

Quantitative Microanalysis Explorer: A Web-based Visualization Platform to Study Optical, Electron, and X-Ray Imaging Data of Lunar Samples

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Key Points:

- Web-based synthesis of large imaging data sets
- Combining image analysis and quantitative elemental data

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Abstract

We have developed the Quantitative Microanalysis Explorer, or QME-Tool, a web-based platform for visualization of large imaging data sets and interrogation of quantitative elemental maps acquired by electron microprobe. Using a combination of open-source JavaScript libraries and custom scripts, the QME-Tool can be used to quickly identify interesting mineral and lithologic phases in a sample by comparing backscattered-electron, optical, and X-ray map images, extract quantitative chemical composition from point and area regions, and easily share data and sample locations with colleagues. We have used the QME-Tool to study regolith contained in the Apollo 17 double-drive tube 73001/2 as part of the Apollo Next Generation Sample Analysis (ANGSA) Program.

Plain Language Summary

We have developed a web-based tool to visualize and interrogate data acquired on samples of the Moon returned by the Apollo astronauts. The QME-Tool makes it easy for scientists to synthesize different types of images, search for and characterize interesting, rare, or unusual rock types, and share their results with colleagues.

1 Introduction

Chemical and petrographic analysis of lunar samples provides important insight into the geologic history of the Moon. Analysis of samples in thin section by a combination of optical and quantitative electron-beam techniques is the most effective way to characterize the sample. This has been a challenging endeavor in the past. Initial analysis of Apollo samples utilized optical microscopy and fixed-beam electron-probe microanalysis (EPMA) followed by early backscattered-electron (BSE) imaging. X-ray mapping evolved still later and fully quantitative EPMA compositional mapping has been developed only recently (Carpenter et al., 2023; Minocha et al., 2022). We recognize several challenges to the lunar science community regarding study of lunar samples. First, lunar samples are analyzed sequentially by groups and involve expensive and time-consuming analytical methods, coupled with the requirement for specialized skills and experience to analyze the data. Second, large data sets are now generated and there is a need for correlative microscopy and microanalysis tools which enable direct comparison of data for specific features in a sample. Finally, an easily accessed web-based framework is needed to allow diverse groups to access the data and collaborate using the ability to extract compositional information and communicate it using data linking. We have developed the Quantitative Microanalysis Explorer, or QME-Tool, to address these needs.

1.1 Apollo 17 double-drive tube 73001/73002

The QME-Tool was developed as part of NASA’s Apollo Next Generation Sample Analysis (ANGSA) program. This program involved the examination of lunar samples that had been preserved since they were collected during the Apollo missions. The goal of the program was to study these pristine samples from a new perspective using novel technologies and methodologies, developed in the years since the samples were first returned to Earth, and aid the preparation for the upcoming Artemis Program (McCubbin et al., 2022).

The ~71 cm Apollo 17 double-drive tube 73001 (lower part) / 73002 (upper part) was collected on the light mantle at the base of South Massif of the Taurus-Littrow Valley. X-ray computed tomography was acquired for the entire core prior to processing the core for thin sections. High-resolution mineralogic characterization of the sample at the micrometer scale is critical for determining the presence of exogenous rock fragments and clasts, stratigraphy, pyroclastic debris, and evidence regarding the landslide deposit.

Continuous thin sections, 5 cm \times 2.5 cm in size, of 73001/73002 were prepared by impregnating the regolith with epoxy and grinding/polishing to a thickness of 30 μm .

We analyzed 12 continuous thin sections from the 73001/2 double-drive tube using the QME-Tool.

2 Methods

In this section we describe the methods used to acquire the data used in the QME-Tool, how that data is processed for use in the tool, and how our code is structured to allow for easy incorporation of new data sets into the QME-Tool. The QME-Tool is based on a simpler web-based tool to display electron and X-ray images (Ogliore, 2021).

