MSL Chemistry and Mineralogy X-ray Diffraction X-ray Fluorescence (CheMin) Instrument

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***Abstract*—This paper provides an overview of the Mars Science Laboratory (MSL) Chemistry and Mineralogy X-ray Diffraction (XRD), X–ray Fluorescence (XRF) (CheMin) Instrument, an element of the landed Curiosity rover payload, which landed on Mars in August of 2012. The scientific goal of the MSL mission is to explore and quantitatively assess regions in Gale Crater as a potential habitat for life – past or present. The CheMin instrument will receive Martian rock and soil samples from the MSL Sample Acquisition/Sample Processing and Handling (SA/SPaH) system, and process it utilizing X-Ray spectroscopy methods to determine mineral composition. The Chemin instrument will analyze Martian soil and rocks to enable scientists to investigate geophysical processes occurring on Mars. The CheMin science objectives and proposed surface operations are described along with the CheMin hardware with an emphasis on the system engineering challenges associated with developing such a complex instrument.**

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1. MISSION OVERVIEW

Launched in the fall of 2011, the Mars Science Laboratory (MSL) is part of NASA's Mars Exploration Program, a long-term effort of robotic exploration of the red planet. Mars Science Laboratory is a rover that will assess whether Mars ever was, or is still today, an environment able to support microbial life. In other words, its mission is to determine the planet's "habitability." MSL mission high- lights are summarized in Table 1 and MSL CheMin instrument highlights are summarized in Table 2 [1]. MSL successfully landed on August 5, 2012 (PDT).

The science objective of MSL is to "explore and quantitatively assess a local region on the Mars surface as a potential habitat for life, past or present." The duration of the primary mission of MSL will be 670 sols, or one Mars year. During this time, the rover will traverse to at least three geologically distinct sites within its landing ellipse, and determine the "habitability" of these sites. Habitability is defined in this context as the "capacity of the environment to sustain life."

MSL will rely on new technological innovations, especially for landing. The spacecraft will descend on a parachute and then, during the final seconds prior to landing, lower the upright rover on a tether to the surface, much like a sky crane. Once on the surface, the rover will be able to roll over obstacles up to 75 centimeters (29 inches) high and travel up to 90 meters (295 feet) per hour. On average, the rover is expected to travel about 30 meters (98 feet) per hour, based on power levels, slippage, steepness of the terrain, visibility, and other variables.

The rover carries a radioisotope power system that generates electricity from the heat of plutonium's radioactive decay. This power source gives the mission an operating lifespan on Mars' surface of a full Martian year (687 Earth days) or more, while also providing significantly greater mobility and operational flexibility, enhanced science payload capability, and exploration of a much larger range of latitudes and altitudes than was possible on previous missions to Mars. While the MSL rover will carry a variety of in-situ instrumentation for collecting Mars data from the surface, this paper focuses primarily on the CheMin Instrument.

Science Objectives

MSL is intended to study Mars' habitability. It will carry the biggest, most advanced suite of instruments for scientific studies ever sent to the Martian surface. Their purpose is to assess whether Mars ever had an environment capable of supporting microbial life. More specifically, MSL has the following science objectives:

Biological objectives:

- Determine the nature and inventory of organic carbon compounds
- Inventory the chemical building blocks of life (carbon, hydrogen, nitrogen, oxygen, phosphorous, and sulfur)
- Identify features that may represent the effects of biological processes

Geological and geochemical objectives:

- Investigate the chemical, isotopic, and mineralogical composition of the Martian surface and near-surface geological materials
- Interpret the processes that have formed and modified rocks and soils

Planetary process objectives:

- Assess long-timescale (i.e., 4-billion-year) atmospheric evolution processes
- Determine present state, distribution, and cycling of water and carbon dioxide

Surface radiation objective:

- Characterize the broad spectrum of surface radiation, including galactic cosmic radiation, solar proton events, and secondary neutrons

The rover will analyze dozens of samples scooped from the soil and drilled from rocks. The record of the planet's climate and geology is essentially "written in the rocks and soil" – in their formation, structure, and chemical composition. The rover's onboard laboratory will study rocks, soils, and the local geologic setting in order to detect chemical building blocks of life (e.g., forms of carbon) on Mars and will assess what the Martian environment was like in the past.

Table 1: MSL Mission Highlights

Mission	Mars Science Laboratory (MSL)
Life-Cycle Phase	Phase C-E (Design/Build/Ops)
Mission Type	Surface, Rover Instrument
Competed vs. Directed	Directed, Mars Program
JPL Role	Manage, build, launch, operate high-capability Mars rover;
Contractors	Lockheed Martin Space Systems: spacecraft Alliance Space Systems Inc.: robotic arm
Inheritance	Viking, Mars Pathfinder, Mars Exploration Rover (MER) DoE (GRC, MSFC) RPS
Hardware	Spacecraft, sky crane, rover, instruments
Science Instruments/ Engr. Instruments	Cameras: Mast Camera Mars Hand Lens Imager Mars Descent Imager Spectrometers: Alpha Particle X-Ray Chemistry & Camera Chemistry & Mineralogy X-Ray Diffraction Sample Analysis at Mars Instrument Suite Radiation Detectors: Radiation Assessment Detector Dynamic Albedo of Neutrons Rover Environmental Monitoring Station
Primary Science Objective	Assess the history of environmental conditions on Mars at sites that may once have been wet and favorable to life.
Cost	Total cost $1,700M (estimated)
Mission Start	Pre-Phase A start 10/01/2001; Phase A start 11/24/2003
Launch Date **Launch Vehicle** **Launch Site**	November, 2011 Atlas V 541 Cape Canaveral Air Force Stn
Project Manager **Deputy PM**	Peter Theisinger, Richard Cook
Project SE **Flight System SE**	Joel Krajewski Ann Devereaux
Project Scientists	John Grotzinger (Caltech) Ed Stolper (Caltech)

Science Payload Principal Investigators (PIs) Science Payload Principal Investigators (PIs) (Con't.)	David Blake (ARC) Ken Edgett (Malin Space Science Systems) Don Hassler (Southwest Research Institute) Paul Mahaffy (GSFC) Michael Malin (Malin Space Science Systems) Igor Mitrofanov (Space Research Institute) Luis Vázquez (Center for Astrobiology, Madrid) Roger Wiens (Los Alamos National Lab)

Chemin Instrument Science Objectives

The CheMin X-ray Diffraction (XRD) instrument will be principally engaged characterizing the geology and geochemistry of the landed region at all appropriate spatial scales (i.e., ranging from micrometers to meters). The science objective of the CheMin instrument is to investigate the chemical and mineralogical composition of the Martian surface and near-surface geological materials to provide scientists the information needed to interpret processes that have formed and modified rocks and regolith.

CheMin is a definitive mineralogy instrument, meaning that the emphasis is on measurements that will aid in understanding aqueous processes on Mars. This is an essential role within the MSL analytical instrument laboratory. Moreover, Table 3 [2] shows the relationship between NASA's MSL science goals and specific CheMin measurements.

