

EXTENDING ANTICIPATED MARS 2020 ROVER CAPABILITIES THROUGH MODELING OF X-RAY SCATTERING RATIOS. L. P. O'Neil¹, D. C. Catling¹, and W. T. Elam², ¹Dept. of Earth and Space Sciences/Astrobiology Program, University of Washington, Seattle WA, ²Applied Physics Laboratory, University of Washington, Seattle WA.

Introduction: The surface of Mars acts as a record of the planet's past environment. However, data from Mars' surface is limited, and it is therefore imperative that we make the most of the data that we collect in the future. The Planetary Instrument for X-ray Lithochemistry (PIXL) is an x-ray fluorescence instrument scheduled to fly to Mars on the 2020 rover. It will be capable of quantifying many elements ($Z \geq 11$) directly through fluorescence. However, lighter elements such as carbon and oxygen are below this atomic number limit, and these light elements in particular may provide indications of Mars' past climate. For example, carbonates, sulfates and perchlorates (and states of hydration of the latter two mineral types) all potentially provide information about Mars' past environment. In turn, the environment sets constraints on past habitability and astrobiology.

The spectrum collected by PIXL will also include x-ray scattering signals, and through modeling, the ratio of Compton to Rayleigh scattering may be used to infer the presence and concentrations of the lighter elements. Such information together with fluorescence data could ultimately be used to deduce how the light elements are bound to other elements in specific minerals of interest.

Methods: Both Compton and Rayleigh scattering occur at some level for all elements, but the relative strength of the scattering peaks varies. The energy of the signal is determined by the energy of the incident beam generated by the instrument, which is known. The scattering intensity and ratio is then controlled by the bulk composition of the sample. The ratio is not diagnostic of specific compounds, but can add information to that already provided by the fluorescence data. We have refined a fundamental parameters model to predict the scattering ratio for any given composition. Often, rather than predicting a ratio for each possible composition, a relationship between average atomic number and scattering ratio is determined experimentally [1]. However, there is not a strict relationship and modeling can eliminate error. Given that scattering measurements are not the primary purpose of PIXL, signal strength is expected to be sub-optimal and elimination of this error is desirable. Modeling can also accommodate unforeseen changes in sample geometry and conditions. While a fundamental parameters model may run faster and be more suitable for large quantities of spectra, we compare with a pub-

lished Monte Carlo model to probe the limitations of the approach [2]. We also compare model spectra for a set of materials to experimental results of x-ray scattering for validation of the model.

A procedure for computing the scattering ratio from the spectrum in a consistent manner has also been developed. A variation on a common background removal method has been necessary because the scattering peaks are significantly broader than fluorescence peaks and are often less intense than the peak in the continuum radiation [3]. Area of the Rayleigh peak is determined by fitting simple Gaussians while the Compton peak is numerically integrated due to its more complex structure.

Results and Future Work: The ratios predicted by the model are in good agreement with both the published model and experimental measurements. When the set of possible compounds is constrained by fluorescence data, we hope to be able to determine the compounds present. The viability of this approach in more complex samples has not yet been explored. Additionally, modeled Compton peak shapes do not yet conform to experimental spectra, and further study of its structure may yield an analysis more robust to noise.

References: [1] Hodoroaba V.-D. and Rackwitz V. (2014) *Anal. Chem.*, 86(14), 6858-6864. [2] Schoonjans T. et al. (2012) *Spectrochim. Acta, Part B*, 70, 10-23. [3] Van Espen P. et al. (1977) *Nucl. Instrum. Methods*, 142, 243-250