Extracting Further Information from an X-ray Fluorescence Spectrum through Modeling of X-ray Scattering

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In circumstances where data is limited, it is desirable to analyze both x-ray fluorescence and x-ray scattering that appear in the same spectrum. 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 quantify many elements ($Z \geq 11$) directly through fluorescence while lighter elements such as carbon and oxygen are below this atomic number limit. The spectrum collected by PIXL will also include x-ray scattering features. Peaks in the spectrum generated by the x-ray tube Compton and Rayleigh scatter off the sample and appear in the collected spectrum. Through modeling, the ratio of Compton to Rayleigh scattering may be used to infer the presence and concentrations of lighter elements. Such information together with fluorescence data could be used to deduce how the light elements are bound to other elements in specific minerals of interest.

The scattering intensity and Compton/Rayleigh ratio is controlled by the bulk composition of the sample. The ratio is not diagnostic of specific compounds, but can add information to that provided by the fluorescence data. We have refined a fundamental parameters model to predict the scattering ratio for any given composition that can be compared to the experimentally measured ratio. While a fundamental parameters model may run faster and be more suitable for large quantities of spectra, we compare with a published Monte Carlo model to probe the limitations of the approach [1]. We also compare model spectra for a set of materials to experimental results for validation of the model.

A procedure for computing the scattering ratio from a spectrum in a consistent manner has also been developed. A variation on a common background removal method is necessary because the scattering peaks are often substantially broader than fluorescence peaks and may even be less intense than the peak in continuum radiation [2]. The area of the Rayleigh peak is determined by fitting a sum of Gaussians while the Compton peak is numerically integrated due to its more complex structure. Ratios predicted by the fundamental parameters 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.

References: [1] Schoonjans T. et al. (2012) *Spectrochim. Acta, Part B, 70,* 10-23. [2] Van Espen P. et al. (1977) *Nucl. Instrum. Methods, 142,* 243-250