2.1 Data Acquisition

2.1.1 Optical Images

Thin sections from 73001/2 were imaged with a Keyence VHX-7000 Series Digital Microscope at Johnson Space Center to acquire reflected, transmitted, cross-polarized (XP), and plane-polarized (PP) images at a resolution of 1.5 $\mu\text{m}/\text{pixel}$ over the entire sample. The Keyence system stitches together individual images into a single large mosaic image.

2.1.2 X-ray Images

We obtained quantitative X-ray elemental maps using a JEOL JXA-8200 electron microprobe at Washington University in St. Louis by stage mapping with a fixed electron beam in two passes. The first pass used 5 wavelength-dispersive spectrometers (WDS) to measure Mg, Al, Fe, Ca, and Ti. The second pass measured Na, Si, Mn, K, and Cr. The measurements were made at 100 nA probe current, 10 micron beam diameter, and 25 ms dwell time for each pass, for a total of 50 msec acquisition time per pixel. The pixel size (and stage step size) is 9.5 μm . Measurement time for each pixel is two orders of magnitude shorter than a conventional spot analysis, which is partially offset by the higher beam current. In practice, grouping of pixels during QME-Tool analysis increases the effective count time and improves analytical precision and accuracy. A single map is 1024 \times 1024 pixels and takes \sim 18 hrs to collect. It takes \sim 5 maps to cover a typical thin section of 73001/2.

2.1.3 Backscattered Electron Images

During the quantitative X-ray analysis, we acquired simultaneous backscattered electron images that are co-registered with the X-ray maps. Additionally, we acquired a high-resolution BSE mosaic map (1.5 $\mu\text{m}/\text{pixel}$, same resolution as the optical images) in a separate acquisition at lower electron beam current and smaller spot size (<1 $\mu\text{m}/\text{pixel}$), typically acquiring \sim 300 BSE images which are then stitched using Fiji.

2.2 Data Processing

2.2.1 EPMA

A conventional EPMA calibration is used for the QME-Tool maps using the Probe for EPMA operating system on the electron microprobe. The X-ray maps are converted to concentration maps using the CalcImage program, which performs a full $\Phi(\rho z)$ matrix correction according to $C = k \times ZAF$, where C is the concentration, k is the background-corrected X-ray intensity emitted from the sample relative to a calibration standard, and individual factors Z , A , and F correct for matrix effects related to the atomic number

(electron backscattering and energy loss), X-ray absorption, and characteristic fluorescence excitation. The WDS background correction uses the mean atomic number (MAN) background correction method from a suite of EPMA standards and establishes an analysis-specific background for all measured elements as part of the ZAF correction. The MAN background correction is routinely used in our EPMA laboratory with demonstrated accuracy superior to conventional WDS background correction and provides an accurate background correction over all quantitative maps in the 73001/2 samples mapped.

Element concentrations are recorded as 32-bit floating-point TIFF images for each of the 10 elements studied, resulting in element wt.% images with an analytical total image that is used for evaluation of accuracy. In the QME-Tool we use these element wt.% images for extraction of analytical data and on-demand calculation of oxide wt.% and cation proportions data for point and region locations based on mouse input. Appropriate TIFF tags are set in these files in the previous step that define a number of parameters, most importantly the image resolution (“Resolution” tiff tag) in nanometers/pixel. These were then processed through Fiji, where they are stitched and normalized to ensure that the intensities are consistent on the overlapping regions of the maps. Greyscale 8-bit png images of each element are saved from these TIFF files by scaling the 32-bit floating point values. The zero value is set equal to the floating-point pixel with the 0.1 percentile value of all pixels in the map, and 255 is set to the 99.9 percentile value. Pixels outside of this range are clipped to black (0) or white (255). These images are also written as red, green, and blue images (where only the single color channel is nonzero) to allow for the RGB image construction in the QME-Tool described below.

