Maps Mineralogy Software for MLA Software users

Thermo Scientific™ Maps Mineralogy Software is a novel data processing suite tailored for automated mineralogy, based on the widely used Maps Software platform from Thermo Fisher Scientific.

Maps Mineralogy Software builds on our continued development and support of MLA and QEMSCAN Software, formerly produced by FEI, and seeks to make automated mineralogy truly "automated." While MLA Software has long been used for mineralogy applications, it requires a high degree of manual analytical work for challenging samples, as well as the maintenance of mineral reference signatures across systems, which can become increasingly difficult. The technology behind Maps Mineralogy Software aims to make mineralogical SEM-EDS (scanning electron microscopy-energy dispersive spectroscopy) data more objective, requiring less manual management of mineral lists and less quality control of results. Additionally, Maps Mineralogy Software seeks to be applicable to all ore/rock types, regardless of the sample's composition or textural complexity. In this application note, we present an overview of the similarities and differences between MLA and Maps Mineralogy Software and highlight how the newer product enables higher levels of accuracy.

Mineral identification approaches

At a high level, the spectral engines of both MLA and Maps Mineralogy Software are quite similar, as they are used to find the reference spectra in a mineral list that have the best statistical match to the shape of a measured EDS spectrum. Maps Mineralogy Software directly incorporates real world chemistry and chemical variations into the definition of a mineral species. It is not necessary to have an example of a mineral prior to quantifying it. MLA Software, meanwhile, is much more rigid, and requires that you have intimate knowledge of EDS spectral behavior.

The size of an MLA library is generally much larger than a Maps Mineralogy library, because MLA Software forces you to account for small variations in chemistry, X-ray photon counts, and beam voltages within mineral signature definitions.

Maps Mineralogy Software also uses a modern algorithm that makes the most of current computing capabilities. Notably, it does not tie mineral definitions directly to the EDS detector resolution (unlike MLA Software), which means that mineral definitions are independent of the EDS detector resolution on the SEM. With MLA Software, mineral definitions are tied directly to acquisition conditions (e.g., mineral definitions created at 400 kcps resolution will not work if you later upgrade to 600 kcps detectors). This makes Maps Mineralogy Software a unique, next-level AM mineral classification system (backed by 12 patents) that is ahead of most commercially available technologies. During spectrum matching, the algorithm automatically deconvolves each acquired spectrum to determine whether it was derived from a single mineral phase or was the result of the X-rays sampling multiple phases from within the electron-beam sample-interaction volume. It also automatically interpolates the intermediate chemistry from complete solid solutions like plagioclase, or incomplete solid solutions like pyroxene, by automatically quantifying positions within the solid solution. In the case of multiple phases contributing to the spectrum, 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.

Best-match spectral analysis

The best-match approach can be described as a probability gradient within n-dimensional composition space. Match probably is a measure of how well the measured spectrum fits against a saved spectrum in the mineral library, with a positive match indicated by the measured spectrum falling within a prescribed region of high probability. For example, in Figure 1, the measured spectrum matches, with high confidence, to the library spectrum of pyrite. For simple cases like this, the spectral analysis works the same for both MLA and Maps Mineralogy Software.
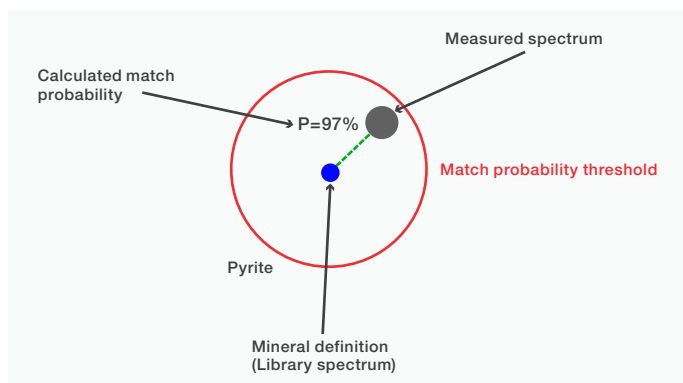

Figure 1. Phase match process used to fit a measured spectrum against a mineral definition (pyrite). The high match probability indicates a pure phase match.