Table 2: MSL CheMin Instrument Highlights

Instrument	Chemistry & Mineralogy X-Ray Diffraction (CheMin)
Life-Cycle Phase	Phase C-E Design/Build/Ops)
Instrument Type	Spectrometer
JPL Role	CheMin instrument management, implementation, and operations.
Instrument Contractors	X Ray Source – Oxford Instruments (Lack of JPL Capability) CCDs – E2V (UK) (Only available source for technology) Coolers – RICOR (Lack of JPL Capability, Best available supplier)
Inheritance	CheMin3 prototype field unit
CheMin Instrument Hardware	X Ray Source, CCDs, Coolers
Primary Science Objective of CheMin Instrument	Investigate the chemical and mineralogical composition of the Martian surface and near-surface geological materials
CheMin Cost	Development: $39.9M cost Capped
Instrument Start	2002
Instrument Manager	Wayne Zimmerman (Current)
CheMin Principal Investigators	David Blake, PI (ARC) David Vaniman, Deputy PI Albert Yen, Investigation Scientist
MSL CheMin Website	http://marsprogram.jpl.nasa.gov/msl/mission/sc_instru_chemin.ht ml

2. HARDWARE OVERVIEW

MSL will truly be a chemistry laboratory on wheels. Going beyond just having a very powerful "fistful" of instruments as MER's Spirit and Opportunity rovers do, MSL will also take samples onboard and analyze them. Some instruments on MSL inherited significant technology from their predecessors on the Mars Exploration Rovers, but they are, indeed, "next generation" in terms of capability.

Table 3: Science Investigations for CheMin Instrument

MSL Science Goals	MSL CheMin Measurements
Mineralogical characterization of hydrous processes.	Identification and quantification of water-precipitated/deposited minerals by **XRD** - clays, micas, hydrates, evaporitic mineral suites (sulfates, halides, borates, nitrates, etc.), carbonates, silica polymorphs.
Identify & characterize phases containing C,H,O,N,P,S	Identification and quantification of carbonates, hydrates, nitrates, phosphates, sulfides and sulfates by **XRD**.
Determine the array of potential energy sources on Mars	Identification and quantification of Fe, Mn,S– containing minerals via **XRD**, elemental analysis of Fe (Iron), Mn (Manganese) and S by **XRF**.
Inventory chemical building blocks of life, identify features that may record biologically relevant processes that have taken place over time.	Identification and quantification of carbon-containing minerals – carbonates, graphite having a range of crystallinity, by **XRD.** Provide mineralogic context for organic carbon measurements by other instruments.
Mineralogical characterization of samples containing C,N,P, or S	Mineralogical identification and quantification of carbonates, nitrates, phosphates, sulfides and sulfates by **XRD**.
Interpret the processes that have formed and	Identification and quantification of aqueous and diagenetic minerals in the context of their host rocks and facies

modified rocks and regolith.	**XRD**. Provide detailed mineralogical analysis to support interpretations of rock fabrics and sedimentary structures.
Investigate the chemical & mineralogic composition of surface and near-surface materials.	Identify sedimentary minerals, sedimentary diagenetic products in the context of their host rocks and facies by **XRD**. Provide a mineralogical underpinning for the interpretation of rock fabrics, sedimentary structures and macroscopic morphological features in rocks and outcrop by **XRD**.
Investigate the chemical and mineralogic composition of igneous materials	Identify igneous minerals and bulk igneous chemistry in basalts and other igneous rocks (magma differentiation, Fe/Mg content of olivine) by **XRD**, evaluate bulk chemistry of igneous rocks by **XRF**.
Investigate the chemical and mineralogic composition of soils	Identify chemistry, mineralogy of near-surface rocks, mineral phases present in the soil, hydrothermal minerals and magnetic phases by **XRD** and bulk chemistry by **XRF**.
Investigate the chemical and mineralogic composition of subsurface rocks	Identify mineralogy of subsurface rocks delivered to the surface by mass wasting and impact gardening by XRD. Evaluate bulk chemistry of subsurface materials by XRF.

Chemistry and Mineralogy X-Ray Diffraction (CheMin) instrument – CheMin represents a major advancement in identifying Martian minerals. After the rover prepares a rock sample, CheMin will then direct a beam of X-rays as fine as a human hair through the powdered material. Because all minerals diffract X-rays in a characteristic pattern and all elements emit X-rays with a unique set of energy levels, scientists will use the information from X-ray diffraction to identify the crystalline structure of materials the rover encounters on Mars. These analyses will assist in the assessment of water history and the search for possible signatures of life.

CheMin Instrument Overview

CheMin will identify and measure the abundances of various minerals on Mars. Examples of minerals found on Mars so far are olivine, pyroxenes, hematite, goethite, and magnetite. Minerals are indicative of environmental conditions that existed when they formed, and can suggest the role that water played in the formation.

Figure 1 shows the CheMin instrument that is installed within the instrument payload area of the rover [3]. A small inlet at the top of the instrument accepts a sample. A beam of X-rays is directed onto the sample. When the X-rays interact with the rock or soil sample, some of the X-rays will be absorbed by atoms in the sample and re-emitted or fluoresced at energies that are characteristic of the particular toms present. This results in a specific unique interference pattern being captured by an internal CCD detector.

Basic Measurement Description

CheMin determines the mineralogy and elemental composition of crushed or powdered samples through the combined application of X-ray diffraction (mineral structure analysis) and energy-dispersive histogram spectra (chemical analysis). This is the preferred method for mineralogical analysis of unknowns in terrestrial labs. With the exception of the sample handling system, CheMin has no moving parts, expendable re-agents, or chemicals. Figure 2 shows the measurement concept underlying CheMin.

In operation, a collimated X-ray beam from an X-ray tube source is directed through powdered or crushed sample material. An X-ray sensitive CCD imager is positioned on the opposite side of the sample from the source and directly detects X-rays diffracted or fluoresced by the sample, shown in Figure 2. The CCD is read out often enough so that each pixel very rarely contains charge from multiple photons. Diffracted primary beam X-rays strike the detector and are identified by their energy. A two-dimensional image of these X-rays constitutes the diffraction pattern.