2.2.2 Image Registration

The different imaging modalities (optical, high-resolution BSE, and X-ray) are slightly distorted compared to each other due to the different ways the images were collected. We have determined that stage automation systems on optical and SEM instruments are not necessarily internally consistent in comparison to the EPMA stage mapping hardware. Therefore, the images need to be warped to fit one “base” map. Warping the quantitative X-ray data is undesirable as it compromises the fidelity of the data (i.e., producing duplicated or interpolated pixel data). Therefore, we chose the BSE map simultaneously acquired with X-ray data (and therefore co-registered with the X-ray maps) as the “base” map and warped the other images to it.

The high-resolution BSE map can be easily warped to the X-ray BSE map using automatically identified control points (detectORBFeatures in Matlab) and an affine transformation (estgeotform2d and imwarp in Matlab). Optical images have such different contrast that they need to be registered by manually selecting control points. We selected ~50 control points between each optical image and the X-ray BSE map, using cracks and grain boundaries that are easily identified in both images, with Matlab’s cpselect function (Figure 1). Then we warped the image using the same functions we used for the high-resolution BSE map.

2.2.3 Cluster Analysis

For each map, we performed a cluster analysis using Matlab’s kmedoids function. We use 20 clusters and run 24 replicates in parallel using the “cityblock” distance metric. The starting cluster is determined by a random sample of 10% of the pixels. The replicate with the best Hamming distance of the 24 replicates is the clustering result that is chosen. For the chosen cluster output, we calculate the cation sum of each cluster. We assigned colors for each cluster using Matlab’s jet colormap, with dark red assigned to the cluster with the largest cation sum and blue with the smallest cation sum.

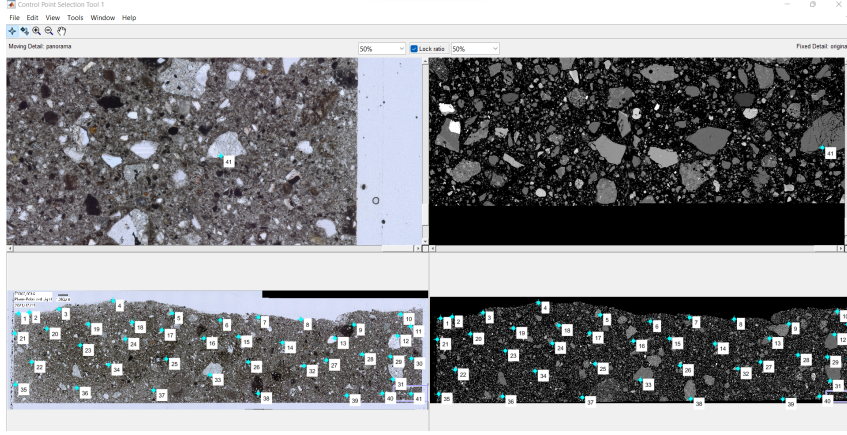


Figure 1. Manual control point selection method using Matlab’s cpselect function. Left is the the plane-polarized image and right is the BSE image of 73002,6016.

2.2.4 Imaging Data Products

The X-ray, optical, BSE, and cluster images are converted to image pyramid files in the dzi format using the vips (Martinez & Cupitt, 2005) software package. The image pyramid tiles are saved as jpg with quality flag set to 90 as a compromise between image quality and filesize. The elemental EPMA data are saved with lossless Deflate compression using tiffcp. Both the jpg quality and the zip compression are used to minimize data transfer times for users with slower internet connections.

2.2.5 Matlab and Javascript Code

The code to register and save the optical and high-resolution BSE images, write the X-ray images, save the zipped TIFF images, and write the image pyramids to the web server is all done in a single Matlab script. Additionally, this Matlab script writes the necessary html and JavaScript files for a given instance of a QME-Tool map directly to the web server. The script requires a folder of the raw data (with the correct filename patterns) as input, and will output a new website with the QME-Tool interface as output. This makes it very simple to create a new QME-Tool data product.

The code to run the web interface for the QME-Tool is in two JavaScript files. The first script (s1.js) contains a call to the OpenSeadragon JavaScript library that displays the zoomable image pyramids and allows for user interrogation of the data. We have made use of a number of OpenSeadragon plugins as described in Section 3. The s1.js script also defines the functions that allow for point and region selection of the EPMA data. The second JavaScript file (s2.js) downloads and reads the EPMA data files using the GeoTIFF JavaScript library (Fabian Schindler, 2018) and defines the functions to make the data presentable to the user.

