

Polarized Infrared Bidirectional Spectroscopy: A New Tool for Characterizing Water in Planetary Materials.

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Introduction: Water or hydroxyl was detected on the surface of the Moon by three spacecraft [1-3] through identification of a 3-micron absorption. There are several hypotheses to account for this spectral feature [?], and those involving the water molecule include water temporarily adsorbed to the surface of lunar soil grains [2, 5-6], trapped within impact glasses [7], or indigenously within pyroclastic deposits [8].

However, there is no available method to distinguish surface adsorbed and internal water of lunar surface materials.

Polarimetry has not been widely applied in planetary remote sensing, but using it in the infrared has the potential to distinguish surface adsorbed water from internal water in lunar regolith and rocks. Given a plane defined by light source, sample and observer, linearly polarized light can be divided into parallel and perpendicular branches based on their oscillation orientation relative to this plane.

For a particulate surface, the observed light comes from specular reflection and light that emerges from the surface after volume scattering. Ideally volume scattered light would be depolarized due to multiple reflection and transmission among the grains. Therefore, the observed perpendicular light comes from specular reflection and part of the volume reflection, and the observed parallel light only comes from volume reflection. As a result, the perpendicular branch may contain information on surface adsorbed water on the optical surface, while the parallel branch may contain both surface adsorbed water on surface of grains below the optical surface and internal water within grains.

In this work, we prepared samples that were known to contain no internal water in order to better understand the infrared polarization properties of surface adsorbed water.

Method: The instrument setup is shown in Fig. 1. It comprises a Designs & Prototypes model 102F portable Fourier-transform infrared spectroscopy (FTIR) spectrometer equipped with a linear polarizer in front of the spectrometer lens, a light source, and a hot/cold sample stage. The perpendicular and parallel polarization positions on the polarizer wheel are determined by finding the maximum and minimum signal counts on the FTIR. We measured the raw data for samples and an Infragold, and dark spectra at two polarization positions that contains signals of the environment and instrument. After subtracting the dark spectrum from both sample and gold reference, the

reflectance spectra were derived from dividing the sample spectra by the Infragold.

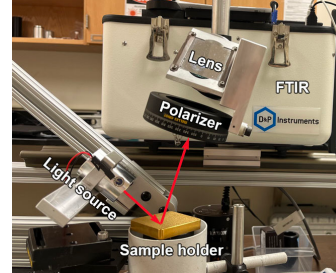


Fig. 1 Polarized FTIR instrument set up.

For the samples, we procured CaF_2 infrared optical windows designed for using near 3 microns and contain no detectable water absorption. We crushed and ground a CaF_2 window and wet sieved them with distilled water to obtain five size fractions: $<25 \mu\text{m}$, $25\text{--}45 \mu\text{m}$, $45\text{--}63 \mu\text{m}$, $63\text{--}125 \mu\text{m}$, and $125\text{--}200 \mu\text{m}$. Smaller grain size fractions should adsorb more water per unit mass due to their higher surface/volume ratio [10]. These different grain sizes allow us to track different amounts of water adsorbed on the surface of CaF_2 grains. Before measuring, all samples and the Infragold were placed on a hotplate and heated to 100°C for at least 12 hours to remove most of the surface adsorbed water. The “hot” spectra for all samples were then measured while the samples were placed on a 100°C sample holder. We then let the samples and Infragold in ambient air for 12 hours so water can adsorb to the grain surface, then measured the “cold” spectra.

Results: The polarized reflectance spectra measured under “hot” and “cold” conditions are shown in Fig. 2 a, b and d, e, respectively. The spectra of hot and cold samples both show that the water absorption is stronger at minimum (parallel) polarization than the maximum (perpendicular), meaning that the volume scattering travels a longer light path and interacted with more particles, thus captured more surface adsorbed water compared to the singular specular reflection off the top layer of the samples.

The spectra of the hot CaF_2 at all grain sizes show a weak 3-micron absorption at both maximum and minimum polarization orientations, indicating that heating the sample at 100°C for 12 hours under ambient air did not remove all surface adsorbed water.

After exposing samples to ambient air at about 22°C for 12 hours, an increase in the depth of 3-micron absorption was observed for all grain size fractions, indicating that water had adsorbed to the surface of the CaF_2 grains. Similar to the hot samples, the minimum

polarized spectra show deeper 3-micron absorption depth than the maximum polarized spectra.

We also observed a trend in the 3-micron absorption depth variation along the grain size of CaF_2 : smaller grain sizes (<25 μm , 25-45 μm , 45-63 μm) tend to show larger absorption depths than larger sizes (63-125 μm , 125-200 μm). This trend was observed for both heated and cold samples and is consistent with the findings of [10]. The adsorption depth did not vary systematically among the grain sizes: the 3-micron absorption depth is similar among the three size fractions smaller than 63 μm ; similarly, the two size fractions larger than 63 μm have comparable 3-micron depths in their spectra.