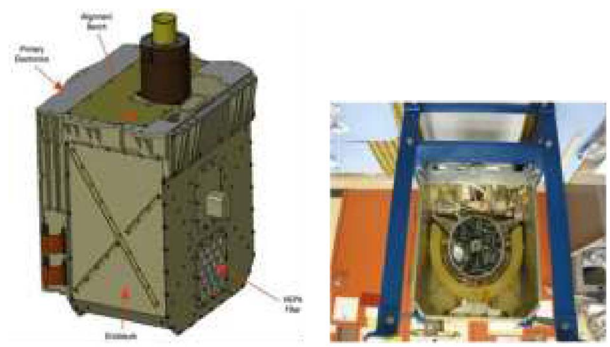

Figure 1: Chemistry and Mineralogy X-Ray Diffraction (CheMin) Instrument

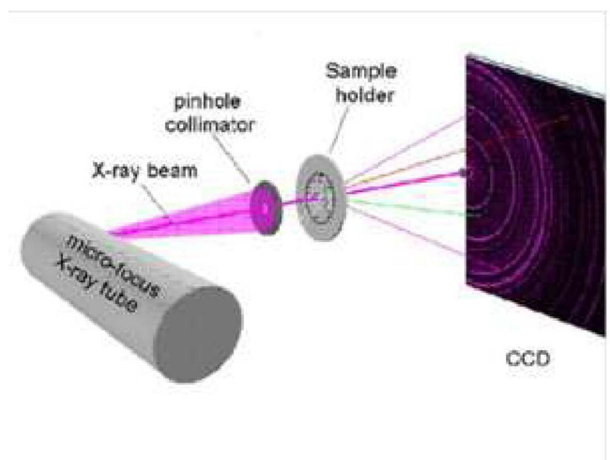

Figure 2: CheMin Measurement Concept

In X-ray diffraction, some X-rays bounce away at the same angle from the internal crystal structure in the sample. When this happens, they mutually reinforce each other and produce a distinctive signal. All elements will emit X-rays with a unique set of energy levels (fluoresced) as well. The CCD collects both diffraction and fluorescence information. Scientists will use the information from X-ray diffraction to identify the crystalline structure of materials that the rover encounters on Mars. An example of a conventional diffraction data plot is shown in Figure 3. All of the X-rays detected by the CCD are summed into a histogram of number of photons (registered counts on the CCD, y-axis) vs. photon energy (x-axis) that constitutes an energy-dispersive histogram sample, shown in Figure 3. Both crystalline and amorphous materials can be analyzed utilizing products similar to the plots in Figure 3. XRF is a by-product of X-ray energy absorption. The energy absorbed is re-emitted in the form of fluorescence which, in turn, is sensed by the detector. The stored charge captured by each pixel is summed and that total energy, measured in electron volts (eV), is unique to each mineral. The science team decided to de-scope the XRF requirement due to schedule constraints.

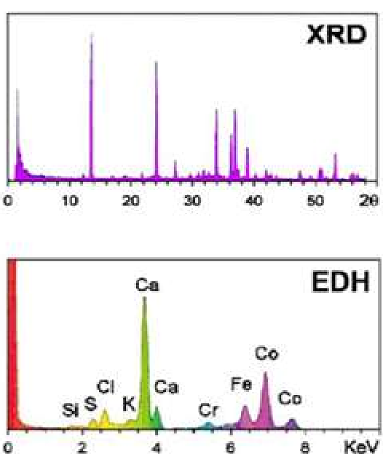

Figure 3: CheMin Resulting Data Sets Concept

Laboratory XRD instruments are generally provided with samples in the form of a powder, with all possible crystallographic orientations presented to the X-ray beam in a random distribution. The grains provided to CheMin will not be as finely ground as a laboratory sample and the beam angle is fixed with respect to the sample cell. Grain orientations must be actively randomized to avoid over representation of particular orientations during analysis. This skewed representation can cause saturation of pixels at these orientations and reduction resolution and relative peak height precision.

Acceptable measurements can be obtained from even poorly sorted or poorly powdered materials if the sample is agitated and particles reoriented sufficiently during the integration period. Achieving acceptable "grain motion," is a critical functional requirement for the instrument design. In practice, this is implemented with a piezoelectric driver that vibrates the sample cell at sonic frequencies in order to provide characteristic grain motion.

The nominal duration of a single experiment, sufficient to quantitatively analyze a single mineral such as quartz or olivine, is 4 hours. Complex assemblages such as basalt with 8 or more minerals may require up to 10 hours of data. This data need not be taken contiguously.

The hardware used to produce the measurement is comprised of a collimated X-ray source, a sample handling mechanism with sample holder, and a cooled X-ray detector. All of this is controlled by a Field Programmable Gate Array (FPGA) and associated electronics (CCD electronics, memory, power supplies, etc.). Schematics of CheMin are displayed in Figures 4 and 5 showing side-and top-views, respectively. Details shown in these figures are discussed further in subsequent sections.

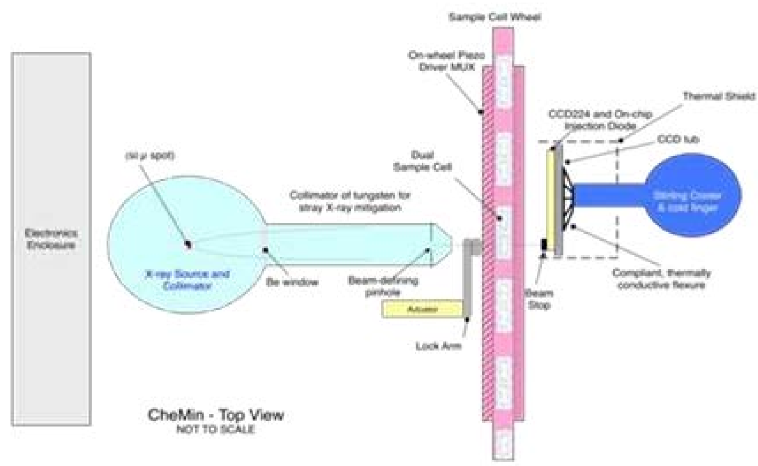

Figure 4: CheMin Schematic - Side View

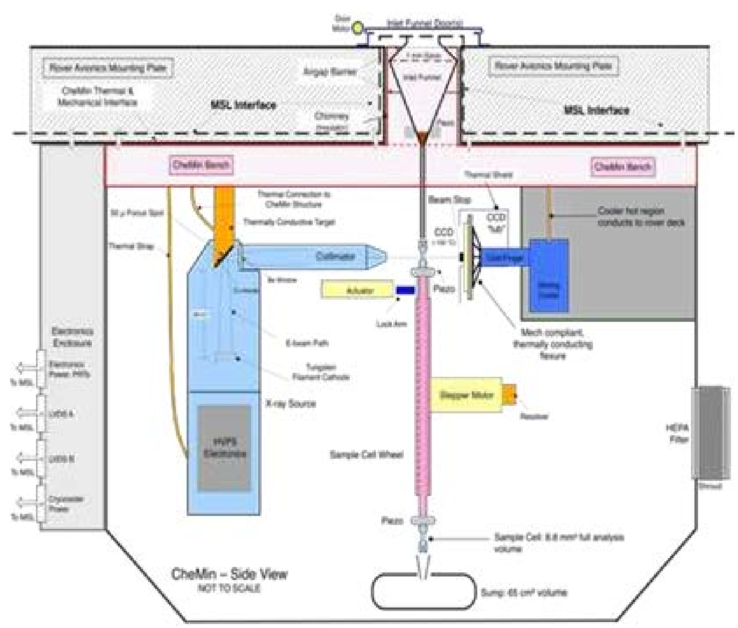

Figure 5: CheMin Schematic - Top View Figure

Major Functional Elements

The CheMin structure and mechanisms [3] consist of the instrument housing (Figure 1), an inlet funnel with piezo actuators to assist powder ingestion, a motor-driven system to move the sample cells into position to receive powder, and piezo actuators to vibrate the sample cells during analysis and emptying into the sump. The Stirling cooler is mounted interior to the main chassis, near the detector. The wheel positions the sample cell under analysis in line with the X-ray beam of the source. The funnel has been configured to avoid the possibility of particles jamming between the funnel and the sample cell.

