X-RAY FLUORESCENCE SOURCE MODELING FOR THE MAPX IMAGING SPECTROMETER: ROCKY PLANETS AND OCEAN WORLDS.

K. A. Thompson,[1] D. F. Blake,[2] P. Sarrazin[1] and T. Bristow.[2] [1]SETI Institute, 189 N. Bernardo Ave., Mountain View, CA, 94043 [2]Exobiology Branch, NASA Ames Research Center, MS 239-4, Moffett Field, CA 94035 (david.blake@nasa.gov).

Introduction: Many astrobiologically significant processes leave traces of their actions as features in the size range 10s to 100s of µm. The Mapping XRF Spectrometer (MapX) will provide elemental imaging at ≤100µm spatial resolution, yielding elemental chemistry at or below the scale length where many relict physical, chemical, and biological features can be imaged and interpreted in the surface regolith of terrestrial planets and rocky or icy planetesimals.

Map-X is an arm-deployed instrument placed directly on the surface of an object to be analyzed [1-2]. During an analysis, either an X-ray tube or a radioisotope source bombards the sample with X-rays (tube) or α-particles and γ-rays (radioisotope), resulting in X-ray Fluorescence (XRF) from the sample. Fluoresced X-rays pass through a focusing lens (X-ray µ-Pore Optic, "MPO") that projects a spatially resolved image of the X-rays emitted from the sample onto an X-ray sensitive CCD. The CCD is read at several frames per second so that in most cases, no more than one photon strikes an individual pixel between read cycles. In this way, energies and positions of individual X-ray photons are recorded. In a 1-3-hour analysis, several thousand frames are both stored and processed in real-time.

Scaling the source to meet science requirements: The source flux must be scaled to meet the science requirements of the instrument including: 1). single-photon counting by the CCD and 2). sufficient flux to meet detection limits for minor elements and accuracy/precision limits for major elements.

For rocky planets with atmospheres (e.g. Mars), MapX requirements are derived from those listed in the Mars 2020 science requirements document [3]. Namely, quantitation to ±10% for major elements Na, Mg, Al, Si, Ca and Fe; and detection of minor elements P, S, Cl, K, Ti, Cr, and Mn at the 100 ppm level.

For icy planetesimals and Ocean Worlds without atmospheres (e.g., Europa), these requirements are retained, plus quantification of the biogenic elements C, N, P, S. Detection of accumulations of the biogenic elements at appropriate concentrations on or in a mineral/ice substrate would constitute permissive evidence of extant life, but context is required.

Empirical testing of X-ray tube and radioisotope sources: An XRF test fixture was fabricated to study fluorescence from 30 mm diameter flat samples made from pressed powders of known mineral and rock compositions. Spectra are collected in air or under vacuum using either tube or radioisotope sources. The tube source has an Au anode, and is operated at 30 KeV, 20-100 µA. Three radioisotope sources have also been evaluated: 30mCi ^{55}Fe (γ = 5.89 KeV), 30mCi ^{241}Am (γ = 14 KeV, 18 KeV and 60 KeV) and a 50µCi ^{252}Cf thin foil α-particle source (α = 5 MeV). Test spectra were analyzed with the spectral fitting and analysis program PyMca [4]. The ^{241}Am source produces unacceptably high background at low energies due to Compton scattering from the ^{241}Am γ-line at 59.5 keV. For the ^{252}Cf source, a similar high background is observed. For this reason we are modeling ^{244}Cm (α = 5 MeV, γ = 11 KeV and 19 KeV) for our radioisotope source in flight- and proto-flight MapX instruments (^{244}Cm sources covered by thin Ti foils, yielding both α-particle and γ-ray excitation are used in the APXS instruments on the MER and MSL *Curiosity* rovers [5-6]).

Comparisons were made of spectra collected with normal collimation in place or with the MPO in place, to determine the attenuation produced by the MPO. The attenuation caused by the MPO is correlated with Z and ranges from ~1-3 for Na to ~18-20 for Fe.

Modeling of X-ray tube and radioisotope sources: We are not able to test ^{244}Cm due to availability and NRC licensing constraints; we are using the Monte Carlo simulation programs XMIMSIM [7] and GEANT4 [8] to explore this and other source combinations, in order to scale the source requirements to the science objectives for rocky planets such as Mars and ocean worlds such as Europa. 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.