Mixed spectra classification requiring manual operation in MLA Software

When a measured spectrum does not match a spectrum in the mineral library, it is marked as "unclassified." In MLA Software, these spectra can be addressed during post-processing, where it can be determined if the match failure is the result of a missing phase or a mixture of multiple minerals. A binary mixture of minerals can be manually specified (i.e. 25, 50, or 75% for each respective pair of phases). If there is still no match, the binary spectrum must then be added as a library entry in order to reclassify the dataset, or be left as an unclassified spectrum. You must manually create all intermediate mixed definitions by hand at fixed ratios, which quickly makes up a majority of the data analysis time.
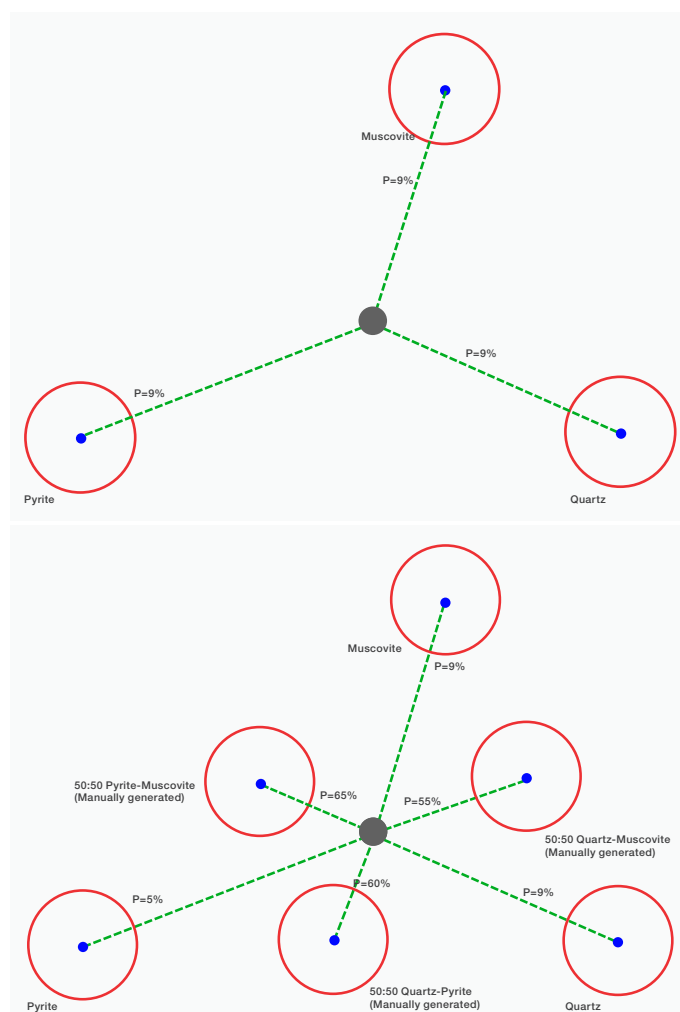

Figure 2. a) Measured spectrum falling outside 3 discreet mineral definitions. b) Manual mixing conducted in MLA Software to identify the three components of the mixture through a series of binary mixtures.

Mixel algorithm in Maps Mineralogy Software for mixed spectra classification

Maps Mineralogy Software uses a novel "mixel" approach for automated identification of multiple mixed phases in a measured spectrum. If the software does not initially find a match to a pure library spectrum, it will automatically begin mixing phases that have already been identified in the sample. This testing ends when the mixture with the highest spectral match has been identified; the proportions of each phase are then attributed to the pixel where the spectrum was recorded. This mixel-based spectral matching differs from MLA Software as it is a full-spectrum match approach that allows for deviations in the stored spectra, enabling a broader range of compositional variability per mineral entry. The degree of mixing is computed per-pixel, which allows boundary pixels between grains to be quantified; or growth zones to be observed.
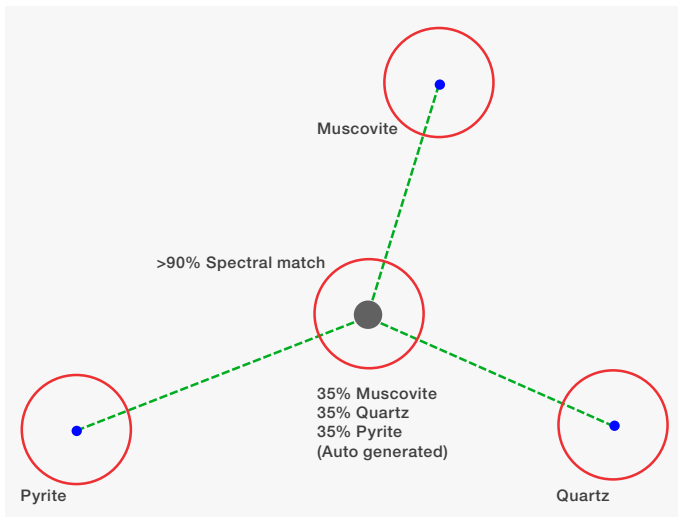
Figure 3. The mixel algorithm in Maps Mineralogy Software automatically compares the unknown spectrum against mixed phases consisting of pure mineral definitions found in the sample.

