MapX: An in-situ Mapping X-ray Fluorescence Instrument for Detection of Biosignatures and Habitable Planetary Environments. R. C. Walroth,[1] D.F. Blake,[1] P. Sarrazin,[2] F. Marchis,[2] and K. Thompson.[2] [1]Exobiology Branch, MS 239-4, NASA Ames Research Center, Moffett Field, CA 94035 (richard.c.walroth@nasa.gov), [2]SETI Institute, Mountain View, CA 94043.

Introduction: The search for evidence of life or its processes on other worlds takes on two major themes: the detection of biosignatures indicating extinct or extant life, or the determination that an environment either has or once had the potential to harbor living organisms. *In situ* elemental imaging is useful in either case, since features on the mm to µm scale reveal geological processes which may indicate past or present habitability. Further, biomineralization can leave traces in the morphology and element distribution of surfaces. The Mapping X-ray Fluorescence Spectrometer (MapX) is an *in-situ* instrument designed to identify these features on planetary surfaces [1]. Progress on instrument development, data analysis methods, and element quantification are presented.

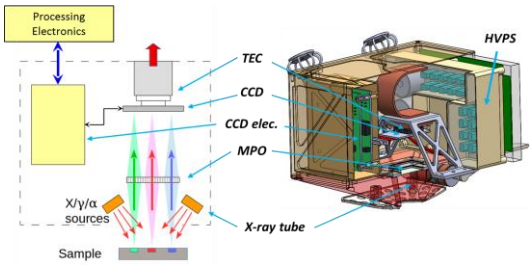

Figure 1. Left: Schematic representation of MapX. Right: Rendering of the arm mounted instrument in a flight like configuration.

Instrument Description: MapX is a full field elemental imager capable of analyzing samples *in situ* without sample preparation. Figure 1 shows a schematic of the instrument, which consists of X-ray sources, a focusing optic, and a CCD. Either radioisotope (e.g., ^{244}Cm) [2] or X-ray tube sources can be used. The focusing lens is an X-ray micro-pore optic (MPO) which focuses X-rays 1:1 onto the CCD. The MPO has a large depth of field, allowing rough unprepared surfaces to be imaged with minimal resolution loss. The CCD is read out fast enough (several frames per second) so that each pixel records either a single photon or background. The number of electron hole pairs generated is directly proportional to the energy of the photon, and after summing a large number of individual frames, an XRF spectrum is generated for each pixel of the CCD. Each individual frame represents a full image; however multiple frames are necessary to produce quantifiable XRF spectra. Longer collection times will allow for improved signal to noise, but in the event a collection is interrupted the partial data will still yield a complete image.

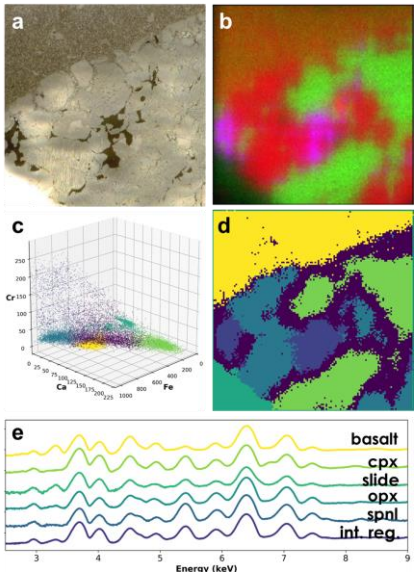

Figure 2. a) Optical image of a petrologic thin section of an ultramafic xenolith (field of view, 18 mm) imaged with MapX-2 prototype in 2b, 2d. b) False color image showing Fe in red, Ca in green, and Cr in blue. c) Correlation between Fe, Ca, and Cr as a 3D scatter plot with clusters of similar composition color annotated. d) Labels applied to the 2D image showing the spatial relationship of the different ROI. e) Summed spectra from the different ROI with assigned mineralogy (cpx: clinopyroxene, slide: glass slide, opx: orthopyroxene, spnl: spinel, int. reg.: interfacial regions).

Data Analysis: The images collected by the CCD are binned by energy and combined into an x, y, energy data cube, the size of which will make downlinking of the raw data infeasible. Obtaining energy band maps at the characteristic energies of different elements from this data cube is trivial. However, these maps do not provide precise elemental composition information as different characteristic lines can overlap and background effects cannot be easily subtracted. With long enough collection times, a full fit of the XRF spectrum may be performed for each pixel, but this requires extensive computational resources as well as unrealistic collection times. Using machine learning, regions of similar composition can be identified based on the rough element maps mentioned above. These regions are identified by finding clusters in N dimensional space where N is the number of relevant elements.

These clusters are then applied to the 2D image to generate a map of ROI. The XRF spectra for these ROI can be summed to generate high signal to noise spectra for ground processing. Thus, the original data cube is reduced to a set of energy band ("element") maps and a set of ROI ("mineral maps") of distinct composition along with companion XRF spectra for quantitative analysis.