Sample Handling and Holder Reservoir (Cell)

The sample handling system [3] allows CheMin to receive material from the MSL Sample Acquisition/Sample Processing and Handling (SA/SPaH) system. A funnel with a small tubular extension serves to receive the powder from SA/SPaH system and deliver that powder to the sample cell. The sample "cell" is a small container with a transparent window on each side. The cell is designed to be reusable and mounts to a sample wheel that rotates to accept a sample, to position the sample under test in line with the source, or to empty out the sample into the sump. Three piezo actuators are attached to the funnel and provide vibration to assist powder flow into a sample cell via the input tube. The tube has an inlet aperture approximately 3 mm in diameter and 35 mm in length. A sample cell is an approximately square, flat enclosure into which a single powder sample (~ 45 - 65 mm^3) is loaded for subsequent analysis, most easily seen in Figure 6. The two flat faces of the cell include windows of thin polymer membranes transparent to X-rays. Sixteen dual sample cell sub-

Figure 6: Dual Sample Cell Subassembly

assemblies are mounted on the sample wheel. Five of the sample cells will contain a variety of calibration samples installed before launch. The wheel rotates to place a selected cell beneath the sample receiving tube. This position is also the analysis position. The wheel also rotates to place a cell at the bottom of the wheel to empty its contents into a sump. The distance between the top cell and sump position, coupled with the small amount of sample, mitigates the possibility of dust migrating upwards onto other sample windows and potentially attenuating the beam strength. This was confirmed via actual laboratory testing [3].

X-Ray Source & Collimator

The X-ray Source (XRS) consists of an X-ray tube, collimator, high-voltage power supply (HVPS) and controller [3]. The X-ray tube consists of a tungsten filament cathode, a focus electrode, a cobalt anode, and a beryllium window, integrated into a single package. The filament produces free electrons that are accelerated by the 28 kV potential differences between the cathode and the anode.

These X-rays illuminate a pinhole aperture, which in turn images the analog electron spot onto the sample. Incident X-rays are diffracted, absorbed, or transmitted by the powder. Diffracted X-rays are scattered from the incident beam at an angle defined by Bragg's Law (sin= n /2d where 2 = angle of diffraction, = X-ray wavelength, d = spacing of a crystal plane in a powder particle and n = 1, 2, 3....). Diffraction of many photons by a random distribution of grains will produce a series of diffraction cones captured as concentric circles on the CCD detector normal to the incident beam.

Cooled CCD Detector

CheMin's detector (model CCD224 from e2V) is an X-ray sensitive CCD that has the ability to measure both the location (x, y) and energy (E) of each X-ray photon it detects. The CheMin CCD detects photons whose energies range from 1.1 to 10 keV, corresponding to elements from Magnesium through Germanium. The detector is similar to the CCDs used on other X-ray space missions. The CCD pixel size of 40 µm x 40 µm and 600 x 600 pixel format was chosen, in combination with the geometry of the instrument, to provide the required angular range and resolution for the XRD experiment. The CCD is a three-phase frame-transfer device. The primary X-ray beam is centered at one edge of the image area. Masks over the light-sensitive and charge transfer regions minimize background noise.

The CCD is conductively cooled. The device is designed for an operating temperature of -60 to -100 °C by a Stirling cycle cryocooler. The CCD must be cooled to minimize dark current noise.

During testing of the CDD installed in the CheMin instrument, it was shown that for a temperature range of -10 to -35 °C, reliable XRD data could be acquired with using the CCD which was promising given the capability of the cryo-cooler to take the detector to even lower temperatures.

Electronics

The CheMin electronics provide signal handling for the CCD and digitization of CCD data. There is non-volatile storage for several thousand datasets, each nominally representing 30 seconds of analysis. Internal temperature sensors and voltage levels are monitored. Science and engineering data are passed to the Rover via a digital interface. In addition, CheMin electronics must provide interfaces for the cryocooler, x-ray source (XRS), 2 motors used to rotate the sample wheel, a paraffin actuator, and a decontamination heater for the CCD. Sample wheel position telemetry must be monitored. Three piezoelectric actuators on the funnel and 16 on the sample wheel are individually commandable. Finally, power must be provided for the electronics, x-ray source (and its heaters), and the cryo-cooler.

3. SOFTWARE OVERVIEW

CheMin does not have a microprocessor, but has embedded software (firmware) within the instrument FPGA. Control is implemented in a one-time field-programmable gate array (FPGA), which contains several distinct processors (state machines), each responsible for its own element. Processes communicate via discrete semaphores (flip flops), and are controlled by uploadable parameters. A single command can initiate a complex process involving many of the CheMin elements in a sequence that can last many hours. This allows CheMin to operate autonomously during the Martian night, having no interaction with the Rover once commanded.

At the beginning of the Martian night, the RCE sends commands to the instrument to turn it on and to analyze the sample. The Rover then begins its nightly hibernation. CheMin verifies that temperatures are OK for analysis, ramps up the high voltage on the x-ray source, and enables the cryocooler. When the XRS is ready, and the analysis temperature has been reached, CheMin begins vibrating the piezo on the cell under analysis and begins saving frames of data. Periodically, the cell piezo changes from normal vibration mode to a so-called 'chaos' mode for one frame, to further agitate the sample. Earth scientists do this 'by hand' while analyzing on earth, so CheMin was designed to mimic this. Since this entire operation is autonomous, CheMin also maintains a robust set of parameters and conditions that will cause it to safe if violated. Under normal operation, when the requisite number of data frames have been acquired, CheMin ceases data collection, ramps down the XRS, takes one frame of dark data, and shuts everything off. CheMin waits in idle mode until morning. All housekeeping telemetry, parameters, and machine state are saved with each analysis frame. Data are stored in non-volatile flash memory. When the rover 'wakes up', it commands CheMin to transfer the data into RCE memory, thus completing one sol of analysis.

CheMin Software Operational Scenario

A normal operational scenario depends heavily on the Rover Compute Element software. The sequence of events will nominally be to turn on CheMin, receive multiple samples from the SA/SPaH system, and dispose of them to clean the cell, then acquire a final sample for analyses using the SA/SPaH system. CheMin is commanded to shake both its funnel and cell to distribute the sample for analysis. Once the sample is in the cell, CheMin operation is suspended until the Martian night when other functionality aboard the rover will be disabled.

During the Martian night, the RCE sends commands to the instrument to (1) turn it on, (2) cool the CCD detector and (3) ramp up the high voltage on the X-ray tube. After CCD and X-ray source devices are stable, samples are shaken again. The RCE commands the instrument to start data collection and store results into flash memory within the instrument.

During data collection, successive X-ray exposures are combined to provide longer integrations of up to 10 hours needed to meet the science requirements. Large data volumes are generated by operating the CCD as a single photon counting device. CheMin stores all of the uncompressed data prior to transmission to the rover.

Housekeeping data is also generated at a rate equal to the rate at which exposures are taken, nominally every 30 seconds, even when X-ray analysis is not happening. Housekeeping data consists of internal temperature and voltage readings of various components within the instrument. There is sufficient flash (non-volatile) memory to store all of the raw data and housekeeping data for an entire analysis, with margin.

