

GYPSUM OPTICAL CONSTANTS IN THE VISIBLE AND NEAR-INFRARED: REAL AND IMAGINED.

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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 [1-5]. In addition, the scheduled Mars Reconnaissance Orbiter (MRO) will be equipped with an imaging spectrometer (CRISM) that will return hyperspectral data at higher spatial resolution [6] than the OMEGA instrument on the Mars Express Mission [3]. 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 mid-infrared 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 near-infrared wavelengths (0.4-5 μm) that are being observed by OMEGA and planned for CRISM.

Background: In the infrared, there have been several studies focused at determining the optical constants of gypsum using classical dispersion models [see figure 1, 7-9].

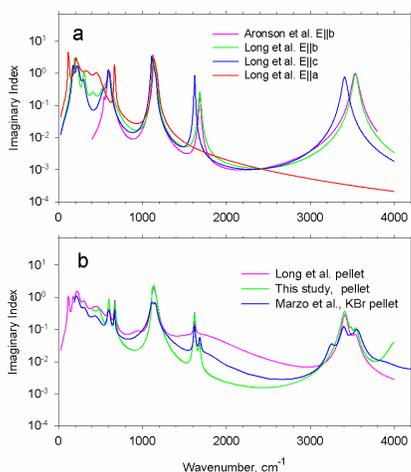


Figure 1. IR imaginary index of refraction (k) determined from various studies. a) crystals b) compressed pellets.

Spectral measurements of gypsum, and other sulfates, have existed for about 100 years at mid-infrared, near-

infrared, and visible wavelengths (0.4-5 μm) [e.g. 10-14]. All these latter spectra exhibit distinct spectral features near 4.5 μm that are attributed to the sulfate anion [10,14]. Yet no sign of this feature is present in the infrared data [compare Figs. 1, near 2220 cm^{-1} , and 2, near 4.5 μm].

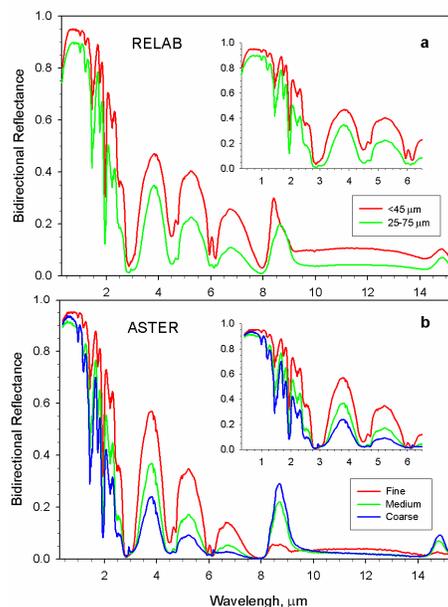


Figure 2. Laboratory Reflectance data used in the current study. a) RELAB. b) ASTER. The inset in each shows the obvious 4.5 μm feature.

Data Used: On-line spectral libraries are available at RELAB (<http://lf314-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/LASF41A) 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 . All these spectra are shown in Fig. 1.

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 [15]. Specifically, $\log R_b(30^\circ) = 1.088 \log R_h$, where R_b is the bidirectional reflectance 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 $<1 \mu\text{m}$. 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 $0.3\text{-}2.5 \mu\text{m}$ wavelength domain as shown in Figure 3.

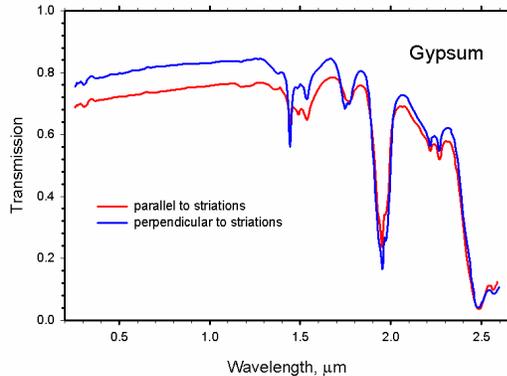


Figure 3. Transmission of a gypsum crystal.

