White paper topic submitted to MEPAG 38 https://mepag.jpl.nasa.gov/meetings.cfm?expand=m38

Hyperlink to latest version: https://odr.io/wp-decadal

CheMinX: A Next Generation XRD/XRF For Mars Exploration. David Blake[1], Philippe Sarrazin[2], Thomas Bristow[1], Marc Gailhanou[3], Barbara Lafuente[2], Kris Zacny[4] and Robert Downs[5]. [1]Exobiology Branch, NASA Ames Research Center, Moffett Field, CA, 94035 (david.blake@nasa.gov); [2] SETI Institute, Mountain View, CA; [3]Aix Marseille Universite, CNRS, IM2NP, Marseille, FR; [4]Honeybee Robotics, Pasadena, CA; [5]Geosciences, Univ. of Arizona, Tucson AZ.

Introduction: X-ray Diffraction (XRD) and X-ray Fluorescence (XRF) analyses provide the most diagnostic and complete mineralogical characterization of rocks and soil by any spacecraft-capable technique, improved upon only by sample return and analysis in terrestrial laboratories [1]. In a complex sample such as a basalt, XRD can definitively identify and quantify all minerals, establish their individual elemental compositions and quantify the amorphous component. When coupled with XRF, the amorphous composition can be determined. X-ray Diffraction analyses of drilled and powdered samples will yield:

- Identification of all minerals present >1 wt. %.
- Quantification of all minerals >3 wt. %, including their structure states and cation occupancies.
- Abundance of all major elements present in each mineral (H and above).
- Valence state of all elements, including speciation of multi-valent species such as Fe.

There are no other instruments currently in NASA's planetary science inventory that can claim even one of these capabilities.

The MSL-CheMin instrument (Fig. 1), the first XRD instrument flown in space, established the quantitative mineralogy of the Mars soil [2], characterized the first habitable environment on another planet [3], provided the first in-situ evidence of Martian silicic volcanism [4], and established an upper limit for P_{CO2} on Mars in Hesperian times [5]. MSL-CheMin, which has been collecting mineralogical data on Mars for more than seven years, is now employed in the characterization of the depositional and diagenetic environments of lacustrine mudstones that comprise the lower strata of Mt. Sharp [6].

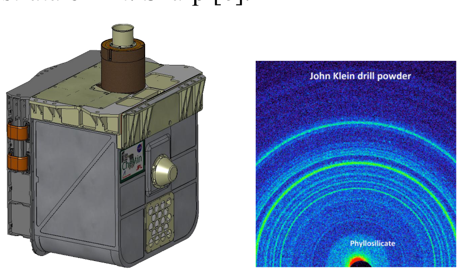

Fig. 1: (left), the MSL-CheMin instrument, 10.5 kg, 300×300×300mm^3; (right), an example of 2D XRD data. Pattern resolution is ~0.35°2θ.

MSL-CheMin as-designed is restricted to Flagship-class missions due to its size, mass and power. Deployment of XRD/XRF on smaller (i.e., MER-class) rovers requires further miniaturization of the instrument, and the availability of a simpler sample collection capability than was implemented for the MSL mission. CheMinX is based on similar principles as CheMin, but benefits from a decade of advancements in geometry design and subsystem miniaturization.

CheMinX design: The XRD measurement of CheMinX is based on the same principles as MSL-CheMin, but uses different components and a different layout for optimum geometry. XRD is collected by a CCD in direct illumination, critical for energy-selective detection of XRD photons in Mars' radiative environment.

For elemental composition, MSL-CheMin used bulk sample compositions determined by a companion instrument (APXS). CheMinX uses an internal Silicon Drift Diode detector (SDD) to provide a concurrent XRF measurement of the sample.

CheMinX sample cells are redesigned for a more compact and lower cost sample handling subsystem. A fixed tuning fork is combined with multiple single-use cells in a cartridge/dispenser arrangement. A preliminary mechanical design of CheMinX is shown in Fig. 2.

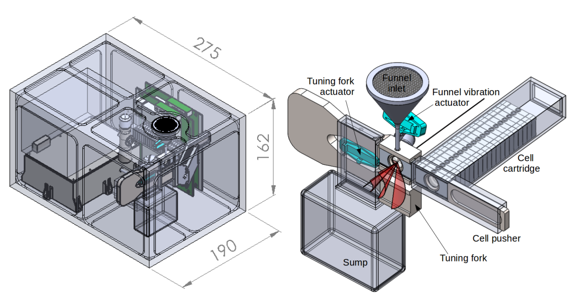

Fig. 2: Preliminary mechanical design of the CheMinX flight instrument; (left), overall instrument with dimensions (mm), projected mass 5kg; (right), sample handling subsystem for the vibrated sample method based on single-use cells in a cartridge.