The map-specific variable such as nanometers/pixel of the “base” BSE image and the list of elements is saved in a third JavaScript file (mapvariable.js).

3 Results

A screenshot of the QME-Tool with a 73001/2 sample is shown in Figure 2. The user can zoom, pan, switch between imaging modalities, and extract EPMA data from

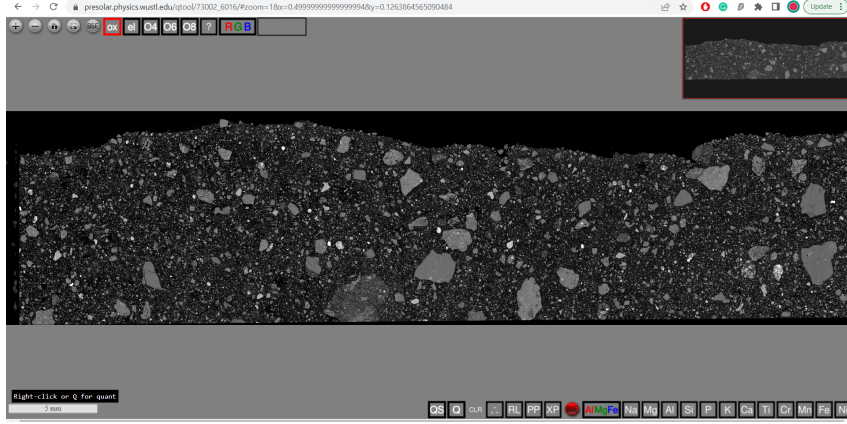


Figure 2. The QME tool displaying the ANGSA sample 73002-6016 backscattered electron image. Quantitative analytical data calculations are selected using the upper controls, and mouse operations and reference images are selected using the lower controls.

portions of the image. In the following sections, we describe the features of the QME-Tool that make it useful for investigating the 73001/2 thin sections.

3.1 The OpenSeadragon Viewer

OpenSeadragon uses image pyramids so only the current field-of-view at the appropriate resolution is loaded into memory at once. The interface allows for smooth zooming and scrolling, so the user feels that the entire large image (gigapixels in size) is accessible at all resolutions nearly instantly. OpenSeadragon is open-source and actively developed. It allows for fast-switching between multiple images. For the QME-Tool, this allows us to switch between different (co-registered) imaging modalities instantly.

3.2 Retrieval of EPMA Data

After examining the X-ray, optical, and BSE images, the QME-Tool user also has the option to look deeper into a part of the sample by extracting the quantitative EPMA data from a region-of-interest (ROI). With the GeoTIFF library, portions of the element data can be extracted from the ten element maps including their analytical total, and displayed to the user. A user can choose between three different types of ROIs: a single pixel (right-click), a rectangular region (“Q” button at bottom of the QME-Tool window), or a region bounded by an irregular polygon (“QS” button). Single pixel data is useful for identifying mineralogy and detecting chemical zoning. Multi-pixel data is useful for determining average compositions and improving precision and accuracy of the averaged analytical data via pixel averaging which effectively increases the total count time.

The selection tools were developed using OpenSeadragon’s MouseTracker class and the pressHandler, dragHandler, and releaseHandler methods. For single pixel selection, a right-click was chosen as the input, which would be used to detect where the user’s cursor was on the screen to output the coordinates. The coordinates are then used as inputs to read data from each of the EPMA TIFF files using GeoTIFF. A rectangular selection is initiated by the user pressing the “Q” button (or the “q” keyboard shortcut). The start (click-down) and end (click-up) coordinates are sent to the GeoTIFF function that reads the EPMA data from this raster.