Analytical Approach: [16] and [17] describe an approach to determination of the absorption coefficient, α , from the measured reflectance spectra that relies upon Hapke's description of radiative transfer within particulate surfaces [18-20, 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, [21] describe an approach for deriving k using [22]'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 $4.5 \mu\text{m}$ region

A treatment of light being transmitted by a slab of material is discussed in detail in [23] and [24]. Representations of the transmission of a slab is given by equations 2.74, 2.75, and 2.76 of [23], 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.

Initial Results: Results of the two different scattering theories and previous values at infrared wavelengths are compared in Figure 4, and results are extended to near-infrared and visible wavelengths where a comparison of the results to those from the transmission measurements is provided in Figure 5.

Summary: We find dispersion analysis models accurately describe the optical constants in the regions of strong absorption ($k \geq 0.1$), where they are least sensitive to the scattering occurring in the sample. We find particulate scattering theories can provide estimates of the optical constants in the

regions of weak absorptions, where the dispersion analysis models are relatively insensitive. In the visible to mid-ir we find the scattering theories consistently predict lower values of k than values determined from transmission models. This latter discrepancy may arise from scattering that is unaccounted for in the transmission measurements and/or models.

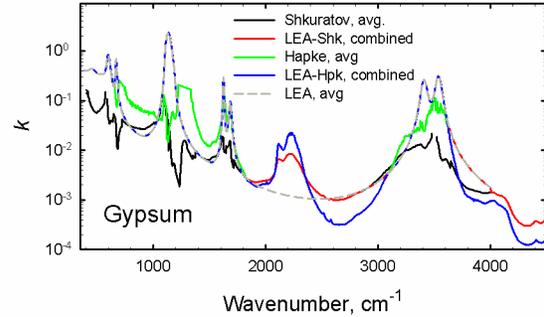


Figure 4. Comparison of imaginary index of refraction values determined in the infrared using various techniques.

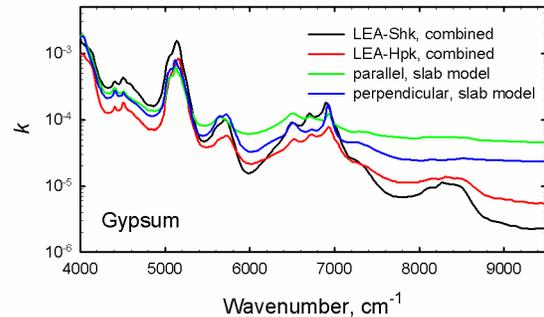


Figure 5. Comparison of imaginary index values at near-ir and visible wavelengths determined using transmission measurements and particulate scattering models.

References: [1] Bandfield 2002 *JGR*, 107, 9-1 [2] Klingelhofer et al. 2004 *Science*, 306, 1740. [3] Bibring et al. 2005 *Science*, 307, 1576 [4] Langevin et al. 2005 *Science*, 307, 1584 [5] Gendrin et al. 2005 *Science*, 307, 1587 [6] Murchie et al. 2003 *6th Intl. Mars. Conf.* 3062. [7] Aronson et al. 1983 *Appl. Opt.*, 22, 4093 [8] Long et al. 1993 *IR Phys.*, 34, 191 [9] Marzo et al. 2004 *Adv. Sp. Res.*, 33, 2246 [10] Coblenz 2006 *Carnegie Inst. Wash., Publ.* 65 [11] Hovis 1966 *Appl. Opt.*, 5, 245 [12] Fink and Burk 1971 *Comm. Lunar. Planet. Lab.*, 185, 8 [13] Salisbury et al. 1991 *Infrared (.1-25 mm) spectra of Minerals*, John Hopkins U. Press [14] Blaney and McCord 1995 *JGR*, 100, 14433 [15] Shkuratov and Grynko 2005 *Icarus*, 173, 16 [16] Hapke and Wells 1981 *JGR*, 96, 3055 [17] Clark and Roush 1984 *JGR*, 89, 6329 [18] Hapke 1981 *JGR*, 96, 3039 [19] Hapke, 1986 *Icarus*, 67, 264 [20] Hapke 1993 *Theory of Reflectance and Emittance Spectroscopy*, Cambridge Press [21] Poulet and Erard *JGR*, 109, E02009 [22] Shkuratov et al. 1999 *Icarus*, 137, 235 [23] Bohren and Huffman 1983 *Absorption and Scattering of Light by Small Particles*, Wiley [24] Heavens 1970 *Thin Film Physics*, Methuen