

Visible and Mid-Infrared Gypsum Optical Constants for Modeling of Martian Deposits

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Introduction: Recent and on-going remote and in situ observations indicate that sulfates are present in significant abundances at various locations on Mars [1-7]. The Mars Reconnaissance Orbiter (MRO) imaging spectrometer (CRISM) is returning hyperspectral data at higher spatial resolution [8] than the OMEGA instrument on the Mars Express Mission [3]. Data from both OMEGA and CRISM have provided spectral evidence for the presence of gypsum and various hydrated sulfates on the Martian surface [e.g. 3-7]. Thus, the optical properties of sulfates, in general, are of interest to quantitative interpretation of this increasing volume of remotely sensed data. This is because optical constants describe how a material interacts with electromagnetic radiation and represent the fundamental values used in radiative transfer calculations describing a variety of physical environments. Such environments include atmospheres where aerosols are present, planetary and satellite regoliths, and circumstellar dust clouds.

Here we focus upon gypsum because of its applicability due to its identification on Mars. Also, gypsum is a mineral that is readily available in sample sizes that are suitable for study using a variety of spectral measurements. In the infrared ($>5 \mu\text{m}$) several studies reporting the optical constants of gypsum can be used in evaluating the approach used here. Most importantly, there is a general lack of data regarding the optical constants for gypsum at visible and mid-infrared wavelengths ($0.4\text{-}5 \mu\text{m}$) that are being observed by OMEGA and CRISM.

Background: In the infrared, there have been several studies focused at determining the optical constants of gypsum using classical dispersion models [9-11]. These have used a variety of samples including; crystals, compressed pellets of pure materials, and grains suspended in a KBr matrix.

Spectral measurements of gypsum, and other sulfates, have existed for about 100 years at visible and mid-infrared wavelengths (0.4-5 μm) [e.g. 12-16]. All the mid-infrared spectra exhibit distinct spectral features near 4.5 μm that are attributed to the sulfate anion [12,16]. Yet no sign of this feature is present in the infrared data used to determine the optical constants. This discrepancy, and lack of optical constants in the visible and mid-infrared prompted us to undertake an effort to estimate k -values at these wavelengths.

Data Used: On-line spectral libraries are available at RELAB (<http://lfr314-rlds.geo.brown.edu/>) and ASTER (<http://speclib.jpl.nasa.gov/>). Both contain spectral data and information regarding sample acquisition, characterization, preparation, and spectral measurements. The RELAB gypsum samples used here are <45 μm (SF-EAC-041-A/LAS41A) and 25-75 μm (CC-JFM-016-B/F1CC16B). The ASTER gypsum sample included in this study (SO-02B) is separated into three sieve size fractions of <45 μm , 45-125 μm , and 125-500 μm .

For the RELAB data, two spectrometers (0.3-2.6 and 0.8-26 μm) were used to acquire the reflectance spectra. The first measures bidirectional reflectance while the second measures biconical reflectance. We used data from the RELAB site that was already combined.

Similarly, for the ASTER data two spectrometers (0.4-2.5 and 2.0-15 μm) were used to acquire the directional-hemispherical reflectance. These individual data sets were combined in the region of overlap. The bidirectional reflectance was calculated from equation 4 of [17]. Specifically, $\log R_b(30^\circ) = 1.088 \log R_h$, where R_b is the bidirectional reflectance with incidence and emission angles of 30° and 0° , respectively, and R_h is the hemispherical reflectance. Examination of the ASTER data revealed that the reflectance of the coarse grained sample is greater than the medium grained sample at wavelengths <1 μm . This spectral behavior is suspicious since as the grain size increases, the pathlength of photons through the material should increase and the effect should be increasing absorption resulting in a decrease in reflectance. As a result, we do not use the coarse grained data in any further analyses.

As another check of our results we use the measured transmission of a gypsum crystal that includes the 0.3-2.5 μm , and in some cases to 3.5 μm , wavelength domain.

Analytical Approach: [18] and [19] describe an approach to determination of the ab-

sorption coefficient, α s from the measured reflectance spectra that relies upon Hapke's description of radiative transfer within particulate surfaces [20-22, and references therein]. Since α is related to k via the dispersion relation, $\alpha=4\pi k/\lambda$, this approach provides a mechanism of determining k .

More recently, [23] describe an approach for deriving k using [24]'s description of radiative transfer within particulate surfaces. We use both of these approaches and compare the results with each other. During our analyses, we assume the average optical constants of Long et al. are accurate at wavelengths in the infrared; with the notable exception of the 4.5 μm region

A treatment of light being transmitted by a slab of material is discussed in detail in [25] and [26]. Representations of the transmission of a slab is given by equations 2.74, 2.75, and 2.76 of [25], in order of decreasing complexity. We used each of these equations and compared the results with each other, and also to the results of the particulate scattering theories.

Results: We identify a discrepancy between the reported available infrared optical constants of gypsum and reflectance measurements of gypsum that clearly indicates an absorption near 4.5 μm . We conclude this discrepancy arises due to the relative weak nature of the 4.5 μm feature that implies previous techniques were insensitive to its presence.

We apply two different scattering theories to estimate the optical constants of gypsum in the visible and mid-infrared wavelengths. We conclude both of these theories are capable of addressing the weak features, but suffer from fundamental insensitivities where materials exhibit their highest k -values. Fortunately, this is exactly the opposite situation for optical constants determined via Fresnel reflectance measurements where they are sensitive when k is high, but insensitive when k is low. We recommend taking advantage of both techniques by applying them in the appropriate regions. This is especially true for samples where relatively thick and optically clear crystals are not readily available.

We combine the results of the scattering theories with previous infrared results and calculate average n - and k -values and their associated standard deviations. We compare these with k -values estimated from transmission measurements at visible and short infrared wavelengths. We find the two derivations are in remarkable agreement. This supports the suggestion of [27] for combining the results of scattering theories with Fresnel reflectance measurements provide more accurate estimates of the optical constants of materials.

Acknowledgements: TLR recognizes the important support from NASA's Planetary

Geology and Geophysics and Mars Fundamental Research Programs that enabled this research. FE and LC gratefully acknowledge funding from the Italian Space Agency (ASI) under contract I/010/05/0. GRR acknowledges support from NASA's Mars Fundamental Research program.

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