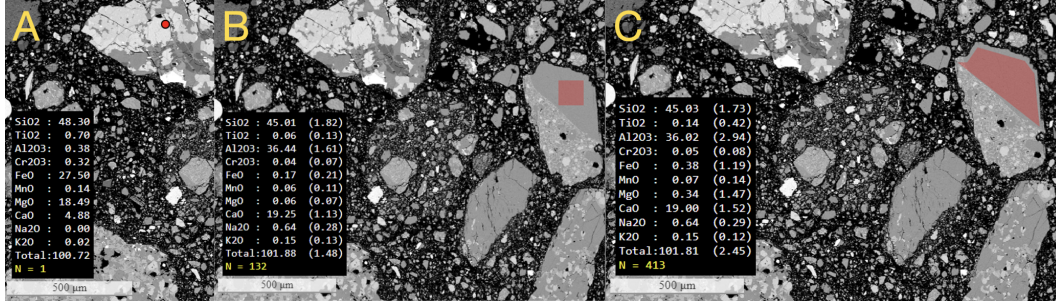


Figure 3. A) Single-point (or pixel) selection for quantitative data acquisition. B) Rectangular region selection for quantitative data acquisition. C) Irregular-polygon selection for quantitative data acquisition. Each operation also automatically copies the data to the clipboard for pasting into a spreadsheet.

For the polygon selection, a circular overlay is added where the first point selected. The movement of the mouse is followed, and a line overlay is drawn along this path. A translucent overlay is added that traces the shape of the polygon that is being drawn as the user clicks new points. A double-click, captured by OpenSeadragon’s dblClick-Handler, records the final pixel location and closes the polygon by adding a line between the last location and the origin of the shape.

Data extraction from an image for a single pixel or rectangular region with GeoTIFF is simple, but for an n -sided polygon, we first extract data from the smallest rectangle enclosing the polygon, then we exclude points in this rectangle that fall outside the polygon.

Each of the ten assembled EPMA element maps for the 73001/2 sections contained over 4 million pixels. Data processing is sped up significantly by using GeoTIFF’s object pooling. This is a form of parallel processing where every core is used to simultaneously extract data from all ten element maps. Data from thousands of pixels is read in a fraction of a second with the QME-Tool. Indeed, it is possible for the first time to quickly obtain averages of fully quantitative EPMA data from large areas in a map, which facilitates comparing different areas conveniently.

3.3 Display of EPMA Data

The default data format is oxide weight percent (“ox” button in the top-left of the QME-Tool), but this can be changed by the user as we convert between element weight percent and oxide weight percent on demand. The other options are element weight percent (“el” button) and number of atoms using a 4, 6, or 8 oxygen basis (“O4”, “O6”, and “O8” buttons, respectively).

For the region selections (rectangular and polygon), after the matrix for each pixel in the region is collected, the arithmetic means are calculated for each of the percentages along with the standard deviation. The means, standard deviations, and number of calculated pixels and totals are displayed in a black box on the lower-left corner of the QME-Tool viewer. The ability to compare element, oxide, and formula basis data for the selected point or region supports the identification of minerals and their chemistry. Additionally, for example, it is possible to determine bulk properties of lithic clasts by selecting the entire clast using the “QS” button and inspect the average composition (this average is not density-corrected but can be using downstream processing).

Additionally, the quant data is automatically copied to the user’s clipboard. This allows for easy pasting into spreadsheet documents. The clipboard text also contains the URL of the field-of-view where the ROI was extracted (but the exact ROI is not contained in the URL). This powerful capability allows for correlative and collaborative analysis and communication with other individuals that may be viewing the same sample from a different geographic location, and for the first time allows them access to the samples. This capability thus allows users in a video conference to simultaneously study one or several samples for efficient analysis and real-time discussion.

3.4 Dynamic Scale Bar

The QME-Tool shows a scale bar in the lower-left corner that changes dynamically as the user zooms in and out. The scale bar is accurate even as the user switches between imaging modalities acquired at different resolutions. The scale bar is an OpenSeadragon plugin originally developed by NIST.

