FEASIBILITY OF GAMMA-RAY AND NEUTRON SPECTROSCOPY ON SEALED MARS SAMPLE RETURN TUBES. C. Legett1, A. Grieve2, S. Nowicki1, K. Mesick1, P. Gasda1, C. Hardgrove1, S. Czarnecki1, and M. Pinilla-Orjuela4, 1Los Alamos National Laboratory (PO Box 1663, Los Alamos, NM 87545; clegett@lanl.gov), 3Los Alamos National Laboratory (now at Commonwealth Fusion Systems), 3Arizona State University 4Los Alamos National Laboratory (now at University of Missouri).

Introduction: NASA is planning to return sealed samples collected by the Perseverance rover to Earth in the early 2030s [1]. These samples will mostly be geological materials (i.e. rock cores and soil samples). The samples will be stored in hermetically sealed titanium alloy tubes. The analysis of these samples will be a top national scientific priority on par with the analysis of the Apollo lunar samples.

We believe an opportunity exists to use neutron-based analysis techniques on the samples while still sealed in their tubes. At a minimum, thermal neutrons could be used to assess the bulk sample composition (including hydrogen) through a combination of neutron absorption and scattering measurements and prompt gamma neutron activation analysis (PGNAA). These analyses could be performed on the samples before their tubes were opened, whereupon contamination or losses could occur, and after opening but before they were subsampled for other analyses. Furthermore, opening and equilibrating the tubes with the lab environment may cause loss of water or other gases from minerals unstable in that environment, including evaporites.

If NASA allows the samples to be taken to other facilities, the use of the Energy Resolved Neutron Imaging (ERNI [2]) and/or Asterix [3] beamlines at the Los Alamos Neutron Science Center (LANSCE) would allow the 3D tomographic mapping of elements like hydrogen and carbon (and some isotopes) at a spatial resolution of up to 10s of micrometers. This information, especially if coupled with X-ray CT, would allow the detailed determination of the hydration, elemental composition, and structure of the samples using non-destructive techniques without needing to open the tubes. Acquiring these data prior to unsealing the sample tubes has the added benefit of determining sample hydration prior to potential alteration due to different humidity conditions in the laboratory. This information would allow planning of sample divisions prior to tube opening, which would reduce the exposure of the sample to the Earth environment and minimize handling of the sample itself prior to additional measurements.

To determine the feasibility of these analyses, we used the LANL-developed Monte Carlo N-Particle (MCNP [4]) software to explore different simple experimental designs, and to estimate the suitability of these samples to neutron-based study.

Models: Our models were variations of a simple geometry. The source and sample tube were separated by a constant distance (approximately 30 cm). The particle flux was determined crossing a 5 cm diameter circular surface 2 cm beyond the sample. Between the source and the sample, we placed varying thicknesses of HDPE moderator and/or lead shielding. The source chosen was a $^{252}$Cf neutron source that was previously experimentally validated at Los Alamos. We did not model the gamma output from the source, and instead configured the model such that it emitted only neutrons. The HDPE moderator thickness was optimized to maximize the thermal and epithermal neutrons flux through the sample. Since we wanted to observe the PGNAA gamma signal, we shielded the moderator from the detector with a sheet of lead.

The neutron and gamma-ray fluxes were calculated at each material boundary (i.e. source side of the moderator, between the moderator and shield, and the sample side of shield). This allowed us to see how each material was affecting the experiment as the particles flowed through each material.

The sample compositions were modeled by mixing 40 compositions based on: Shergottite [5], BHVO-1 [5], Gale crater basaltic dunes (Gobabeb), GBW07108 (a limestone), gypsum, the median composition of the Murray and Stimson formations from ChemCam and APXS measurements, and Mars bulk silicate estimates from [6]. Compositions not cited above were determined from ChemCam laboratory data at Los Alamos or from the ChemCam PDS repository.

Optimal Design: Varying the HDPE moderator thickness between 1 and 20 cm (Figure 1), we determined that the optimal moderator thickness is 5 cm. The 10 cm thick moderator provided the greatest number of thermal neutrons, but significantly fewer epithermal neutrons compared to 5 cm. 5 cm provided the best tradeoff between the two regions.

The gamma-rays produced through the (n,g) reactions in the moderator were reduced by 90% through the addition of a 10 cm thick lead sheet over the sample side of the moderator. This was desirable because we were interested in examining the predicted change in 2.223 MeV gamma-ray flux due to hydrogen.
Results: Water equivalent hydrogen could be derived from either neutron flux (Figure 2) or 2.223 MeV gamma-ray flux. Using single gamma-ray emission energies, Si (3.539 MeV), Ca (1.943 MeV), Na (92 keV), and Cl (1.166 MeV, Figure 3) exhibited clear correlations with concentration, while Fe (7.632 MeV) and Al (7.724 MeV) exhibited weak or no correlation with concentration.

Future Work: This project is now being extended to include more comprehensive MCNP6 simulations with MSR-specific sample compositions. The purpose of this next round of simulations is to generate simulation results using compositions specific to the MSR samples that have been acquired by the Perseverance rover in Jezero crater. The compositions which will be used are from the Planetary Instrument for X-Ray Lithochemistry (PIXL) [7] as reported in the Mars 2020 Initial Reports Volumes 1 and 2 [8,9]. PIXL is an X-Ray fluorescence spectrometer that creates chemical composition maps of targeted areas. The compositions we will use in our simulations are mean bulk compositions from PIXL measurements on rock abrasion patches adjacent to (within 10s of cm of) the core drill areas. Data is not acquired directly from the core location to reduce possible sample degradation. Abrasion removes the top several cm of the rock surface to better represent the underlying bulk rock from which sample cores are gathered.

These new compositions may result in neutron and gamma-ray signals which differ from those of the previous study and therefore could require reconsideration of experimental setup parameters such as the distance from source to sample or sample to detector, etc. We will be responsive to these changes in order to maximize measurement efficiency. Ultimately, this study will lead to the development of laboratory experiments using Mars analog samples.

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References: