CHEMINX: A NEXT GENERATION XRD/XRF FOR MARS EXPLORATION. P. C. Sarrazin[1], T. F. Bristow[2], D. F. Blake[2], M. Gailhanou[3], J. Chen[4], B. Lafuente[1], K. Thompson[1], R. Walroth[2], K. Zacny[5], R. T. Downs[6], G. W. Downs[6], and A. Yen[7], [1] SETI Institute, Mountain View, CA (psarrazin@seti.org), [2] Exobiology, NASA ARC, Moffett Field, CA, [3] CNRS, IM2NP UMR, Marseille, France, [4] Baja Technology, Tempe, AZ, [5] Honeybee Robotics Spacecraft Mechanisms Corp., Pasadena, CA, [6] Geosciences, Univ. Arizona, Tucson AZ, [7] JPL, Pasadena, CA.

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

The MSL CheMin instrument (Fig. 1), the first XRD instrument flown in space, established the quantitative mineralogy of the Mars soil [1], characterized the first habitable environment on another planet [2], and provided the first in-situ evidence of Martian silicic volcanism [3]. CheMin is now employed in the characterization of the depositional and diagenetic environments of lacustrine mudstones that comprise the lower strata of Mt. Sharp [4].

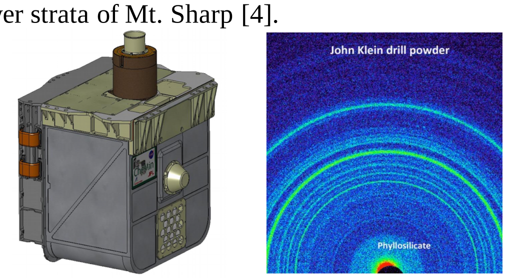

Fig. 1: The MSL CheMin instrument, 10.5 kg, 300×300×300mm^3 (left) and example of 2D XRD data (right). Resolution is ~0.3°2θ.

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. We are developing CheMinX, based on similar principles as CheMin, yet benefiting 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 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, CheMin used bulk sample compositions determined by a companion instrument (APXS). With CheMinX, the instrument provides XRF measurement independently using an internal Silicon Drift Detector (SDD).

Evolutions of the resonant sample cells of CheMin 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.

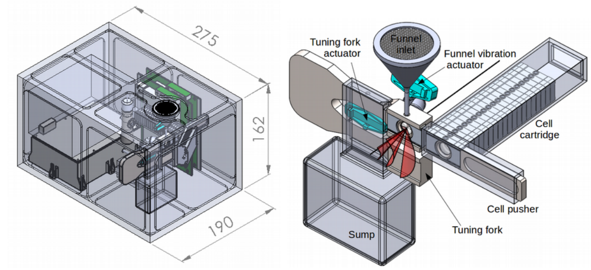

Fig. 2: Preliminary mechanical design of the CheMinX flight instrument; left: overall instrument with dimensions (mm), projected mass 5kg; right: sample handling subsystem for the vibrated sample method based on single-use cells in a cartridge.

Benefits of higher XRD resolution: CheMin's 0.35° 2θ FWHM (full width half maximum) resolution has been shown to be sufficient for deciphering and quantifying the mineralogies analyzed on Mars but causes some challenges with the correct identification of pyroxenes. A study was conducted to evaluate the benefits of improved resolution. XRD patterns were simulated representing a mixture of nine minerals and an X-ray amorphous phase, calculated at different resolutions (0.15<FWHM<0.4° 2θ), all other parameters being equal (total count, background, injected noise). The mineral selection, which includes a mixture of three types of pyroxene, is representative of basaltic sediments observed at Gale crater. Simulated patterns were analyzed blind using Jade Rietveld refinement and the same methods employed to analyze CheMin data from Mars. Identification of all major mineral groups is possible at the lowest resolution. However, identification of the correct mixture of pyroxenes was only possible at resolutions ≤0.25° 2θ FWHM. The correct identification of mixtures of common basaltic minerals, like pyroxenes, is required to permit calculation of unit-cell parameters and chemical compositions of minerals. This information also helps to determine the source area(s) of basaltic sediments and the igneous processes that operated in these areas.

XRD Geometry and CCD detector: The CheMinX XRD geometry is based on an architecture demonstrated by hundreds of commercial XRD instruments (Terra, commercial spin-off of CheMin, Fig. 3). This geometry resulted from a ray-tracing study of

CheMin geometries with high aspect ratio 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 being fully compensated for by an optimized elongated collimator design. Placement of the CCD at a 30° tilt from the direct beam enables an increased sample to detector distance providing a slight improvement in 2θ resolution. This geometry modification enables the use of commercial VIS-NIR spectroscopy CCD detectors in place of the custom X-ray CCD of CheMin. The cost of these detectors as well as their power requirement for deep cooling are dramatically reduced.

In its Terra-like implementation with a single CCD, CheMinX will provide a resolution of 0.3° 2θ FWHM, slightly improved over CheMin's 0.35°. We are also designing a dual CCD configuration of CheMinX for higher XRD resolution. Ray tracing simulations established that 0.15-0.2° 2θ FWHM can be achieved with no loss of angular range by combining a low range and high range CCD, positioned at increased distance from the sample. This dramatic improvement in instrument performance comes at a significant cost in size, weight and power of the instrument. The single CCD version remains our prime focus due to its increased miniaturization. The higher resolution dual CCD version is taken into account in the subsystems development (particularly the CCD electronics) should a flight CheMinX be allocated sufficient volume, mass and power to host two CCDs.

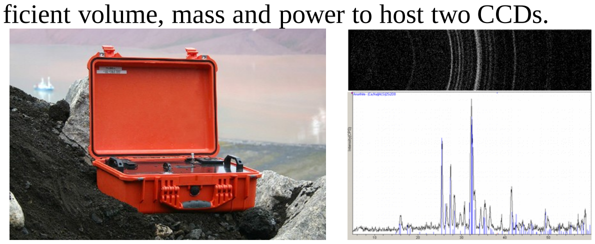

Fig. 3: Terra commercial portable XRD instrument, mass: 14.5 kg (including case, batteries and embedded computer), power: 75W, typical analysis time: 15 min to 1 hr, Left: prototype deployed in Svalbard during 2007 AMASE, Right: 2D and diffractogram XRD data collected at this site. CheMinX will use the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

Chemical analysis by X-ray fluorescence: Elemental data is 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 the critical components. High TRL subsystems are being developed in collaboration with industrial partners: Special full-frame and frame-transfer X-ray CCD detectors are being developed with (Teledyne e2v), custom FPGA based electronics for low noise CCD operation and embedded data processing (Baja Technology), miniature microfocused X-ray tubes (RTW), high voltage power supplies (Battel Engineering), etc. These components will find applications in CheMinX as well as other planetary XRD and XRF instruments developed by our team [5-7].

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 of CheMinX on smaller rovers. We are evaluating sample processing and delivery technologies as part of this instrument development, and will demonstrate CheMinX with powdering drills and arms prototypes developed at Honeybee Robotics.

Summary: Substantial reductions in mass, volume and energy consumption relative to MSL CheMin are now possible for similar XRD performance (resolution of 0.30-0.35° 2θ FWHM). 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 both cases, the instrument benefits from improved XRF performance by 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 or other locations in the Solar System.

References:

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