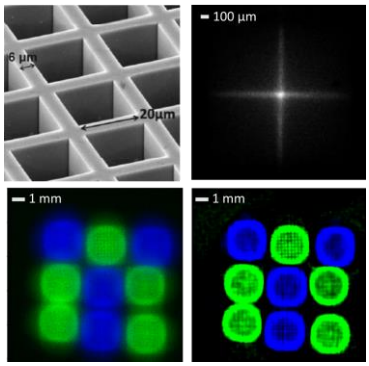

Figure 3. Top left: SEM image of MPO. Top right: Point spread function collected at SSRL. Bottom left: Raw image collected from MapX-2 of electron microscopy grids, Ni in green and Ti in blue. Bottom right: image after deconvolution.

Image Deconvolution: The MPO employed by MapX consists of an array of 20 µm square pores coated with Ir. It operates by reflecting X-rays in x and y to refocus them 1:1 onto the CCD. Optimal focusing requires a single reflection in x and y. In the event that a photon only reflects off of one wall, or reflects off of one wall twice, it will only be refocused in one axis. This results in a cross shaped PSF (Figure 3, top right). A customized script based on the AIDA deconvolution package was developed to use the PSF to recover resolution [3]. Figure 3, bottom right, shows an example of the deconvolution for a set of Ni and Ti electron microscope grids (127 µm pitch, 90 µm hole width).

MapX Prototypes to Date: Two prototype instruments are now operational. MapX-2 uses commercial off the shelf components and is operated in air with two X-ray tube sources. It has a spatial resolution of 200 µm and an energy resolution of 200 eV. Operating in air requires a 200 µm thick Be window to protect the CCD, limiting MapX-2 to elements above a Z of 20 (Ca). To date dozens of petrologic thin sections, imaging standards, and unprepared rock surfaces have been characterized using MapX-2. MapX-3 uses flight qualified or qualifiable components, including the legacy CCD224 from CheMin, in a high vacuum environment. The CCD224 is sensitive to all elements Z=13 (Al) and above. MapX-3 has comparable energy resolution to MapX-2 with a spatial resolution of 100 µm.

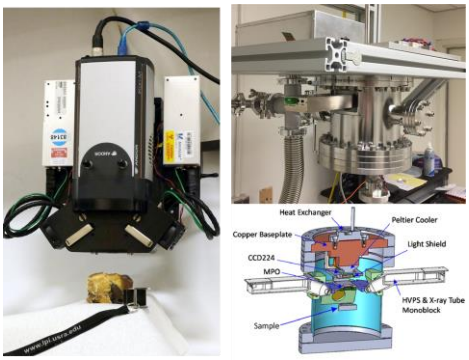

Figure 4. Left: MapX-2. Right: MapX-3 (above) with cut away schematic (below).

Element Quantification: With sufficient knowledge of the instrument geometry and the physics of the detector, it is possible to simulate spectra based on element composition. Simulations using GEANT4 and XMIMSIM are used to predict detection and quantification limits using MapX (Figure 5) [4]. We calculate the significance level k as the number of counts in a characteristic peak divided by the square root of the background below the peak. k>2 signifies successful detection at the 95% confidence level, k>10 signifies successful quantification.

Work is ongoing to use PyMca fitting and analysis of spectra for accurate determination of the elemental composition in terms of weight percent.

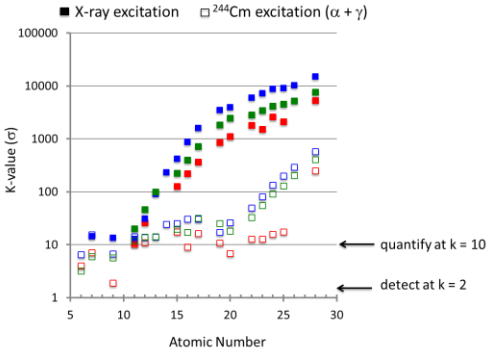

Figure 5. Graph of k values for element detection limits using MapX. Red is for a basalt matrix, green for silica matrix, and blue for ice matrix respectively.

Acknowledgements: This work was supported by the Ames Center Investment Fund (CIF), NASA's PICASSO (13-PICASSO-0111) and MatISSE (16-MATISE16_2-0005) programs, and the NASA Postdoctoral Program.

References: [1] Sarrazin, P. *et al.* (2016) *LPSC XLVII* #2883. [2] Radchenko, V. et al. (2000) *Applied Radiation and Isotopes* 53 (2000), 821-824. [3] Hom, E.F.Y. *et al. J. Opt. Soc. Am.* (2007) 1580-1600. [4] Thompson, K.A. *et al.* (2017) *LPSC XLVIII* #1602.