

**HIGH-THROUGHPUT MODELING OF SURFACE COATINGS AND LAYERING EFFECTS IN MARS X-RAY FLUORESCENCE DATA.** S. J. VanBommel<sup>1</sup>, R. Gellert<sup>2</sup>, J. A. Berger<sup>3</sup>, M. A. McCraig<sup>2</sup>, C. D. O'Connell-Cooper<sup>4</sup>, L. M. Thompson<sup>4</sup>, A. S. Yen<sup>5</sup>, N. I. Boyd<sup>2</sup>, and A. L. Knight<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>University of Guelph, Guelph, ON; <sup>3</sup>NASA Johnson Space Center, Houston, TX; <sup>4</sup>University of New Brunswick, Fredericton, NB; <sup>5</sup>Caltech/NASA Jet Propulsion Laboratory, Pasadena, CA.

**Introduction:** On the surface of Mars, rovers and their scientific payloads experience a myriad of challenges that typically do not encumber similar instruments in a terrestrial laboratory. In the case of active Mars-based X-ray spectrometers, such as the Alpha Particle X-ray Spectrometer (APXS) on the Mars Science Laboratory (MSL) rover *Curiosity* [1] and the Planetary Instrument for X-ray Lithochemistry (PIXL) instrument on the Mars 2020 (M2020) rover *Perseverance* [2], these challenges include limited sample preparation, variable environmental conditions (e.g., thermal), and general constraints on experimental operations (e.g., measurement duration, targeting limitations etc.) [3]. Significant advancements have been made to mitigate many of these challenges, through either modifications in regards to how the instrument is used (e.g., [4, 5]), changes to instrument design in part based off of lessons learned (cf. [2] and [1]), and/or through computational techniques applied to flight data once on the ground (e.g., [4-6]). On the other hand, flight hardware and operational limitations can limit the scope and availability of sample preparation. In the case of MSL, this includes limitations on which targets *Curiosity* can safely remove surface dust using the Dust Removal Tool (DRT) [7]. On M2020, the rover has a non-replenishable gas DRT (gDRT) as well as an abrasion bit to grind away the surface coatings of rocks [8], with the use of either limited by several factors. MSL does not have an abrasion bit or a means to grind the surface beyond exposing subsurface tailings through traditional (and percussive) drilling [7].

In instances where sample preparation is limited, rover instruments are often forced to investigate target surfaces that are blanketed by a nearly ubiquitous and globally compositionally homogenous coating of Mars dust. As the composition of dust is well constrained (e.g., [9]), one can predict the expected signal detected (e.g., by APXS or PIXL) from the surface dust layer and the underlying rock substrate. Here we employ a simplified approach to solving this problem, one that trades a slight reduction in accuracy (due in part to ignoring minor effects; e.g., secondary excitation) in exchange for a highly efficient algorithm capable of arriving at a solution within a fraction of a second as opposed to hours or days for alternative routines (e.g., [10]). The application is computational in nature, can be applied to a multi-layer model, and is not restricted to a dust surface layer. Furthermore, variability in sur-

face layer coverage can be modeled as a linear superposition of the layered solution with pure surface and pure substrate endmember compositions.

**Method:** We model the expected X-ray quanta obtained for a given depth through the implementation of Beer-Lambert law. The expected signal received from a layer of thickness  $dx$  spanning depth  $a$  to  $b$  is approximated by

$$S_{(a \rightarrow b)} \propto \int_a^b P_s dx$$

where  $P_s$  is proportional to  $e^{-\mu x}$  and  $\mu$  is the attenuation coefficient (product of mass attenuation coefficient and material density and is dependent on material composition). Thus, for layer  $i$  in a model with  $N$ -layers of thickness  $R$ , the expected signal from depth  $(i-1)R$  to  $iR$  is approximated by

$$S_i \propto \int_{(i-1)R}^{iR} e^{-\mu_i x} dx$$

and the solution is derived through the summation across all  $i$  for all elements. In the case of a two-layer model, the approximation simplifies to

$$S_1 \propto \frac{1}{\mu_1} (1 - e^{-\mu_1 T})$$

$$S_2 \propto \frac{1}{\mu_2} e^{-\mu_1 T}$$

where the subscript  $1$  denotes the surface layer, subscript  $2$  the substrate, and  $T$  the thickness of the surface layer. Incident penetration depth exceeding escape depth is a critical assumption for the model; a complete description of assumptions are provided by [11].

