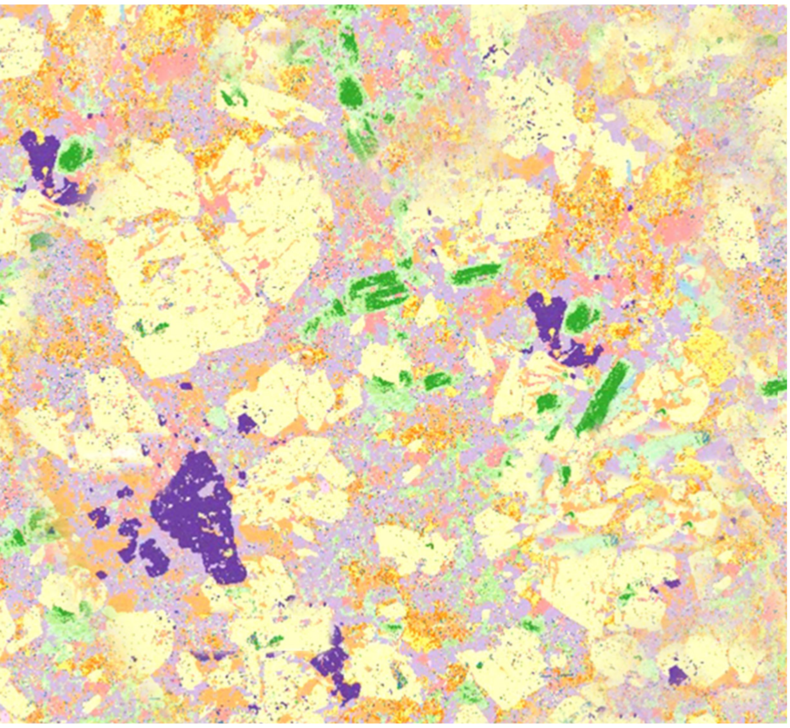
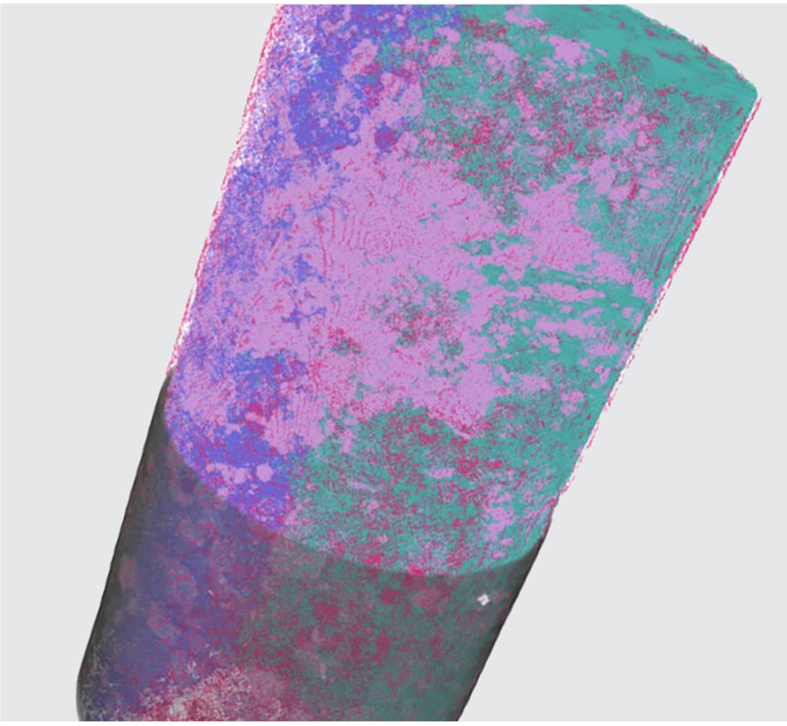
3D Automated Quantitative Mineralogy

ZEISS Mineralogic





Seeing beyond

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Rock and mineral assemblages are three dimensional (3D) structures, but traditional microanalytical techniques used to examine and address them, such as scanning electron microscope (SEM) based automated quantitative mineralogy (AQM), or traditional optical petrography, are inherently 2D. The prevalence of these techniques is understandable as they give a great level of analytical precision and reliability, but their 2D nature limits the insights that are available to the researcher, as well as their ability to make quantitative assessments.