Mixel technology is especially powerful when investigating 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. Additionally, spectral deconvolution allows for accurate identification and quantification of sub-species in solid solution series, including compositional zonation (e.g. plagioclase, chromite-spinel), and trace/minor element substitutions (such as arsenic in pyrite or iron in sphalerite).

Handling of solid solutions

To create solid solution definitions in the MLA mineral library, you would measure spectra from each subspecies or use the STD to store standard spectra during acquisition. This is very time-consuming and complex for solid solutions that have more than two end members (e.g. pyroxenes or garnets). Further, mixed pixel phases of pyroxene with other minerals like quartz are equally possible within the sample but require even more time from the operator to define.

Maps Mineralogy Software, meanwhile, automatically detects which sub-species of a solid solution is present in your sample; you are only required to add the solid solution end members to the mineral library and link them as a solid solution series. For complex (more than binary) solid solutions, the composition space is built into the mineral list, complete with species names, their composition ranges, as well as immiscible/nonphysical regions. You do not need to add intermediate compositions as separate mineral definitions, as the software will automatically determine the appropriate species using its mixel spectrum deconvolution. When the solid solution series is available in the overview list of mineral species, it can be added to any recipe (with any system configuration) for classification/analysis. Maps Mineralogy Software will identify when a spectrum belongs to this solid solution series and allocate the appropriate sub-species to the classification.
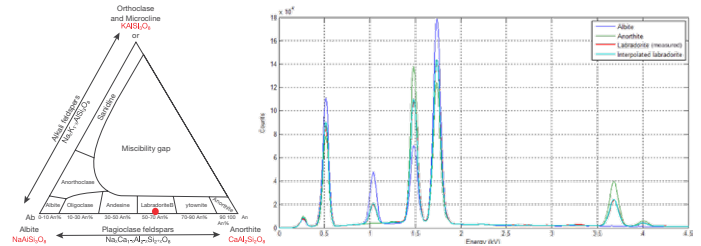

Figure 4. Left) Plagioclase feldspar solid solution ternary diagram. Right) Mixel algorithm used to perform spectral matching to a measured labradorite sample.

Managing mineral libraries and mixed phases

To create a mineral library in MLA Software, EDS spectra would have to be measured from known minerals, or the STD measurement mode would be used to measure and store mineral spectra in the library from a sample acquisition. For each species, multiple example spectra should be collected to ensure the library contains an accurate definition of the mineral. There is no option to create entries based on properties such as mineral name, chemical formula, or composition. Once a mineral library has been created, it can be used for other samples, projects, and measurements. However, the same setup process, including spectra collection, has to be repeated when using a different accelerating voltage, detectors, or SEM, as the spectra are directly tied to each microscope and cannot be reliably used between systems. The mineral library definitions are also fixed to be used with EDS spectra of approximately 2,000 counts, and classification becomes more inaccurate when longer dwell times are used. This essentially limits the accuracy of the approach and limits the level of sample complexity that can be addressed.

Although Maps Mineralogy Software also utilizes a mineral list to manage mineral species and their associated spectra, the creation and management of phases follows a very different process. Maps Mineralogy Software ships with a library of >4,000 mineral species.

While theoretically possible to run an acquisition utilizing the entire library, a sub-set library, called a recipe, is typically used to reduce computation time and reduce false positives within a particular geological body. Out of the box, Maps Mineralogy Software comes with several recipes that include subsets of mineral definitions suitable for common rock/ore types.

Recipes can be easily edited to conform to expected variations in a sample's mineralogy. You also have several options to add new species to a recipe. Similar to MLA Software, a new phase can be added by manually collecting an EDS spectrum, which can be useful for uncommon phases with unique compositions. Maps Mineralogy Software also makes it easy to add phases from the mineral library by searching for the mineral name. Once selected, a synthetic spectrum is generated for the mineral and added to the recipe. Additionally, spectra can be added based on a specific chemistry.