The data collection and storage are done autonomously within the instrument. Data processing and transmission to Earth is done by the RCE. On completion of an analysis session, the RCE will turn off the instrument.

CheMin data will be provided through the MSL Ground Data System (GDS), however, CheMin will have its own GDS. The CheMin GDS will be designed to provide the requisite technical science and engineering products from the instrument.

4. TECHNICAL CHALLENGES

The technical challenges of developing a CheMin instrument actually started long before the MSL mission concept was finalized, with the development of field instruments. The history of how these field instruments evolved into flight instruments is described below.

Challenges encountered during development of CheMin included meeting requirements for weight, volume, power, and thermal properties. Additional challenges involved uncovering late signal noise issues, flying a unique sample handling system, and the problems associated with the development of an X-ray source for flight. Lastly, there was the challenge of developing the FPGA firmware on schedule.

Technology Readiness Level

Mineral analysis using the XRD/XRF technique in the laboratory has been performed for some time [4]. It was not until the early 1990's that groups began to deploy instruments to the field to perform in-situ XRD/XRF mineral analysis. These units were initially rather large, bulky, and power hungry. With advancements in components, smaller and lower power field instruments, generically known as "CheMin", began to be implemented around 2001. By 2003, there was an instrument (known as CheMin 3) that began to demonstrate the true feasibility of future extraterrestrial usage. Figure 7 shows the CheMin 4 in Death Valley, CA in 2004 [5]. This instrument was implemented as the next step after CheMin 3. The prototype instrument, which can be hand-carried to remote locations, weighs about 20 kg. A geologist's hammer is shown for scale.

(Death Valley, CA 2004)

Figure 7: CheMin 4 Prototype Instrument

Weight, Volume & Energy Limits

The spaceflight CheMin instrument (shown in Figure 1) looks much different than the prototype and weighs about

10 kg [5]. The MSL flight requirement for the instrument is a weight of less than 12.4 Kg. Weight reduction from the prototype was achieved through a series of careful materials choices and updates to the CheMin mechanical design. However, meeting the weight requirement for CheMin was a challenge since during the redesign of the high voltage power supply, ruggedization for flight added mass to the instrument. The extra weight could not be eliminated, so the CheMin Project negotiated with MSL to increase the original 5 Kg allotted weight to the current 12.4 Kg.

CheMin flight volume has remained stable and fits nicely into the allocated volume of 30 cm. x 29 cm. x 27 cm. This was achieved by careful tradeoff analysis. Early on, it was planned that the instrument would contain two X-ray sources (XRS), but it was discovered that two XRS would not fit into the limited volume available. A decision was made to eliminate one XRS. Originally, the intention was to do true quantitative XRF with one XRS. XRD would be done using the other XRS. XRF requires higher energy and less beam collimation precision, while the XRD requires less energy and a narrow, more precise beam. True quantitative XRF requires both a measurement of reflected and transmitted x-ray energy. This requires an extra X-ray detecting diode to measure reflected X-ray energy. A common CCD detector measures the transmitted X-ray energy. Problems with procuring a flight qualified diode for XRF, schedule pressure, and the need to reduce volume resulted in the instrument team deciding to reduce the XRF to a qualitative measurement utilizing transmitted energy only. This decision was determined not to have any volume requirement for the instrument to be met.

The MSL rover power system provides CheMin with 2 amp and 4 amp switches to supply the instrument with suitable current. The MSL Project keeps an energy budget. The flight energy requirement for CheMin is 750 Watt-hours and the current best estimate of usage is 719 Watt-hours. CheMin is within the MSL energy budget for the instrument with a little margin. However, the power requirement comes from meeting thermal interface requirements that were a challenge for the instrument team.

Thermal Challenges

CheMin was originally designed to operate within a temperature range of -40 °C to +50 °C. As the design matured, X-ray source design limitations limited the thermal operating range to -20 °C to +20 °C. This range is maintained passively by the design of the thermal paths and structure connecting the instrument to the Rover Avionics Mounting Plate (RAMP), which is temperature controlled. As designed for normal Mars operations, the CCD is cooled to -100 C below the RAMP temperature. However, higher than expected heat leaks to the CCD were caused by three primary sources:

(1) The thermal model done for the CDR predicted approximately a factor of five lower heat flow from the alignment bench to the CCD than estimated in the final thermal model. In a vacuum environment the CCD cools to -100°C. However, in the Martian environment (predominately CO_2) temperatures are limited to -55°C to -60°C below the RAMP temperature. This is due to high heat conduction through the small gaps between parts of the CCD light baffle and support which are very close to the

bench. The heat leak was increased by the 0.0012” thick copper plating under the gold plating on the CCD baffle. Redesign of the interface was not feasible.

(2) The CDR thermal model predicted a lower heat flow through the cryo-cooler bumper tube to the cryo-cooler cold finger by about a factor of six as compared to the final thermal model. The difference was primarily caused by the unaccounted for plating of 0.0012” copper on the inside and outside of the bumper tube. The effect was mitigated by replacing the bumper tube with one having no copper plating and covering the inside and outside of the cryo-cooler bumper tube with a layer of gold foil.

(3) The CDR thermal model predicted around a two and one-half times lower heat flow through the Titanium CCD support than was estimated in the final thermal model. This was caused by a modeling error. Redesign of the interface was not feasible due to schedule constraints.

Schedule slip of the Developmental Model (DM), due to budget constraints, eliminated an early thermal test in vacuum which had it been done in a simulated Martian Environment, would have flagged this thermal issue. Fortunately the performance of the E2V CCD in terms of low noise/dark current was significantly improved from the previous versions allowing satisfactory science return.

There is an operational constraint for the X-ray source at the interface to the RAMP of +20 °C. The CCD detector needs to be very cold, while the X-ray source operates warm. Attempting to balance all the thermal requirements is non-trivial. The CheMin instrument has heat in all the wrong places, so proper temperature ranges on components are maintained using active heaters and coolers. Maintaining proper temperature ranges is a particularly difficult engineering challenge.

There are 11 temperature sensors that are read by CheMin. These monitor the X-ray source, CCD detector and various mechanical assembles. The CCD detector and X-ray source are the most critical components for temperature control. The CCD (as discussed above) is conductively cooled by a Stirling-cycle cryo-cooler connected to the CCD via a flexible thermal strap. The X-ray Source dissipates 13 W when operating, to keep temperature from exceeding the +20 °C limit. Most power is dissipated via conduction through a thermal strap and jacket around the high voltage power supply (HVPS) to an alignment bench with the X-ray tube. To ensure the HVPS package temperature does not exceed allowable operational limits, a thermal jacket is mounted on the package with a high conductivity thermal strap connecting it to the alignment bench. The 3 watts produced in the tube are dissipated to the alignment bench via the copper alignment spacer.

X-Ray Source Challenge

The field instrument experience was a catalyst for the choice of CCD detector and X-ray source. The E2V Company was used for the CCD detectors because they had lots of experience, and had flown on previous missions (such as MER). Initially, there was concern about using residual parts, so the project decided to purchase new devices. This worked out well; however, the procurement of the X-ray source would be more difficult.

