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High-Fidelity Simulations of Mars Science Laboratory Alpha Particle X-ray Spectrometer Spectra: Enhanced Characterization and Results from Gale

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Abstract

Simulation software permits the rapid and accurate generation of Mars Science Laboratory (MSL) Alpha Particle X-ray Spectrometer (APXS) Martian spectra for any combination of target composition and experimental conditions. Analyses of these spectra enhance the characterization of the MSL APXS and support broader scientific investigations.

1. Introduction

The APXS on the MSL rover *Curiosity* determines the chemical composition of Martian materials [2-4]. The spectra acquired by the APXS were used to calibrate and validate the "APXS Characterization by Empirical Simulation" (ACES) spectral simulation program. The development and testing of the ACES program is discussed in detail by [5]. A simulated ACES spectrum is compared to an observed Mars spectrum in Fig. 1.

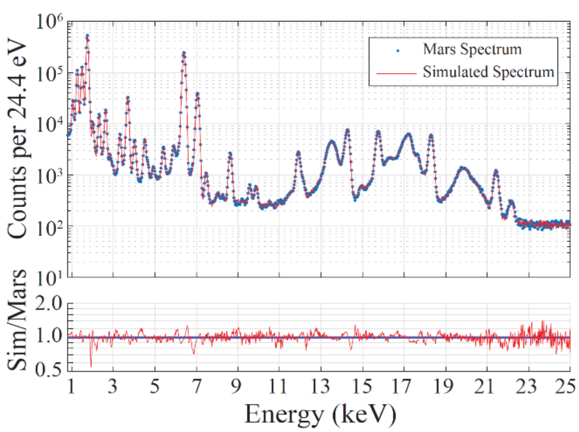

Figure 1: Simulated (red) and observed (blue) Ekwir_1_postbrush spectra, capturing program performance under ideal measurement conditions [5].

ACES spectra can be analyzed with the APXS spectral analysis routine that provides target compositional information to the MSL Science Team and ultimately the public via NASA's Planetary Data System. The ability to generate spectra with a high throughput (simulation rate of ~1000/hr) permits further characterization of the performance of the APXS. For example, for a fixed composition, the reported uncertainties can be examined as a function of varying spectral conditions. Likewise, for fixed experimental conditions, the sample composition can be altered to probe situation-specific detection limits and errors (e.g., Fig. 2) [6]. Such analyses would be prohibitively intrusive to physically conduct in a laboratory setting.

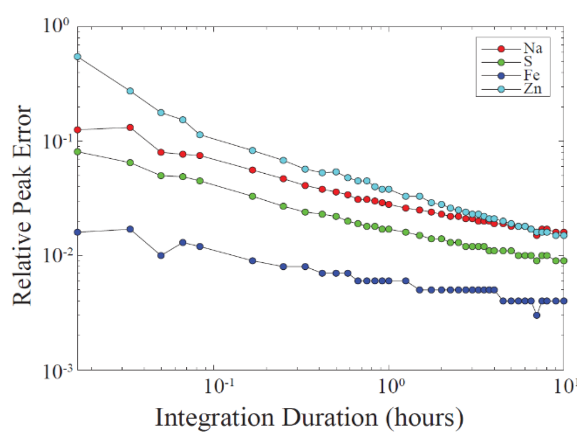

Figure 2: Peak area uncertainty in a typical Mars soil matrix and ideal measurement conditions [5].

2. Results and Conclusions

Spectra were simulated for various temperatures (simple proxy for spectral resolution) and effective durations (incorporates source decay, sample proximity, and measurement duration into a single parameter). The abundance of trace elements such as Ni, Cu, Zn, Ga, Ge, and Br were individually varied. Each simulated spectrum was analyzed with the APXS spectral analysis routine. The precise quantification limit (PQL) of each trace element was determined as a function of experimental conditions (e.g., Fig. 3, for Zn). The PQL was defined as the concentration of a given element for a defined matrix composition and measurement conditions whereby <10% peak uncertainty is observed.

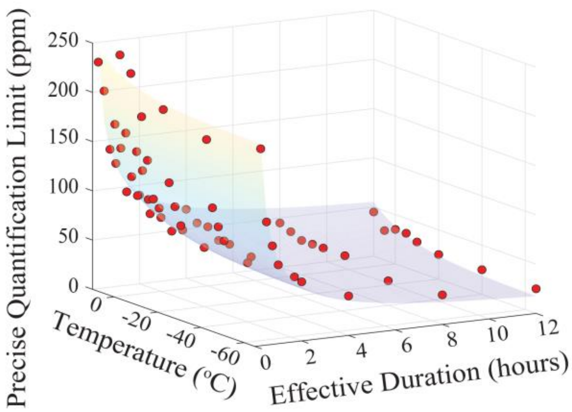

Figure 3: PQLs for Zn as a function of temperature and effective duration fit with a bivariate least squares function [6].

The quantitative PQL results determined from the analysis of simulated spectra demonstrate PQLs in the 10s of ppm range for the aforementioned elements under ideal conditions [6]. However, while individual measurement durations rarely exceed 8 hours in length due to the practical operational limitations of operating on Mars, multiple measurements on targets of similar composition can reduce the PQL by approximately a factor of 2.

In instances where targets are of the same composition and are of sufficient spectral resolution (to avoid peak broadening), the spectra can be summed to improve statistics, essentially increasing the effective duration component (e.g., Fig. 3) and in turn lowering the PQL. This permits the quantification of trace elements to <10% precision error where individual measurements are insufficient.

While Ni, Zn, and Br are provided with every APXS analysis due to their typical abundance in the 100s of ppm (or greater), the concentration of less abundant Cu, Ga and Ge trace elements can be below the PQL in individual measurements, especially for quick and/or warm-temperature assessments of targets [6].

Given the cumulative duration of high-quality measurements acquired at several prominent geologic units at Gale, PQLs are determined for each unit. Through direct spectral analysis accompanied by simulated ACES spectra, we investigate the potential to derive the typical abundance of Cu, Ga, and Ge in these units. Soils and sands are also studied.

Acknowledgements

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