Geophysical Research Abstracts, Vol. 7, 02966, 2005
SRef-ID: 1607-7962/gra/EGU05-A-02966
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X-ray diffraction / X-ray fluorescence: An important instrumental technique for Mars astrobiology missions.

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1 Mars Astrobiology Goals & Definitive Mineralogy: The search for evidence of life, prebiotic chemistry or volatiles on the surface of Mars will require the identification of rock types that could have preserved these. Anything older than a few tens of millions of years (>99% of Mars history) will either be a rock, or will only be interpretable in the context of the rocks that contain it. In the case of Mars soil, identifying the nature and quantity of both crystalline and amorphous components will be essential to understanding sources and processes involved in its generation. The key role that definitive mineralogy plays is a consequence of the fact that minerals are thermodynamic phases, having known and specific ranges of Temperature, Pressure and Composition within which they are stable. More than simple compositional analysis, definitive mineralogical analysis can provide information about pressure/temperature conditions of formation, past climate, water activity, the activity of biologically significant gases and the like. X-ray Diffraction and X-ray Fluorescence (XRD/XRF) are extraordinarily powerful and complimentary techniques that constitute the preferred method for mineralogical analysis of unknowns in terrestrial laboratories. Indeed; all other mineralogical analysis techniques that claim to be definitive ultimately rely on XRD for the definitive identification of unknown crystalline solids.

The CheMin XRD/XRF instrument. An important goal of NASA's Mars Science Laboratory (MSL '09) mission is the determination of definitive mineralogy and

chemical composition. CheMin is a miniature XRD/XRF instrument that has been chosen for the analytical laboratory of MSL. 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. The CCD detector is operated in single photon counting mode (the detector is read out often enough so that in the vast majority of cases, pixels contain charge from either zero or 1 photon). The CCD detector is exposed to the X-ray flux, read out and erased many times (100-1000 exposures). When operated in this manner, the CCD can be used to measure the charge generated by each photon (and hence its energy). 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. At incremental radii this pattern is summed circumferentially about the central undiffracted beam to yield a 1- dimensional 2θ plot comparable to conventional X-ray diffractometer data. All of the X-rays detected by the CCD are summed into a histogram of number of photons vs. photon energy that constitutes an XRF analysis of the sample. Quantitative mineralogical results are obtained from XRD data by Rietveld refinement and other full-pattern fitting techniques (1,2). Both crystalline and amorphous materials can be analyzed in this way. Quantitative elemental compositions are obtained from XRF data by fundamental parameters (FP) calculations (3).

Analysis of Mars analog materials by CheMin: We will describe three example investigations in which CheMin data can be used to evaluate putative evidence of present or past habitability. The three are: Evaporite rock strata such as found by MER-B at Meridiani Planum; an impact-gardened basalt environment such as found by MER-A at Gusev crater; and Mars soil. CheMin results from Mars analog materials will used to illustrate how conditions of present or past habitability (T, P, αH_2O, sources of energy, presence and quantification of redox elements) can be evaluated in these examples on the basis of definitive mineralogical analysis.

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