Oxford X-Ray Technology Group, Inc., working with NASA Ames, developed a small X-Ray tube through a NASA SBIR program. The X-Ray tube had been used in field instruments and seemed like a logical choice. The X-Ray source procurement was a critical item for CheMin, and because Oxford had experience, the initial decision to purchase the X-Ray source (e.g., X-ray tube and high voltage power supply integrated into a single package) from them made sense.

As a result, the company was not well aligned with the delivery of single, highly qualified components, including a detailed paper trail of testing and characterization history. They were more aligned toward delivering many components for manufacturing a series of commercial X-Ray products.

Oxford’s inability to supply flight qualified components led the CheMin Project in 2006 to a new strategy for obtaining a flight ready X-ray source assembly. JPL itself would manufacture the assembly and qualify it for flight. The X-ray tube would still be purchased from Oxford since this device was clearly beyond the Lab’s capability. A set of eight X-ray tubes were purchased. JPL put the tubes through extensive environmental and life testing. There was particular concern about the tungsten filament within these tubes passing vibration qualification. After all testing was completed, device characterization and inspection screening were used to select suitable tubes for flight. A flight tube, one spare and a development model tube, were finally selected.

Development of the high voltage power supply (HVPS) was assigned to the radar division at JPL. It was a challenge because the HVPS needed to be integrated into a small, tightly fitted space with assurance that suitable isolation to protect against arcing would be provided.

To provide electrical insulation, the high voltage power supply is filled with a dielectric insulator, a mixture of sulfur hexafluoride (SF6) gas and gaseous nitrogen (N_2). The mixing ratio is selected to keep it gaseous over the full operating temperature ranges. The gas mixture was chosen to be gaseous down to -40°C for protection of the HVPS.

The high-voltage power supply and controller interface the main instrument electronics to the X-ray tube. The HVPS produces the various voltages required by the tube elements. The HVPS produces the -28 kV cathode voltage, the filament current (nominally 1.3 A), and the focus voltage (nominally -90 V, referenced to the cathode voltage). The high-voltage power supply is housed in a laser-welded stainless steel "can" and is integrated directly with the X-ray tube (via a laser welding process). The controller is separated from the high-voltage section and is integrated with the support structure used to mount the X-ray Source to the alignment bench. All the manufacturing, design and testing of the X-ray source proved to work out well and be within the Lab's capability.

Signal-to-noise (SNR) and Signal Quality Challenge

As the CheMin instrument design was evolving a significant effort was put into developing a high fidelity performance and error budget model [6]. As the reader can see from Figure 4, there are several variables that effect both the alignment of the instrument and subsequent beam alignment error could not exceed 0.35 degrees off center. Considering all sources of alignment error, it was determined that indeed the mechanical and optics design could maintain that error requirement but not with any significant margin. That said, the subsequent performance model showed that even operating the detector at higher temperatures than desired, the SNR was projected to 2x higher than the requirement. Figure 8 shows the modeling results.

In order to save schedule, the CheMin DM (demonstration model) was descoped as a deliverable, and the decision was made to proceed directly with the building and testing of the flight model (FM). While this plan was very successful with regard to the FM delivery, it left CheMin scientists without a means to replicate CheMin performance on the Earth. The DM electronics still had to be produced for FPGA development and testing, but were done so with no regard to replicating FM performance. A program was undertaken to bring the CheMin DM up to flight-like status.

While the flight unit met the above performance requirement with margin, an issue arose after the flight unit was integrated into the rover and launched. The team proceeded with its sample testing/characterization using the development model (DM) instrument. However, as the testing proceeded on the DM, it was noted that the returned spectra exhibited noise which masked the actual signal. The SNR was not anywhere close to what was observed on the flight unit. Since the DM electronics were designed to emulate the flight and now had significant operational hours logged, the poor SNR raised suspicions that perhaps there was the potential for a component failure on the flight unit which would be mission ending. A Tiger Team was formed to determine root cause. The team proceeded to develop a detailed fault tree and examine every possible noise source.

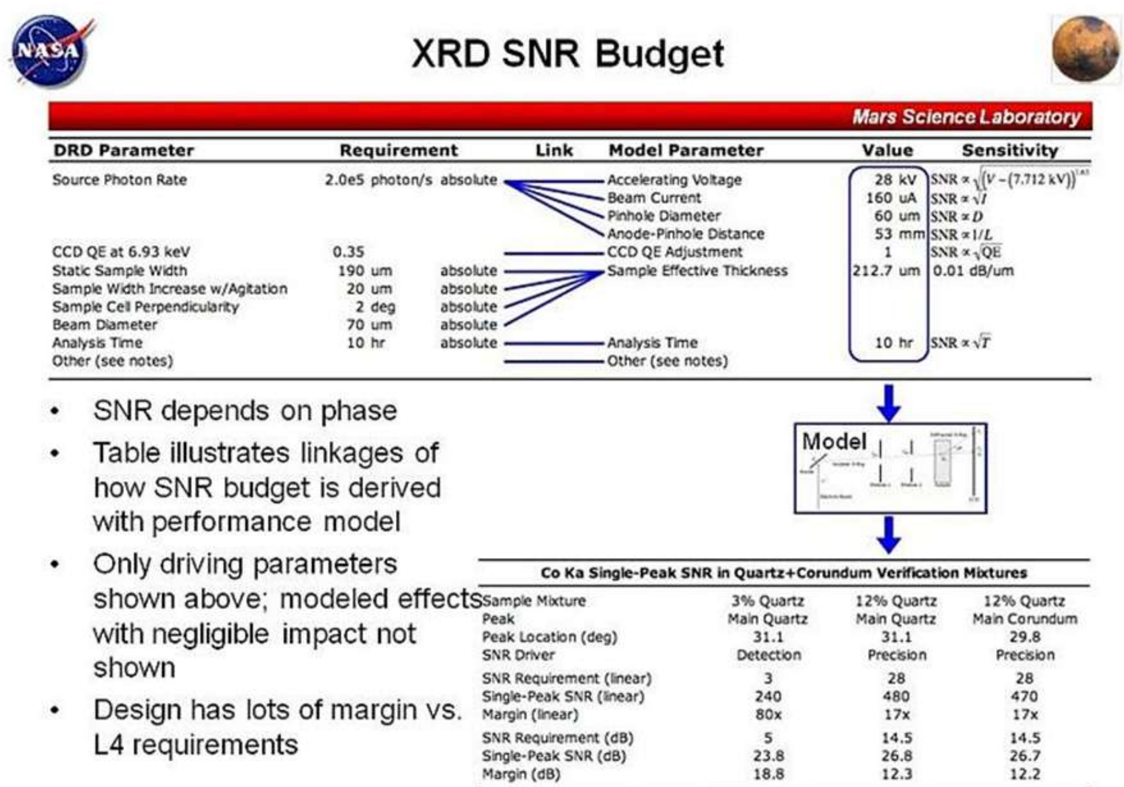

Figure 8: Results of SNR Model

Time was of the essence because MSL had already launched, and there was only 5 months before landing. By probing the boards and examining the output signal, the team isolated the analog, utility, and power boards as the likely source for the noise. The team found that a combination of non-flight parts, significant hay-wiring/poor routing providing sources for stray inductance, and failed solder pads were the primary causes for the noise. Ultimately, the decision was made to completely re-build the analog and utility boards using all qualified flight parts. The re-built boards were re-integrated with the DM instrument and re-tested. The DM performance matched the flight and proved that the flight unit was indeed robust. Figure 9 shows how the SNR changed with the rebuild.