X-ray microscopy is a technique whereby 3D volumes can be reconstructed from a set of projections using back-projection. The greyscale value of a voxel (3D pixel) within these volumes is proportional to the relative X-ray attenuation within that voxel, which is in turn related to the constituent material density, atomic weight and the incident X-ray energy. Frequently, subtle variations in either mineral composition (such as through solid solution, or when mineral compositions are strongly related) lead to reconstructed greyscale values that are sufficiently close to each-other that they are indistinguishable to traditional segmentation techniques [1]. To add complexity, the absolute greyscale value of the reconstructed image can be affected by a range of properties associated with factors such as imaging geometry, X-ray filtering or the presence of material outside the field of view (so-called region of interest scanning, or interior tomography), even if relative values remain the same. Such challenges have limited the application of X-ray microscopy to petrological or mineralogical applications, with most published work requiring intricate image processing and segmentation workflows [2]. While the minerals are challenging to discriminate by computational techniques, they are often easily discriminable by eye, which acts to smooth out noise, remove artifacts and perform classification on a much greater range of parameters than just a single pixel or voxel greyscale value (Figure 1). Manual inspection will show local and non-local greyscale values, gradients, textures and associations, which are integrated by the brain to form an ultimate local or region classification.

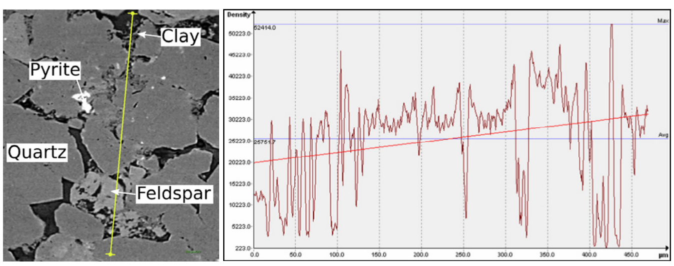


Figure 1 *A) Cross section through 3D X-ray microscope (XRM) image of a multi-mineralogical sandstone composed of quartz, feldspars, clays and pyrite. While these mineralogical differences can be seen relatively easily by eye, a profile through these minerals (B) shows no simple threshold that can be applied to separate each mineral phase.*

The last 20 years have seen a transformation in a wide range of fields, widely grouped together under the umbrella of "machine learning." Recent studies have shown that, when applied to the challenge of voxel classification, machine learning techniques are more robust, less noise- and artifact-prone, and, critically, provide a set of computational techniques that are able to perform classifications using this higher dimensional space [3-4]. This is done by first computing a range of features from an image using a set of filters, creating a "pixel feature-vector." This is then fed into a machine learning algorithm (such as the "forest of random trees" algorithm [5], which ultimately creates a pixel classification.

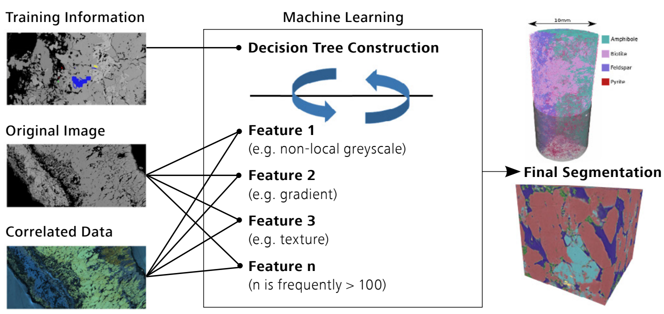


Figure 2 *Voxel segmentation using machine learning as present in ZEN Intellesis. Data is processed through a bank of filters, creating a complex pixel-by-pixel feature vector. Labeled pixels are used to construct a decision tree algorithm, which is then applied to the entire volume to create the final segmentation.*

While such techniques significantly simplify the challenge of 3D mineralogical analysis, significant challenges remain, specifically training the models required for accurate classification and the mineralogical assignment of the computationally classified phases. To solve this challenge, automated quantitative mineralogy (AQM) techniques, such as ZEISS Mineralogic, can be used, and then correlated to the 3D data. ZEISS Mineralogic uses energy dispersive X-ray spectroscopy (EDS) scanning, integrated within a SEM to first produce quantitative chemical maps across extended regions of a sample surface. These chemical maps are then compared to an extensive mineralogical database to assign unique mineralogical classifications with a resolution down to 200 nm [6].