Results:

Mars. Baseline requirements are to measure Na, Mg, Al, Si, Ca, Fe to ±10%, if present at >1000 ppm, and to detect P, S, Cl, K, Ti, Cr, Mn (at 2σ significance) if present at >100 ppm. Here we assume integration over a sample area of 2cm x 2cm and an accumulation time of 10000 seconds. Table 1 shows results for *k* in a basalt-like matrix (15% Fe, 27% Si, 11% Al, 47% O) and an SiO_2 matrix using either six 5mCi ^{244}Cm sources, or a tube source (30 KeV, 100 µA). As can be seen in Table 1, science requirements are reasonably well met using either ^{244}Cm or X-ray tube sources.

Table 1 Significance level k for Kα peak detection in two different rock matrices (Mars)

Element	Energy (KeV)	Significance Level *k*			
		Basalt Matrix		SiO_2 Matrix	
		^{244}Cm	Au Tube	^{244}Cm	Au Tube
Trace elements: detection @100 ppm: k >2 indicates detection at 95% level of confidence					
P Kα	2.02	1.9	10	1.9	22
S Kα	2.31	3.8	20	4.2	51
Cl Kα	2.62	3.0	35	4.2	90
K Kα	3.31	3.5	85	3.9	210
Ti Kα	4.51	1.4	170	3.9	320
Cr Kα	5.41	2.3	340	5.6	460
Mn Kα	5.90	1.7	260	8.4	530
Major elements: quantify to 1.0% ± 0.1% k > 10 indicates successful quantification					
Na Kα	1.04	140	57	170	110
Mg Kα	1.25	140	180	260	350
Al Kα	1.49	x	x	220	850
Si Kα	1.74	x	x	x	x
Ca Kα	3.69	240	11000	210	19000
Fe Kα	6.40	x	x	560	53000
x = element is already present in the matrix at well over 1% and the resulting k is >>10					

Europa. Two scenarios are considered for the detection and quantification of the biogenic elements on Europa: 1) Detection in a water ice matrix (e.g. analysis of icy surface regolith from a lander), and 2). Detection of C, N on a substrate through which melt water or water from a subsurface ocean had been filtered. Fluorescent yields from an X-ray tube source were found to be inadequate; only results from ^{244}Cm fluorescence are shown (for low-Z elements, fluorescence by α-particles is extraordinarily efficient).

Table 2 Significance level k for Kα peak detection in a water ice matrix. 30 mCi ^{244}Cm source, 10^4 sec.

Element	Energy (KeV)	Weight %	k-value
C Kα	0.282	0.1%	8.3
N Kα	0.392	0.1%	18
Na Kα	1.04	0.1%	23
Mg Kα	1.25	0.1%	33
P Kα	2.02	0.1%	80
S Kα	2.31	0.1%	72
Cl Kα	2.62	0.1%	57

As shown in Table 2, quantification of the biogenic elements and other low-Z elements of interest is possible with a ^{244}Cm source. Other elements scale similarly to those shown in Table 1 for an SiO_2 matrix.

Table 3 shows k-values for C, N on a zero background substrate through which melt water from Europa ice (or water from a subsurface Europa ocean) has been filtered.

Table 3 Significance level k for Kα peak detection on a zero background filter through which melted Europa ice has been filtered. 1 microbe per 100X100 µm pixel over a 2 cm X 2 cm area. 30 mCi ^{244}Cm source, 10^5 sec.

Element	Energy (KeV)	Concentration	k-value
C Kα	0.282	1 microbe / 100X100 µm pixel	28
N Kα	0.392	1 microbe / 100X100 µm pixel	11

Acknowledgments DFB is grateful for support from NASA PICASSO grant # NNX14AI28A.

References: [1] Blake, D.F. et al. (2017) LPSC XLVIII (this conference). [2] Blake, D.F. et al. (2016) IPM2016 #4006. [3] Mustard, J. et al. (2013). http://mepag.jpl.nasa.gov/reports/MEP/Mars_2020_SDT_Report_Final.pdf. [4] Solé, V.A. et al. (2007) *Spectrochim. Acta Part B, 62*, 63-68. [5]. Rieder, R. et al. (2003) *JGR-Planets, No. E12, 8066, doi:10.1029/2003JE002150, 2003*. [6]. Gellert, R., et al. (2006). *J. Geophys. Res. 111, E02S05, doi:10/1029/2005JE002555.* [7] T. Schoonjans et al. (2012) *Spectrachim. Acta Part B, 70*, 10-23. [8] Portnoi, A.Y. et al. (2004) *J. Analytical Chem, 59*, 1057-1065.