Interestingly, when we plot the ratio of the minimum and maximum polarized spectra for all grain sizes (Fig. 2 c and f), the observed difference in 3-micron spectral absorption with grain size is minimized; though the cold samples still have stronger 3-micron absorption depths than the hot samples.

Discussion: Theoretically, the perpendicular branch (maximum polarization) contains water absorption from surface of the grain and half of the volume scattering, while parallel (minimum polarization) only contains water absorption from half of the volume scattering. However, for particulate samples, the surface specular reflection does not occur at the same phase angle, which reduced the surface specular reflection. Since the specular reflection removed most of the perpendicular light, the incident light of volume scattering tends to be dominated by parallel polarization. For translucent and bright minerals, volume scattering may be not efficient enough to entirely depolarize the light [9]. Our observation show that the parallel branch shows stronger water absorption for both hot and cold samples, indicating that parallel polarized light dominates the volume scattering, and only small amount of volume scattered light contributed to the perpendicular branch.

Our measured polarized spectra show an obvious variation in 3-micron absorption depth between the hot

(water-poor) and cold (water-rich), indicating an increase in the adsorbed water content on CaF_2 grains. Smaller grain sized fractions show stronger water absorption because their larger surface/volume ratio allows photons to have more chance to interact with grains and their surface adsorbed water, consistent with the suggestion of [10].

The ratioed spectra of volume scattering (minimum polarization) and specular reflection (maximum polarization) exhibit little variation with grain sizes. An increase in 3-micron depth still can be seen as more water adsorbed on the cold samples compared to the heated samples. This ratio appears to be insensitive to the different water content caused by grain size. We infer that this ratio may be related to the amount of water per unit surface area within the sample but not the total mass of water in the sample, which may be a useful parameter.

Conclusion: The polarized spectra of a series of different grain sized CaF_2 samples show that the volume scattering branch (parallel) sees more surface adsorbed water than the specular reflected branch (perpendicular), and the ratio of the two branches may be independent on the grain sizes because no internal water exists within CaF_2 powders.

In the future, we will measure samples contain internal water, to further investigate the dependence of polarized ratio spectra on grain size.

References: [1] Pieters C. M. et al. (2009), *Science*, 326(5902), 668-672. [2] Sunshine J. M. et al. (2009) *Science*, 326(5962), 565-568. [3] Clark, R. N. (2009). *Science*, 326(5952), 562-564. [4]? [5] Watson, K. et al. (1961). *JGT*, 66(9), 3033-3045. [6] Hendrix, A. R. et al. (2019). *GRL*, 46(5), 2417-2424. [7] Honniball C. I. et al. (2021). *Nature Astronomy*, 5(2), 121-127. [8] Milliken, R. E., & Li, S. (2017). *Nature geoscience*, 10(8), 561-565. [9] Hapke, B. (2012). Cambridge university press. [10] Fisher E. A. et al. (2023) 54th LPSC.

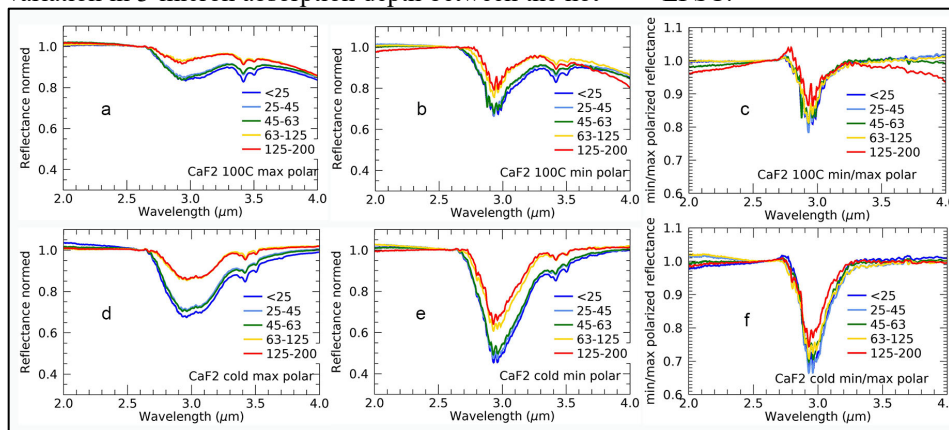


Fig. 2 Top row is (a) maximum polarized (b) minimum polarized and (c) ratio of minimum and maximum spectra of five grain size fractions of CaF_2 powders measured at 100°C, and bottom row is the same set of samples measured at room temperature. All reflectance spectra were normalized to 2.6 microns.