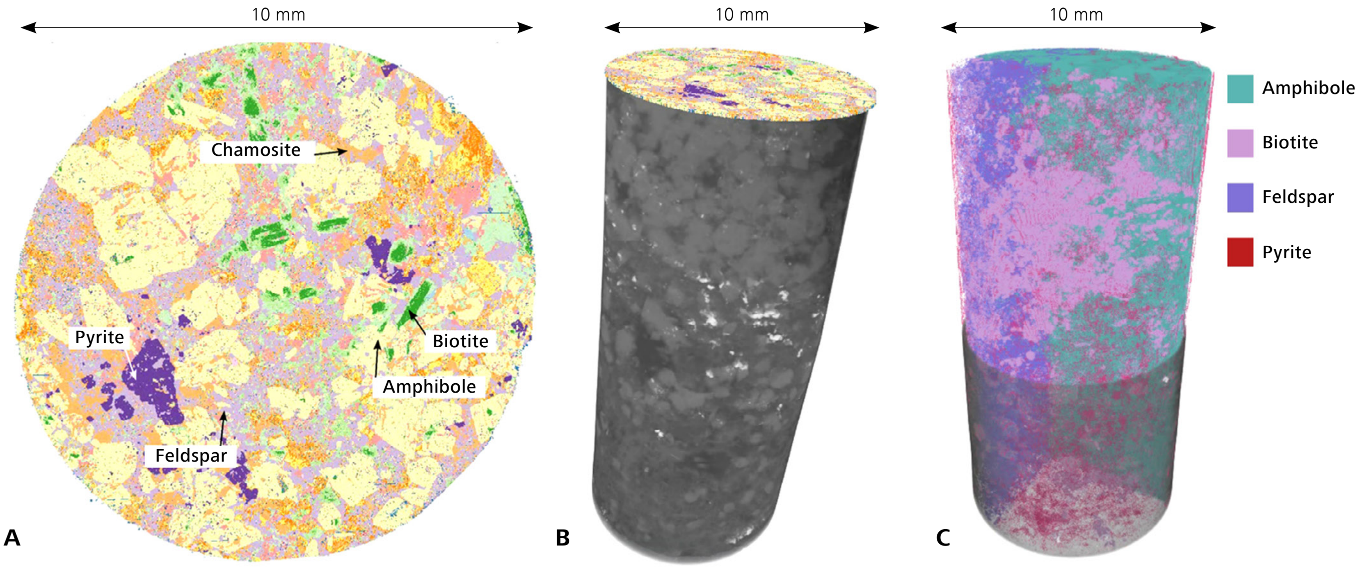


Figure 3 *A) AQM mineral map of the top surface of a drill core. (B) Correlation of the 2D AQM mineral map with the 3D tomography. (C) 3D classification of mineralogy using ZEN Intellesis.*

The propagation of this classification to 3D can occur through two workflows. The simplest technique assigns mineralogy and chemical compositions to phases identified and classified through manual training of classes identified from the 3D data. A single composition and classification is then assigned to each phase, which is then propagated throughout the 3D volume. Another more sophisticated workflow is to import the classifications found from ZEISS Mineralogic and use them to train the classification found in 3D. This provides a more complete training set, but only for the intersecting region between the 2D AQM mineral map and the 3D X-ray volume. These two techniques can be combined with extensive training data provided by AQM supplemented by additional manual training data provided from within the 3D volume.

The AQM mineral map is usually performed on an outside surface of a sample, such as the polished top surface of a drill core, allowing for the easy registration of the 2D data with the 3D tomography. A more complex workflow is possible where a thin section is prepared from a central portion of the sample after 3D tomography data has been acquired. This approach has the disadvantage of both being destructive and making the 2D-3D registration more challenging, however it may reduce certain X-ray imaging artifacts and may be required if AQM data is required on deeply buried 3D features.

