report or image (e.g. deportment, assay, etc.) is based on mineral compositions saved in the mineral list. Elemental output is not representative of the sample itself. Within Maps Mineralogy Software, elements are quantified using the internal standards built into the MRE. Additionally, a sum spectrum is generated for every mineral present in the sample. This output permits identification of trace elements that would otherwise be impossible to see with the relatively small number of X-rays taken at each point. Once summed, the software uses a standards-based quantification on the spectra and outputs a more accurate elemental assay that is representative of the sample composition. Finally, all elemental maps are also generated based on the true elemental signature of the sample.
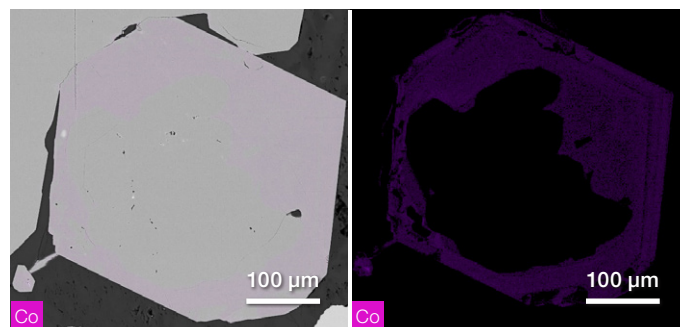

Figure 9. Left) Cobalt elemental map overlain on a pyrite grain. Right) Intensity map of cobalt distribution within pyrite. Maps Mineralogy Software outputs true EDS maps that are representative of the actual elemental distributions within a sample. QEMSCAN Software could also generate elemental maps, however, these would be based on back-calculated compositional information. Therefore, trace or atypical elements would not be captured in a standard acquisition.

Conclusions

The QEMSCAN SIP list can be configured for solid solution series and boundary texture classification to achieve comparable results to the mixel algorithm of Maps Mineralogy Software. However, this would require substantial time and experience to set up in order to tweak the SIP list and its entries. Maps Mineralogy Software does this automatically while requiring very little user input or experience.

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