XRD Geometry and CCD detector: The CheMinX XRD geometry is based on an architecture demonstrated in hundreds of commercial XRD instruments (Terra, a commercial spin-off of MSL-CheMin, marketed by Olympus Corp., Fig. 3). This geometry resulted from a ray-tracing study of MSL-CheMin geometries with high aspect ratio (1024 X 256 pixel) detectors. It was found that reduced surface area CCD detectors can be used with no loss in throughput, angular resolution or angular range. The loss in detector coverage is compensated for by an optimized collimator design. Placement of the CCD at a 30° tilt from the direct beam enables an increased sample to detector distance providing an improvement in 2θ resolution. This geometry modification enables the use of VIS-NIR spectroscopy CCD detectors in place of the custom X-ray CCD of MSL-CheMin. The cost of these detectors as well as their power requirement for deep cooling are dramatically reduced.

In its Terra-like implementation, CheMinX will provide a resolution of 0.3° 2θ FWHM, slightly improved over MSL-CheMin's 0.35°.

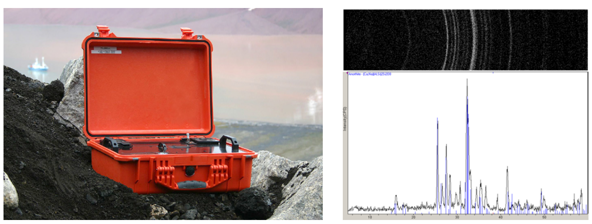

Fig. 3: Terra commercial portable XRD instrument, mass: 14.5 kg (including case, batteries and embedded computer), power: 75W, typical analysis time: 15 min to 1 hr; (left), prototype deployed in Svalbard during 2007 AMASE; (right), 2D image and 1D diffractogram XRD data from Terra. CheMinX will use the same detector and XRD geometry as Terra.

Chemical analysis by X-ray fluorescence: Elemental data are obtained from XRF spectra collected by a Silicon Drift Detector (SDD) in reflection geometry. These spectra are quantified using Fundamental Parameters (FP) approaches and calibrated spectra obtained from experiments conducted under the same conditions in terrestrial laboratories. Depending on the background, trace elements can be detected down to a few 10s of PPM, given sufficient collection time.

Direct beam intensity monitoring: CheMinX has the capability to measure the direct beam intensity at Co K_α. This enables the measurement of sample absorption, which varies with chemistry, compactness and thickness. Absorption inside the sample affects the overall diffracted intensity and the shape of the diffraction peaks, and is as such important for accurately modeling the diffraction pattern for data interpretation. The direct beam intensity measurement is obtained passively with a solid polycrystalline material (diamond, silicon) positioned in the beam-stop structure to diffract a single partially masked ring, proportional to the transmitted beam intensity, on a lesser populated region of the CCD.

Development of High TRL Components: Rapid and cost-effective development of flight instruments requires the availability of mature technologies for critical components. High TRL subsystems are being developed in collaboration with industrial partners: Specialized full-frame and frame-transfer X-ray CCD detectors (Teledyne e2v); custom FPGA-based electronics for low noise CCD operation and embedded data processing (Baja Technology); miniature micro-focused X-ray tubes (RTW) and high voltage power supplies (Battel Engineering). These components will find applications in CheMinX as well as other planetary XRD and XRF instruments developed by our team [7-9].

Sample collection and delivery: CheMinX requires the collection and delivery of powdered rock materials or soils. The identification of simpler sampling technologies than those applied on MSL is critical for the deployment on smaller rovers. We are fabricating and testing sample processing and delivery systems as part of this instrument development, and will demonstrate CheMinX with powdering drills and arm prototypes developed at Honeybee Robotics.

Summary: Substantial reductions in mass, volume and power relative to MSL-CheMin are now possible while achieving improved resolution and 10X reduction in data collection time. An instrument with improved resolution (<0.25° 2θ FWHM) is also being developed to provide better capabilities with complex mineral assemblages and trace phases, at the cost of reduced miniaturization. In either case, the instrument benefits from improved XRF performance through the use of a dedicated SDD placed in backscattering geometry. CheMinX will provide quantitative mineralogy and elemental chemistry from drilled rocks and scooped soils on Mars in a package suitable for deployment on a MER-class rover.

References: [1]. Velbel, M.A. (2018). DOI: http://doi.org/10.2138/am-2018-6468CCBYNCND. [2]. Bish, D.L. et al. (2013) *Science,* 341, 1238932; doi:10.1126/science.1238932, [3]. Vaniman, D.T. et al. (2013) *Science*, 10.1126/science.1243480. [4]. Morris, R.V. et al. (2016) *PNAS*, doi: 10.1073/pnas.1607098113. [5]. Bristow, T.F. et al. (2016) *PNAS*, www.pnas.org/cgi/doi/10.1073/pnas.1616649114. [6]. Bristow, T.F. et al. (2018) *Science Advances*, Sci. Adv. 2018;4: eaar3330. [7]. Walroth et al. (2018) *LPSC-49* #2233. [8]. Blake et al. (2019) *LPSC-50* #1144. [9]. Blake et al. (2019) *LPSC-50* #1468.