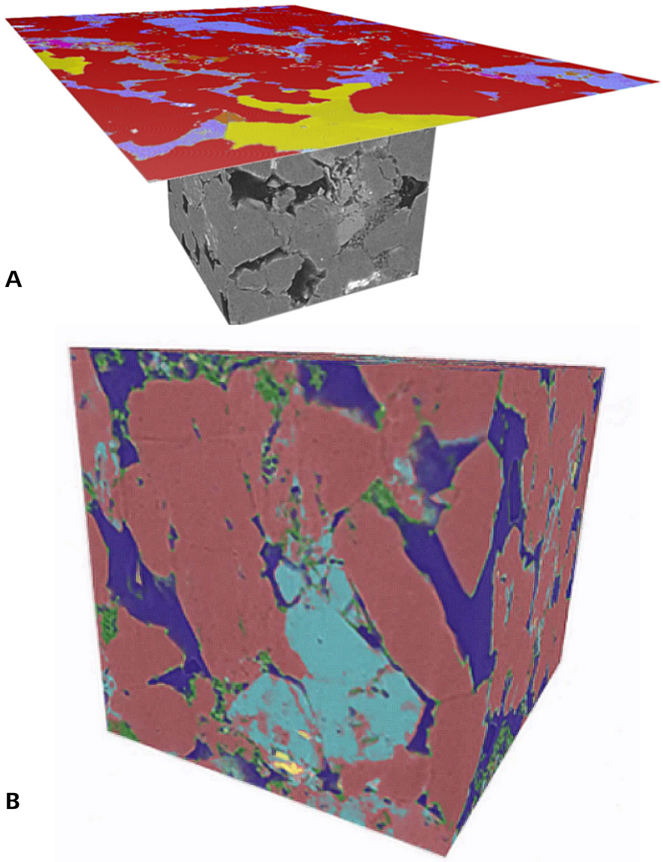
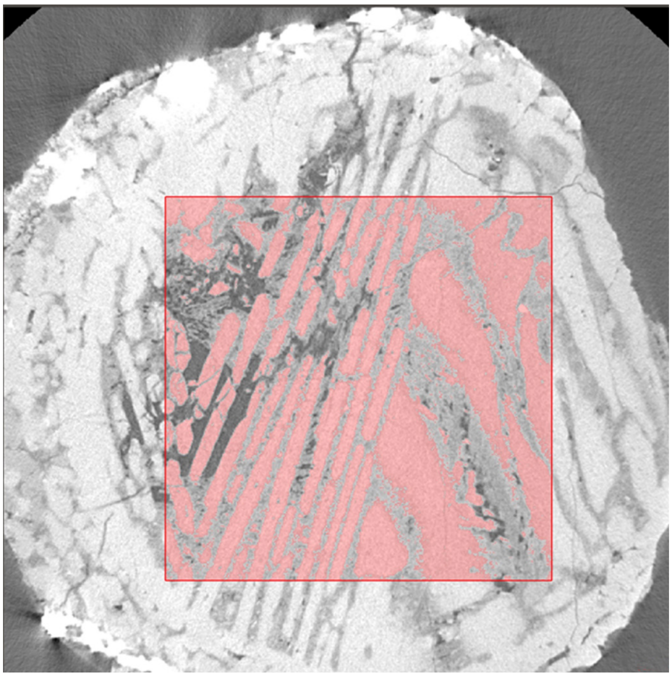


Figure 4 *(A) Correlated AQM mineral map and 3D X-ray tomography. (B) X-ray mineral classification.*



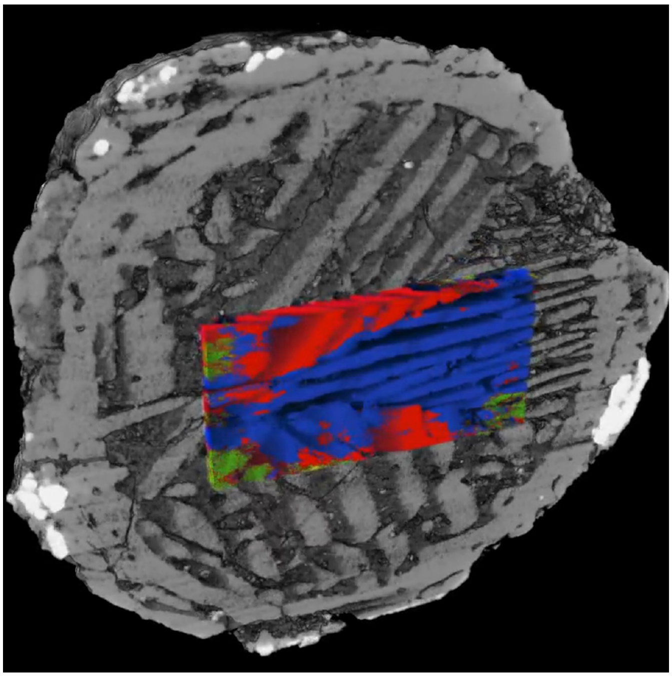


Figure 5 *(A) Absorption tomography volume of a barred olivine chondrule from the Bjurböle meteorite. Olivine is shown with a red overlay.*
(B) LabDCT reconstruction of olivine crystal orientation from within the chondrule.
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ZEISS provides a complete set of integrated software packages that enable and simplify such sophisticated analytical workflows. ZEISS Mineralogic provides AQM mapping of SEM data allowing for quantitative major element compositions to be determined and mineral classifications to be assigned. 3D data integration and correlation can be performed using ZEN Connect and ORS Dragonfly (for 3D visualization). Machine-learning based image segmentation of complex 2D and 3D data can be performed using ZEN Intellesis.

Conclusions and Future Work

One of the exciting future areas of development for 3D mineral classification is its integration with techniques such as diffraction contrast tomography using ZEISS LabDCT. This allows for crystal orientations to be explicitly resolved through Laue condition X-ray diffraction. One of the challenges when applying these techniques to geological systems is their relative crystallographic imperfection and complexity. An aspect of this complexity is when multi-modal systems are present. In this case, performing a 3D mineralogy workflow prior to LabDCT reconstruction allows for specific domains within the 3D volume where crystallographic reconstructions can be performed with a known crystal symmetry for the associated mineral. This in turn allows for both mineralogy and details of crystallography to be extracted from a sample.

References

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