You simply input the oxide wt% from an external source (e.g. EMPA data) and a synthetic EDS spectrum is generated based on the input composition. In contrast to MLA Software, once the mineral list is generated, it can be used reliably at any of the supported accelerating voltages (i.e. 15, 20, 25 kV) as well as on any microscope. No replication or change based on common operating conditions is necessary. In contrast, an MLA standards library is fixed to a single SEM and a single beam voltage; running that library on a different system produces degraded results.

Figure 5. 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.

The standard acquisition approach in MLA Software utilizes image processing to identify grains and then target the center of mass (centroid) of each. This approach has two main benefits:

1. Centroid-based acquisition limits the number of X-rays necessary for reconstruction and therefore dramatically increases acquisition throughput

2. Avoids generating X-rays at grain boundaries where mixed spectra complicate mineral ID accuracy

This approach does, however, have some inherent shortcomings. Proper image-based segmentation approaches fail or become unreliable when the backscattered-electron contrast of the phases becomes too small, or if the sample contains complicated mineral textures (due to fine grain sizes or intergrowths). To account for this, MLA Software also runs in a raster mapping mode (XBSE), but this approach run into the software's limited approach for handling mixed spectra. The process to add mixtures is laborious and subject to the experience of the user. The amount of effort to generate a single mineral list for a sample grows factorially as the number of systems increases. Managing the mineral list across sample types and between systems becomes a complicated exercise, especially for labs with new or inexperienced users.

In Maps Mineralogy Software, this boundary-texture classification is done automatically by the mixel algorithm. You are only required to perform a quality control check of the data to ensure that no real mineral phases are being misclassified as mixed spectra. There are also several settings in the recipe that can be adjusted to make this less likely or avoid it altogether. You could also remove an incorrect mineral definition from the recipe altogether, if the phase does not occur in the analyzed samples. 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.
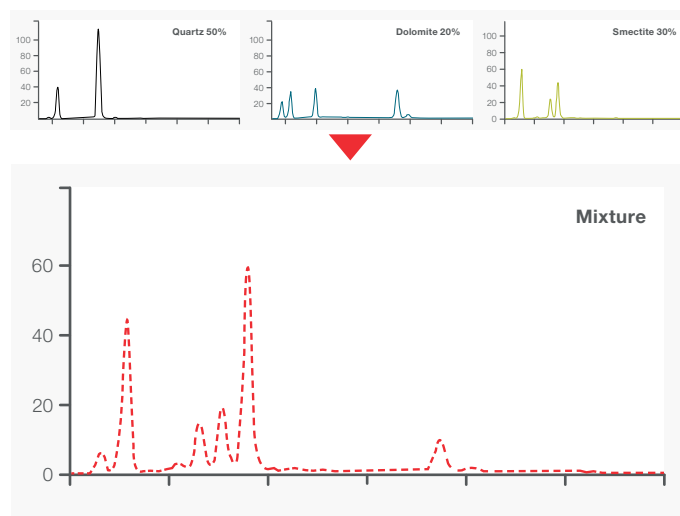

Figure 6. Simplified example of the mixel algorithm at work. At grain boundaries, within fine-grained samples, and within complicated mineral textures, mixed spectra are common due to the generated X-rays sampling multiple phases within the electron beam sample interaction volume. The mixel approach accurately identifies the phases that make up a mixture and generates a relative proportion of each phase identified.

