
Introduction: The Mars Science Laboratory (MSL) rover will land in Gale Crater on Mars in August 2012. The planned landing site is an alluvial fan near the base of the crater's central mound. Orbital remote sensing of this 5 km high mound indicates the presence of hydrated sulfates, interstratified with smectite and hematite-bearing layers. Minerals formed in an aqueous environment are of particular interest given that water is a fundamental ingredient of living systems and that MSL's prime science objective is to investigate martian habitability.

CheMin Instrument: The CheMin science investigation will provide definitive in situ mineralogy of the surface materials at Gale Crater and test for the presence of minerals formed through aqueous processes. CheMin is a transmission X-ray powder diffraction (XRD) instrument utilizing Co-Kα X-rays and a cooled charge-coupled device (CCD) detector. CheMin can detect diffractions from 5° to 55° 2θ at an angular resolution of better than 0.35° 2θ. Depending on environmental temperatures, the energy resolution is expected to be better than 250 eV at Fe-Kα. The sample wheel contains 27 reusable cells for martian samples and 5 reference standards for periodic assessments of instrument health and performance. Typical analysis durations for a martian sample may be ~8 hours spread over multiple martian nights. The ability to detect minor phases in complex samples is enhanced at lower detector temperatures and longer integration times.

Flight Model (FM) data: Prior to integration into the MSL vehicle, the CheMin FM was extensively tested in a pressure- and temperature-controlled chamber simulating the martian surface environment. The five internal reference standards and selected empty cells were analyzed over a wide range of temperatures and data acquisition modes. In order to launch an uncontaminated instrument, no samples other than the sealed standards were analyzed by the FM. The five reference standards are described below.

Beryl-quartz mixtures. Two reference cells were filled with mixtures of synthetic emerald (Cr-beryl) and quartz at ratios of 88:12 and 97:3 by weight. Beryl has three well-defined and separated peaks of high intensity, providing a strong signal with relatively short integration times. The two different mixtures were used to evaluate precision, detection limits, and alignment (Fig. 1) of the instrument.

Fig. 1: Fits to the beryl-quartz diffraction rings on the CCD uniquely establish the internal alignment of the flight instrument.

Amphibole. A natural pargasite from Gore Mountain, NY (Fig. 2) has a number of closely-spaced diffraction peaks and was included as a reference standard for verifying and monitoring 2θ range and resolution.

Ceramic. A mixture of nontronite and smaller fractions of 11 other phases was fired at 800° C and then crushed and sieved to create a synthetic standard containing many of the elements of interest to the investigation (Fig. 3). The energy scale and resolution of the instrument are established by this reference standard.

Arcanite. A synthetic sulfate prepared by crystal growth from saturated solutions of K₂SO₄ is the final reference standard. The sulfur content, which may be representative of sulfate-rich materials to be examined by MSL, results in a high fluorescence background and significant attenuation of Co X-rays in the diffraction pattern.

Fig. 2: Amphibole XRD pattern produced after converting 2D CCD images to a plot of counts versus 2θ. Rietveld refinement establishes the phases in this multicomponent sample.
Development Model (DM): As the FM has analyzed only five powdered samples prior to launch, understanding the performance of the instrument relies heavily on the DM. It is a functional replicate of the FM but resides in the laboratory to analyze a variety of samples under simulated martian environmental conditions. Precise thermal control of the instrument mounting plate in the chamber allows characterization of the primary factor affecting data quality, CCD temperature. As temperatures increase, the energy resolution decreases, resulting in an elevated XRD background. Typical analyses on Mars will be conducted with a detector temperature of approximately -40°C. Nearly 200 powdered samples ranging from natural basalts to chemical geostandards to exotic phases will be analyzed by the CheMin DM.

Prior to extensive data collection from the DM, a number of key aspects of the science investigation were validated using a laboratory CheMin IV instrument. This platform collects diffraction data in transmission, but the source, sample cell, detector and electronics are all very different from the MSL hardware.

Quantitative XRD. Fig. 4 shows that data from a multiphase sample collected with a CheMin IV instrument can be analyzed to accurately determine the quantities of the individual phases. True values confirming these results were obtained using a commercial laboratory diffractometer. The detection limit of the FM is generally better than 3% by weight for well-ordered minerals, but greater for poorly crystalline or amorphous phases.

Phyllosilicates. As shown in Fig. 5, phyllosilicates can be readily discriminated based on differences in their 001 diffraction peaks. Widths of 001 peaks may be interpretable in terms of disorder in stacking and intercalations. However, the range of chemical and physical treatments available in the laboratory will not be available, limiting CheMin's ability to discriminate among different smectites.

Elemental Chemistry. A number of chemical geostandards were analyzed by a CheMin IV instrument. Elemental peak areas were measured and plotted versus their reference concentration. The consistency of these calibration curves, not yet accounting for matrix effects and instrumental background, demonstrates that similar profiles can be generated for the DM. Ultimately, qualitative determinations of elemental chemistry from the FM data will be available to compare against and supplement chemical data obtained from other MSL instruments.

Summary: With its suite of state-of-the-art instruments, the Mars Science Laboratory will conduct a detailed study of the history of habitable environments at Gale Crater. CheMin will establish a ground truth for orbital spectroscopy and will provide definitive mineralogy which is crucial for understanding the nature and extent of aqueous processes at the landing site.