Sample Handling Challenge

Sample handling within CheMin is new and has never been flown before. The vibration of the sample cell is a tuning fork style arrangement, is localized and less coupled, and has the advantage of minimizing the ejection of material. It has solved the problem of how to remotely, randomly arrange material within the instrument for XRD.

The major challenge faced when deploying the new sample handling system is to understand the physics of sample excitation under Mars environmental conditions and then designing a test program for handling and characterizing all of the possible materials this system could encounter. Examples of the critical variables that had to be understood are [8]:

1. Variable particle sizes which may affect the momentum transfer between particles;
2. Variable particle geometries which may also effect the motion dynamics, and particle-to-particle interactions (e.g., friction), see Figure 10;
3. Electrostatic charging of the window material resulting in particles sticking to surfaces;
4. Potential increase in the electrostatic field effects due to window oil-canning, i.e., windows flexing as the cell is vibrated;
5. Secondary charge transfer effects which may result in layering of particles;

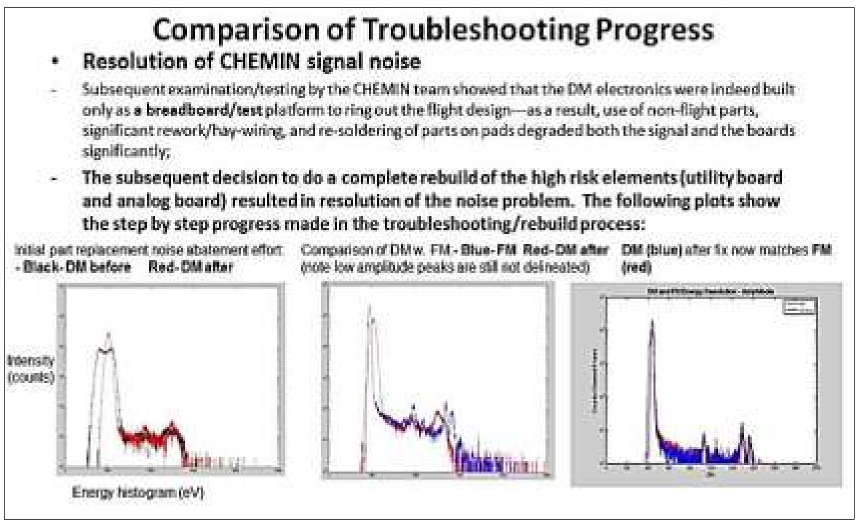

Figure 9: Results of SNR progressive improvement

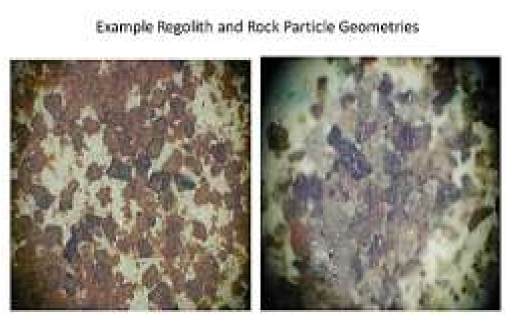

Figure 10: Left Image – Weathered regolith particles / Right Image – Angular Interlocking basalt particles

6. The effect low pressure has on reducing atmospheric drag on particulates;
7. The effect low pressure has on reducing the molecular- level lubrication between particulates;
8. The effect low gravity may have on offsetting the effects of low pressure;

In order to quantify the above variables a modeling and laboratory test program was established. A particle-to-particle interaction physics model was derived from first principles. The model was then executed in a step-wise fashion in which each particle-to-particle interaction is mapped and calculated, with the subsequent force vectors captured and stored, and then used as the initiating function for the next collision. In this manner, the eventual total particle interaction network was mapped using "net-velocity vectors" within the cell volume. The model was then validated by testing in the laboratory. The challenge comes when the modeling results and laboratory results are compared and then interpreted. Figure 11 shows the results of one modeling run and the equivalent laboratory run of a sample with the same particle characteristics as the model. The exceptional agreement between the model and lab tests gave confidence to our selection of excitation parameters for the various sample types we expected to encounter on Mars. The modeling and testing process spanned a period of approximately 5 months. However, when completed, the particle dynamics for different materials were reasonably understood, the effects of signal attenuation factors like variable particle size, sample chamber window bowing, and particle electrostatics (clumping together and sticking to the sample chamber window) were characterized and their respective impacts on signal amplitude were resolved. See Figure 12. Last, the effects of the Mars lower gravity on sample excitation were found to be negligible.

In closing this discussion, one must not only demonstrate functionality, but do so within schedule, budget and attempt to validate a broad set of control parameters. The

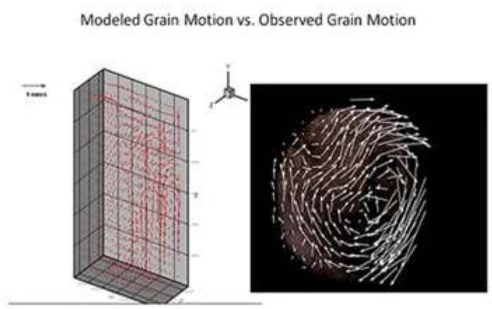

Figure 11: Particle Excitation model and lab test agreement

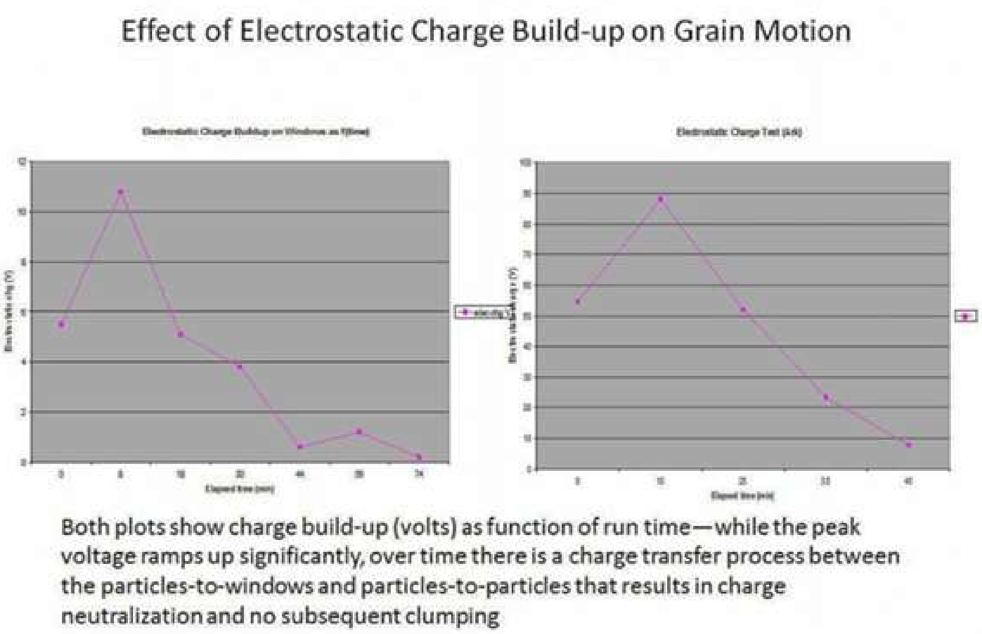

Figure 12: Electrostatic charge neutralization between particles and windows

preliminary samples chosen for testing were basalt, arkose, kaolinite, hematite and satin spar. Conditions such as loose sample left within the instrument and volume residual material remaining in the cell after cleaning were only marginally tested in an attempt to lengthen the life of the instrument. At the end of the day, one must accept that testing might be imperfect, but good enough to give a high likelihood of success.