Acquisition and visualization improvements

Acquisition in Maps Mineralogy Software is performed through Thermo Scientific Maps Software, the central automation platform that handles all 2D imaging automation functions across the entire Thermo Scientific electron microscopy portfolio. Built around its robust architecture is a streamlined approach for setting imaging/EDS parameters, as well as entering sample metadata (e.g., survey, size fraction, sample weight, etc.) for reporting. Templates containing common acquisition parameters are available to augment the fast and simplified acquisition setup. The Maps Software architecture automatically stitches acquired tiles based on feature detection algorithms, unlike MLA Software, where compensating for misaligned tile boundaries is a common struggle. Additionally, acquisition in Maps Mineralogy Software does not suffer from the size restrictions encountered in MLA Software. The acquisition and processing of EDS data occurs on a tile-by-tile basis, where each tile represents a single field-of-view within the microscope.
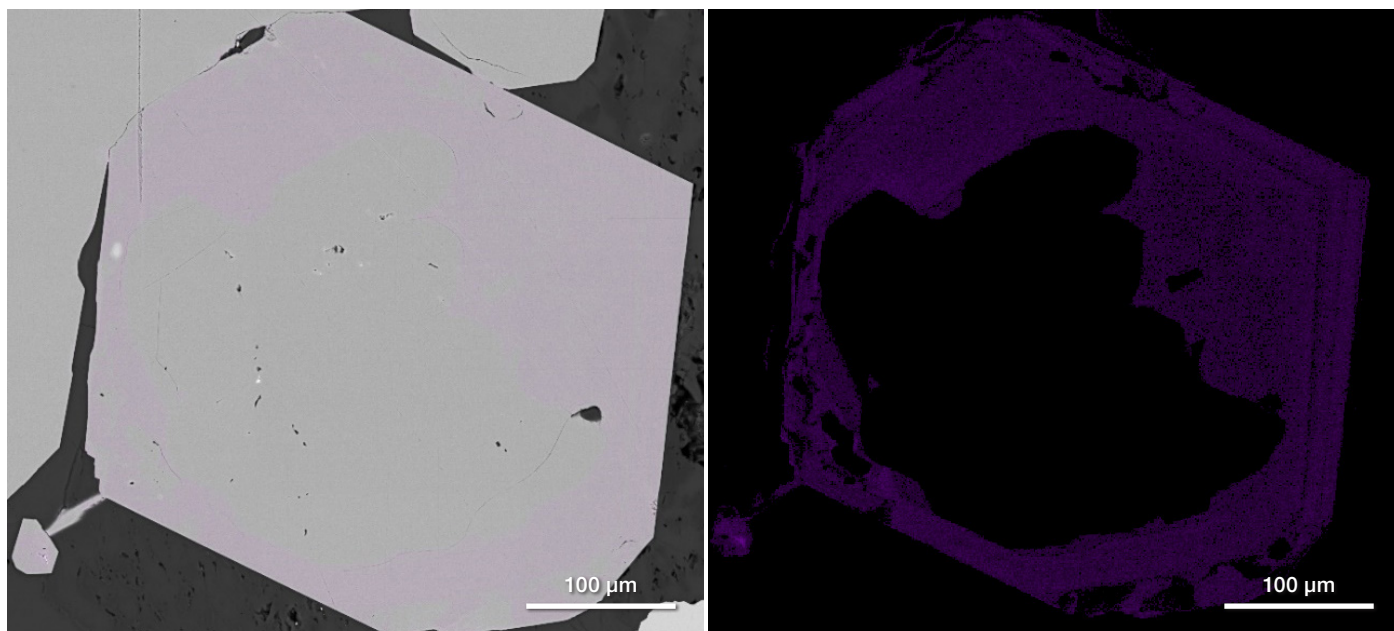
Figure 7. Example illustrating the fidelity of EDS map visualization in Maps Mineralogy Software. Left) BSE image of a pyrite grain with an overlaid map of cobalt. Single-click access to this true EDS map allows for easy exploration of elemental variation across a sample. Right) Same location, but with the BSE image layer turned off. Growth rims on pyrite are clearly visible in the trace element maps even though they were not observable in the BSE, iron, or sulfur maps.

There is no limit on the number of minerals per tile, nor the number of X-rays acquired per tile. MLA Software, meanwhile, has implementation limits when acquiring data in grid mode, or if the number of minerals within a single field exceeds 255.

Maps Mineralogy Software provides more information on a sample thanks to true EDS compositional maps that are available for overlays, in addition to basic mineralogy maps. This allows you to easily inspect compositional variability and account for any regional enrichments in trace elements (Figure 7).

Conclusions

In conclusion, the MLA mineral library can be configured for solid solution series and boundary texture classification to achieve comparable results to the mixel algorithm of Maps Mineralogy Software. This would, however, require substantial operator time and experience to set up and tweak the mineral libraries. Maps Mineralogy Software does this automatically while requiring very little user input or experience. Both new users as well as labs encountering complicated mineral textures and compositions would benefit from the improved automation and increased objectivity of the data. Maps Mineralogy Software offers accurate, reliable results that are less dependent on your level of experience while also enabling the analysis of challenging samples without the high amounts of manual post-processing typically required with MLA Software.

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