**Results and Discussion:** The work of [11] investigates a Gale crater target with a thin Mn-rich layer (Stephen; sols 627-629), utilizing a laser-induced breakdown spectroscopy (LIBS) instrument on MSL, Chemistry and Camera (ChemCam), to provide a more realistic depth profile of the Mn-rich layer that can be used iteratively for better predictions of X-ray results. While capable of predicting observed concentrations for a myriad of user-defined layer or coating scenarios and assisting in the interpretation of potential future (potentially alteration-driven) coatings, the most obvious and immediate use case of the model is to examine how dust coatings can mask compositions of the underlying rock. To that end, we present simulated concentrations for pure mineral substrates that have an overprinted uniform and continuous layer of Mars airfall dust. We simulate dust at various thicknesses encoun-

tered (or expected) on Mars (e.g., [12-16]). The results presented in the tables that follow (i.e., **Tables 1-4**) demonstrate that while some elements are largely impervious to the effects of thin (i.e., 10  $\mu\text{m}$  thick or less) dust beyond normalization effects (e.g., Fe), others are extremely sensitive to even a  $\mu\text{m}$  or two of dust coating (e.g., Na), complicating diagnoses of underlying minerals, should their areal extent be large enough to fill the instrument's analytical field of view. This, of course, is further complicated by the lack of uniformity in the areal coverage and thickness of Mars dust.

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**Table 1:** Simulated observed major element concentrations for Albite (Plagioclase Feldspar) underlying varying thicknesses of Mars airfall dust.

Albite - Plagioclase Feldspar					
Dust	0 $\mu\text{m}$	3 $\mu\text{m}$	5 $\mu\text{m}$	10 $\mu\text{m}$	Inf
Na <sub>2</sub> O	11.82	6.12	4.79	3.83	2.75
MgO	0.00	9.86	11.85	11.41	8.32
Al <sub>2</sub> O <sub>3</sub>	19.44	20.93	17.64	12.92	8.92
SiO <sub>2</sub>	68.74	52.43	49.76	49.51	39.37
SO <sub>3</sub>	0.00	5.16	7.39	9.27	8.35
Cl	0.00	0.55	0.80	1.07	1.08
K <sub>2</sub> O	0.00	0.14	0.22	0.33	0.47
CaO	0.00	1.76	2.75	4.19	7.05
FeO	0.00	2.20	3.55	5.82	21.03

**Table 2:** Simulated observed major element concentrations for Forsterite-90 (Olivine) underlying varying thicknesses of Mars airfall dust.

Fo90 - Olivine					
Dust	0 $\mu\text{m}$	3 $\mu\text{m}$	5 $\mu\text{m}$	10 $\mu\text{m}$	Inf
Na <sub>2</sub> O	0.00	3.71	3.99	3.51	2.75
MgO	49.35	22.93	15.00	10.66	8.32
Al <sub>2</sub> O <sub>3</sub>	0.00	7.60	9.72	10.49	8.92
SiO <sub>2</sub>	40.87	40.71	43.23	45.33	39.37
SO <sub>3</sub>	0.00	5.13	7.01	8.53	8.35
Cl	0.00	0.54	0.76	0.99	1.08
K <sub>2</sub> O	0.00	0.14	0.21	0.30	0.47
CaO	0.00	1.75	2.61	3.86	7.05
FeO	9.77	16.63	16.29	14.81	21.03

**Table 3:** Simulated observed major element concentrations for Pigeonite underlying varying thicknesses of Mars airfall dust.

Pigeonite					
Dust	0 $\mu\text{m}$	3 $\mu\text{m}$	5 $\mu\text{m}$	10 $\mu\text{m}$	Inf
Na <sub>2</sub> O	0.00	2.72	3.03	2.97	2.75
MgO	15.18	8.96	8.92	8.89	8.32
Al <sub>2</sub> O <sub>3</sub>	0.00	5.57	7.38	8.86	8.92
SiO <sub>2</sub>	51.73	41.07	38.85	39.21	39.37
SO <sub>3</sub>	0.00	3.76	5.33	7.21	8.35
Cl	0.00	0.40	0.58	0.83	1.08
K <sub>2</sub> O	0.00	0.11	0.16	0.26	0.47
CaO	6.03	6.71	6.43	5.91	7.05
FeO	27.06	30.08	28.44	24.57	21.03

**Table 4:** Simulated observed major element concentrations for Halite (NaCl) underlying varying thicknesses of Mars airfall dust. NaCl has been detected by APXS at Gale crater [17].

Halite					
Dust	0 $\mu\text{m}$	3 $\mu\text{m}$	5 $\mu\text{m}$	10 $\mu\text{m}$	Inf
Na <sub>2</sub> O	46.64	17.77	8.92	4.10	2.75
MgO	0.00	9.62	11.80	11.48	8.32
Al <sub>2</sub> O <sub>3</sub>	0.00	7.47	10.19	11.45	8.92
SiO <sub>2</sub>	0.00	30.94	42.87	49.43	39.37
SO <sub>3</sub>	0.00	5.04	7.35	9.32	8.35
Cl	53.36	24.32	11.14	2.17	1.08
K <sub>2</sub> O	0.00	0.14	0.22	0.33	0.47
CaO	0.00	1.72	2.74	4.21	7.05
FeO	0.00	2.14	3.53	5.86	21.03