FPGA Schedule Challenge

During the Integration and Test phase of the flight instrument, it became clear that the final challenge was to finalize the FPGA firmware on schedule. Algorithms and sequences originally targeted for the FPGA were either removed or simplified. A test suite to validate the FPGA was created. The problem was that early on in the project, major elements like the sample delivery/excitation issue, X-ray source delays, and thermal control dominated the instrument control system design and validation effort. These issues drove the schedule and placed a lot of pressure on the final S/W design and FPGA burn going into integration and test. Ultimately, the FPGA implementation was successful.

5. SUMMARY AND CONCLUSIONS

It was a challenge transforming the legacy CheMin design used in the field to a flight instrument. Initially, the proposed completion cost was $15M, but the instrument project failed its preliminary design review (PDR), causing a re-plan and capping the cost at almost 3x the initial estimate. Not appreciating the true technology readiness level, vendor capability (i.e., the X-ray source), and the large array of sample excitation variables that needed to be tested made the flight implementation very challenging. The MSL CheMin instrument was originally scheduled for delivery to MSL rover integration in July 2008. However, with the delay of the MSL launch from 2009 to 2011, more time was given to the MSL CheMin Team for limited testing and problem resolution. This delay proved invaluable to allowing the instrument to reach flight maturity. In closing, to date the CheMin instrument is working well on Mars. The instrument received its first regolith sample for analysis on October 18, 2012. Figure 13 shows the actual diffraction pattern resulting from that first analysis.

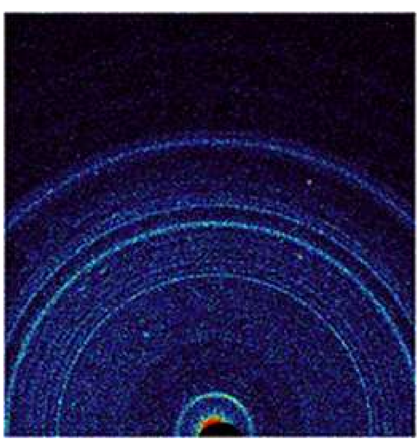

Figure 13: Mars Regolith Sample

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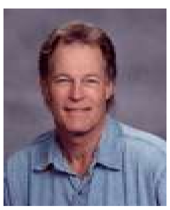
BIOGRAPHY



Wayne Zimmerman *is currently the Chief Engineer for the Instruments and Science Data Systems Division at JPL. His current responsibilities include trouble shooting science instrument problems and insuring instruments meet performance, schedule, and cost requirements. He also chairs both instrument design reviews and design teams for on-orbit and in-situ science instrument payloads for planetary, lunar, and Earth science missions. He was actively involved in sample handling/processing/delivery technology development and insertion into flight projects like the MSL CHEMIN X-ray diffraction instrument and the Mars Scout UREY astrobiology instrument. He is the acting project element manager for CHEMIN. Wayne received his B.S. in Fluidics from Case Institute of Technology, Cleveland Ohio, and his M.S. in Aerospace Systems Engineering from the University of Southern California. Wayne has been at JPL for 35 years building robotic instrument delivery/sampling systems for Mars as well as designing integrated instrument platforms for terrestrial and planetary applications.*

Leonard J. Reder *returned to JPL in 1999, as a Real-Time Senior Software Engineer to work on the Keck Interferometer Project. He contributed to software for high speed, closed-loop control of optical delay lines, created auto- alignment software, and developed a high-level science sequencer implementation. He has developed machine learning applications, Mars surface simulation, infrared sensor data analysis and management software, and MSL flight software code generation tools. Prior to coming to JPL, he worked on several U. S. Navy sensor systems at both the software and system level. His interests include real-time image processing and digital signal processing for scientific instrumentation, autonomy, data management technologies, as well as software and systems modeling and development techniques. Reder earned a B.S. in Electronic Engineering from California Polytechnic University at San Luis Obispo, and an M.S. in Electrical Engineering from the University of Southern California.*

William Harris *has been associated with the design, assembly, and test of flight instruments since coming to JPL in January of 1959. His work has included involvement in the Sargent Program, Mariner series, Ranger Series, Voyagers 1 and 2 (MDS), Microwave Sounder Unit Series, UARS Microwave Limb Sounder, Mars Observer (PMIRR), 14 Cassini (ISS), CloudSat, GALEX, and MarsScience Lab (CheMin).*

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John Michael Morookian *received his B.S. in Electrical Engineering from the University of Southern California (1991), began working at JPL in 1990 as an academic part-time employee and is currently a Senior Engineer in the Payloads and Observing Systems group within the Systems Engineering section. He is the recipient of both a NOVA and a Technology and Applications Programs Exceptional Service Award for achievement in the area of fiber-optic links. He has spent the last decade developing in situ instruments for planetary exploration, most notably the Microscopy Electrochemistry Conductivity Analyzer (MECA) instrument for the Phoenix mission and CheMin for the Mars Science Lab.*

David Randall *a Principal Electronics Engineer, working for Caltech at JPL, NASA's Jet Propulsion Laboratory. David is responsible for the design and delivery of flight electronics for instrument systems. He was the Product Delivery Manager for CheMin/MSL electronics. MSL landed in Gale crater on Mars August 5th, 2012.*

Dr. Phillipe Sarrazin (Co-I) *studied Materials Sciences and Mechanical Engineering in France. During the decade following his doctorate he worked as a research scientist in several academic and government laboratories, developing new technologies with a particular interest in X-ray instrumentation. He played a key role in the development of the NASA XRD/SRF planetary instrument and remains involved in the program today as a member of the MSL (Mars 2011) CheMin instrument Science team. In 2004 Dr. Sarrazin founded one of the companies which now make up inXitu, Inc. He managed the company, pursued his research on XRD equipment for space exploration under a number of government research grants, and prepared the introduction of these technologies to the market. Dr. Sarrazin now supervises the Research and Development at inXitu, Inc. and plays a lead role in a number of research programs for innovative instrumentation in X- ray analysis. Dr. Sarrazin is also a senior research scientist at the SETI Institute, Mountain View, CA.*