CHARACTERIZING THE SPECTRA OF IMLENITE, HEMATITE, MG-SPINEL AND REGOLITH SIMULANTS TO PREPARE FOR UPCOMING LUNAR MISSIONS.

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Introduction: The composition of the lunar polar regions (80-90°N/S) is relatively well known on a regional scale (100s-1000s of m/pixel), but poorly known at the local scale. The Lunar Prospector mission provided indications of the elemental abundances in the polar regions on a regional scale \cite{1}, including the amount of iron and thorium, which allowed to identify different crustal terranes \cite{2}. The south polar region includes material from the South Pole Aitken terrane (>5 wt% FeO and <2 ppm Th) and the Feldspathic Highlands Terrane (<5 wt% FeO and <2 ppm Th) \cite{2}. Since then, isolated olivine-rich exposures have been identified \cite{3}, as well as exposures of hematite \cite{4} and pure anorthosite \cite{5} from the analysis of hyperspectral data acquired by the Moon Mineralogy Mapper (M3) onboard Chandrayaan-1 and the Spectral Profiler (SP) onboard Kaguya. The analysis of the entire SP dataset (millions of spectra) also allowed to generate the first gridded polar mineral maps which provide the abundance of the main lunar minerals (plagioclase, olivine, and pyroxene) at a spatial resolution of 1000 meters per pixel \cite{6}.

While these datasets have been useful to understand the composition of the poles at the regional scale, various robotic missions will soon study the south polar region equipped with multispectral imagers and spectrometers, allowing to better understand compositional variations at the local scale. For example, the NASA Volatiles Investigating Polar Exploration Rover (VIPER) mission will analyze the composition of the regolith near the South Pole of the Moon, at Mons Mouton \cite{7}. The rover will be equipped with the Near Infrared Volatile Spectrometer System (NIRVSS) consisting of two sensors recording spectra between 1300-2500 nm and 2200-4000 nm \cite{7} allowing investigate the composition of the regolith in unprecedented details.

In this study, we focus on characterizing the spectroscopic properties of ilmenite, red hematite and pink Mg-spinel in our laboratory in preparation for upcoming robotic missions. These minerals have been detected from lunar orbit \cite{8,9,10} and could be present in the polar regolith. We then evaluate the efficiency of the Hapke radiative transfer model in estimating the abundance of minerals in mixed samples for different wavelength ranges.

Method: The method consists of three main steps: (1) Measuring the spectra of mineral endmembers and regolith simulants for various grain sizes and acquisition angles, measuring the spectra of mineral endmembers and regolith simulants mixtures; (2) Modeling the spectral mixture of mineral endmembers and regolith simulants using the Hapke radiative transfer model; (3) Comparing the results of the Hapke model and laboratory measurements to evaluate the model accuracy.

Mineral endmembers and regolith simulants. Minerals and simulants are sourced from various companies. LHS-1, developed by Exolith Lab in 2021, is primarily composed of 74.4% anorthosite, followed by glass-rich basalt (24.7%), ilmenite (0.4%), pyroxene (0.3%), and olivine (0.2%). In addition, we obtained 100g of ilmenite from the same supplier. For hematite, we procured 1 kg of raw red hematite from England, supplied by Minerals Unlimited in late 2023. Finally, we acquired 40 g of raw pink Mg-spinel from India through a web supplier called Etsy.

Laboratory setup and experimentation. Spectra are measured with an ASD FieldSpec 4 Hi-Res NG spectrometer allowing for a spectral range between 350 and 2500 nm with a resolution of 3-8 nm. This instrument is installed on a homemade-custom goniometer, enabling measurements within a range of -60° to 60° for emission angles, -90° to 90° for zenithal incidence angles and 0° to 270° for azimuthal incidence angles, with nominal step of 1°. Up to 3 samples can be placed at the same time on the goniometer turntable and the Spectralon used for calibration, takes the fourth and last spot.

We created 32 samples of pure minerals and LHS-1 characterized by grain sizes \cite{11}: >250 μm (bulk sample), 250-125 μm, 125-75 μm, 75-50 μm, 50-20 μm, 20-10 μm and <10 μm (separates are wet sieved and dried). Then, we mixed the simulant with pure minerals, while setting the mineral abundances at 1, 2, 3, 4, 5, 10 and 15 vol.% For each pure mineral sample, we acquire the reflectance by varying the angles of emission and incidence with a constant step of 10°, giving a total of 1080 spectral measurements.

Spectra of minerals/LHS-1 mixtures are acquired by the ASD FieldSpec 4 with fixed incidence and emission angles of 30° and 0° (nadir) respectively. To match the spectral range of instruments on board the rovers, we use two other spectrometers: (1) FTIR 4300 acquiring spectra between 1920 and 15385 nm with a resolution of 4-16 nm used to extend the spectral range into the thermal infrared domain; (2) Ocean HDX recording wavelengths between 200-1100 nm to focus on the UV range. Last one is set up on the goniometer with same fixed angles used for the ASD. FTIR is used with a contact probe contiguous to the sample. These
measurements are used to derive a spectral library that can be compared to that generated by the Hapke model.

The Hapke radiative transfer model. This step involves evaluating the model’s accuracy by considering the input parameters such as single scattering albedo, observation geometry, backscattering, and phase function [10]. This model allows for the calculation of bidirectional reflectance for each wavelength by varying the mineral grain size and abundance, as well as incidence and emission angles, and sample porosity. Considering each variation of the previously mentioned parameters, the model produces a spectral signature for each possible combination. As an output, we compile modeled spectra in a spectral library.

Evaluate the Hapke model accuracy for mineral abundance estimation. After modeling spectra using the Hapke model, we compare them to the measured spectra to identify the best fit. To achieve this, we compute the Root Mean Square Error (RMSE) for each spectrum pair and select pairs with the lowest RMSE values. Subsequently, we can compare properties between the two spectra and assess the global accuracy of the model.

Expected results:
We aim to create a spectral library containing measured spectra of ilmenite, red hematite, and pink Mg-spinel across different grain sizes and acquisition parameters. We expect changes in reflectance values, predicting an increase with finest fractions (<25 μm) due to their more significant impact on the signal than thicker grains [11]. Also, an increase in incidence angle is expected to decrease reflectance values, characterizing the spectral behavior of minerals. Similarly, LHS-mineral mixtures could provide information about limits of detection for mineral absorption bands and help to determine the minimum abundance required to detect studied minerals. Overall, this data proves valuable for identifying these minerals during robotic missions on the Moon, including VIPER, the Canadian Lunar Rover [12] or other upcoming missions.

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References:

Figure 1: Spectral signatures of the minerals studied. (A) Comparison of hematite spectra measured by the M3 sensor and the USGS reference spectral library [Li et al., 2020]; (B) Spinel reference spectrum [Pieters et al., 2011]; (C) Spectra of the main minerals: plagioclase (Plg), clinopyroxene (Cpx), orthopyroxene (Opx), olivine (Ol) and ilmenite (Ilm) [Lemelin et al., 2013]; (D) Spectrum of ilmenite [Lemelin et al., 2013].

Figure 2: Images of pure mineral samples for various grain sizes.

Figure 3: Diagram of the installation of the ASD FieldSpec 4 High-Res NG spectrometer on the homemade goniometer. The setup is installed in a dark room during measurements, and everything is painted with non-reflective paint.