3.5 Thumbnail Overview

The QME-Tool has a thumbnail view in the top-right corner that reappears when the mouse cursor is active. The thumbnail view has a red square showing the current field-of-view. This red square can be dragged to rapidly move to another field of view with the same magnification.

3.6 Custom RGB Maps

An Al-Mg-Fe X-ray RGB map is pre-assembled and is always available for viewing via a button among the element list at the bottom of the QME-Tool. The user can also create custom RGB color maps of any combination of three elements by first clicking the RGB at top, then selecting the red element, then the green element, then the blue element. Different RGB maps would be helpful for different studies of the 73001/2 samples. For example, a team looking for mare basalts to study fissure-type eruptions (P. M. Thesniya, 2020), could create an RGB map consisting of titanium, iron, and magnesium (Meyer, 2003). This would provide a basis for a more in-depth quantitative analysis of the regions that reflect the presence of all three.

3.7 Cluster Map

The output of the unsupervised clustering algorithm described previously can be viewed by clicking on the button with three dots in the bottom part of the viewer. An example of a cluster map is shown in Figure 4.

3.8 Measurement of Depth in Core

Thin sections from the 73001/2 double drive tube were divided into pieces, so it is important to track the depth of a given region of the core from the surface. When the 73001/2 sections are shown in the viewer, the depth from surface in centimeters is calculated from the current mouse position and shown in the bottom-left.

3.9 Unique and Shareable URL

A unique URL is produced for every field-of-view, i.e., $x - y$ position and zoom level. The URL can be copied and shared with collaborators. Opening the link will open the QME-Tool at the same field-of-view and showing the base map (the high-resolution BSE image). This feature solves the often cumbersome problem of communicating the location of a map feature for discussion by reducing it to a shared link.

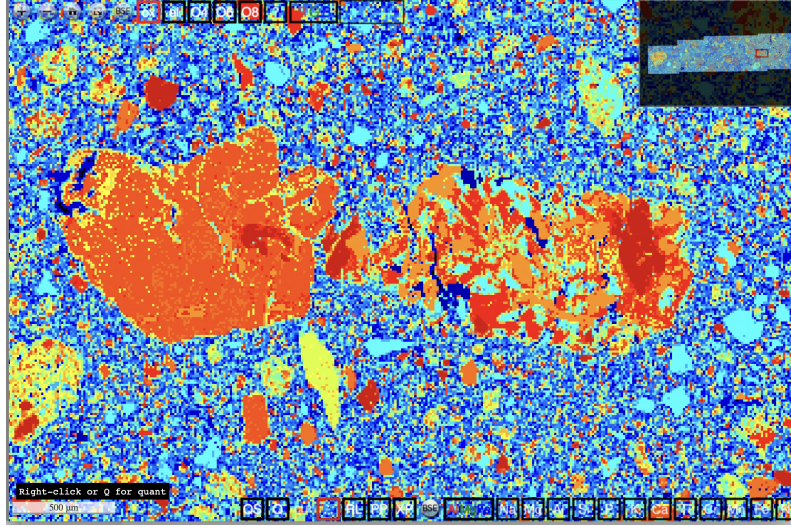


Figure 4. Cluster map for a portion of 73002,6018.

3.10 Keyboard shortcuts

Switching between maps, starting an EPMA data retrieval, zooming, panning and other functions can be accessed through keyboard shortcuts. Keystrokes are often faster than mouse clicks and can speed up analysis when the user is analyzing many subsamples. The keyboard shortcuts are given in the mouse-over text of the buttons and in the help menu (“?” button) at top.

3.11 Index Site for 73001 and 73002

The links for all analyzed 73001 and 73002 thin sections are shown on an index page, along with thumbnails showing the proper orientation of each section and its depth from the surface.

4 Discussion

The QME-Tool is used to study the 73001/2 samples in a number of ways. One application is searching for prebasin highlands components and Tycho ejecta (Jolliff et al., 2022), and another is searching for volcanic glass (Yen et al., 2022). In both cases, the QME-Tool’s optical, BSE, and X-ray maps were used to first identify regions that may contain the samples of interest. Next, EPMA data extraction was used to study whether the regions-of-interest had the required chemical composition.

The QME-Tool provides a way to rapidly switch between imaging modalities for very large images. This is useful when studying geologic samples of all types. For example, twinning in rock fragments is more pronounced in cross-polarized images than in other modalities (Figure 5). The BSE map is helpful because it has relatively high signal to noise compared to the X-ray maps, allowing for interpretation of phases based on their grey levels. The transmitted light image allows recognition of glassy regions, and the reflected light image allows location of metal and various opaque accessory phases such as ilmenite and sulfides.

The QME-Tool is optimized for collaboration as it is accessible through any browser, and does not require any specialized or commercial software. While the responsiveness of the QME-Tool depends on the download speed and number of cores in the device, the

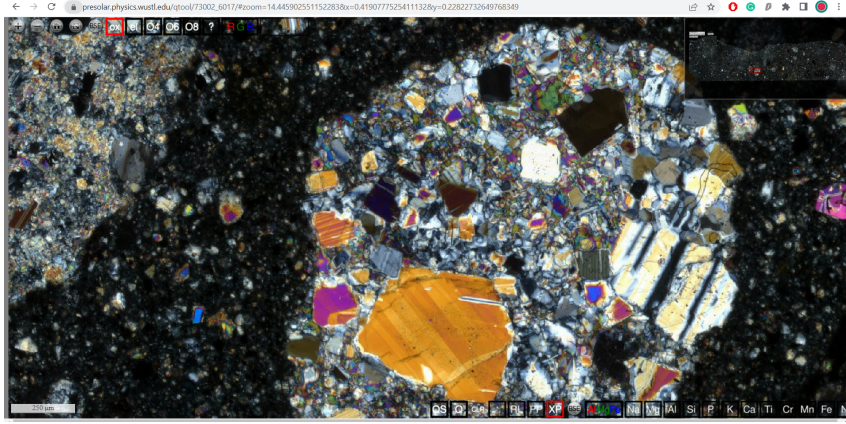


Figure 5. A cross-polarized image of a clast in ANGSA sample 73002-6017 showing examples of polysynthetic twinning.

QME-Tool even on a slow connection is still significantly faster than traditional ways of co-registering images and processing EPMA data. We recently tested the tool at a conference in Australia using wireless network access and observed, with good internet speed, very good performance.

While there is vast potential for the uses of the tool, it is necessary to take into account its current limitations and areas for improvement. The bulk composition derived from a large number of pixels does not take into account different densities of the phases. Image registration process currently uses affine transformations. Non-rigid transformations would better handle, e.g. barrel distortion of the optical images. Better registration would allow for better confidence in selecting an EPMA data extraction directly from an optical image. The current JavaScript code (the scripts `s1.js` and `s2.js`) can be converted to typescript for easier debugging.

The QME-Tool is flexible enough to incorporate any imaging modality or spot analysis as long as it can be registered to the base map. Additionally, the QME-Tool is not only for microscopy images. Large-scale planetary imaging data could be incorporated into the QME-Tool as well, overlaying different spectral maps of a planetary body.

5 Conclusion

We have developed the QME-Tool, a browser-based data visualization and data interrogation tool to study the Apollo double-drive tube 73001/2 as part of NASA's ANGSA program. The QME-Tool combines publication quality EPMA data and large-image visualization tools to enable exploration of large data sets quickly and easily. The QME-Tool can provide scientific access to precious samples to scientists from all over the world without having to have the samples in hand. The upcoming Artemis missions will return new samples from the Moon in the coming years, and open-data products like the QME-Tool can be leveraged to enable fast, simultaneous, and worldwide access to these samples.

6 Open Research

The thin sections of 73001/2 in the QME-Tool can be accessed at the following URLs:

<https://presolar.physics.wustl.edu/qtool/73001/>

<https://presolar.physics.wustl.edu/qtool/73002/>

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