VNIR OPTICAL CONSTANTS OF HYDROUS CALCIUM-SULFATES: GYPSUM AND BASSANITE.

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Introduction: Gypsum ($CaSO_4$•$2H_2O$) and bassanite ($CaSO_4$•$0.5H_2O$) are generally common evaporitic minerals on Earth. Gypsum and bassanite have also been detected in several regions on Mars from remote sensing data. Gypsum has been identified in Olympia Planitia in the north polar region [1]. Bassanite has been found at Mawrth Vallis [2]. Since their formation is typically associated with water, they can hold important information of aqueous activities on ancient Mars, specifically in terms of temperature, humidity and salinity.

Visible and near-infrared (VNIR) reflectance spectroscopy is an important and useful method to identify minerals on a remote sensing platform. However, determining abundances of minerals in a mixture is difficult because spectral response does not mix linearly with abundance in the VNIR wavelength region. Radiative transfer theory can be used to address the problem of non-linear spectral mixing and to extract quantitative mineral contents [3, 4]. Radiative transfer theory describes the interaction of light with a particulate medium. Although reflectance is not linearly correlated with concentration in a mixed spectrum, the single scattering albedos of individual components in a mixture do combine linearly. Optical constants (complex indices of refraction, *n* and *k*), fundamental properties of minerals, are important input parameters of single scattering albedo in a radiative transfer calculation.

This work presents the preliminary results of optical constants of the common known hydrous Ca-sulfates using radiative transfer theory.

Methods: Gypsum and bassanite were ground and sieved into three size fractions (63-90, 90-180, 180-250 μm). VNIR (0.35-2.5 μm) reflectance spectra were acquired at 7 phase angles from 15 to 45º for each sample referenced to a spectralon standard using ASD spectroradiometer at Stony Brook University's Center for Planetary Exploration (CPEx).

Optical constants *n* and *k* were calculated using Hapke's model of radiative transfer theory encoded by MATLAB through several steps of minimization [5]. First, *k* for each grain size was guessed individually by fixing all other parameters except *k* through a lookup table. Then a global minimization routine was used to find a single size-independent *k* for three grain sizes simultaneously. The VNIR *k* was combined with MIR (2.5-50 μm) *k* calculated from classical dispersion theory and this long range *k* was used to derive VNIR *n* by a Kramers-Kronig analysis. Both *n* and *k* were put into the minimization step to determine the phase function. We used *n* and the new phase function to run the minimization routine for a new *k* and vice versa. The process was iterated until *n* and *k* do not change substantially.

Results: The fitting results and VNIR optical constants of gypsum and bassanite are shown in Figure 1 and 2. The calculated spectra from size-independent *k* by global minimization can fit the laboratory data very well. The size-independent *k* is different from any size dependent *k*, and also not the same as the average of size-dependent *k* values.

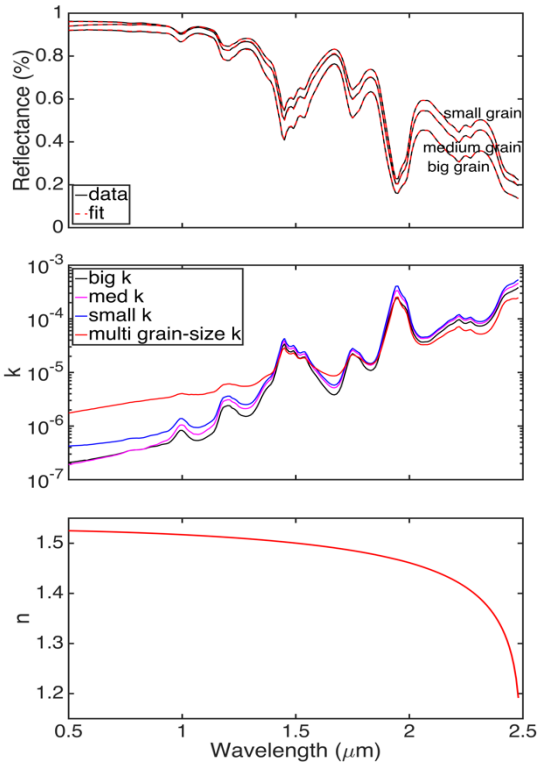

Figure 1. Fitting results and optical constants of gypsum. (Top) Reflectance from size-independent *k* overlying on laboratory data. (Middle) Imaginary index of refraction, *k*, for individual grain sizes and from multi grain size minimization. (Bottom) Real index of refraction, *n*.

The phase function minimization step gives the fitting results and determines phase functions used in this radiative transfer model for gypsum and bassanite shown in Figure 3 and 4. Nearly all modeled spectra from three size fractions and seven phase angles fit laboratory measurements well. The phase function is constrained afterwards.

Discussion: During the computation of optical constants in this work, porosity of particulate sample

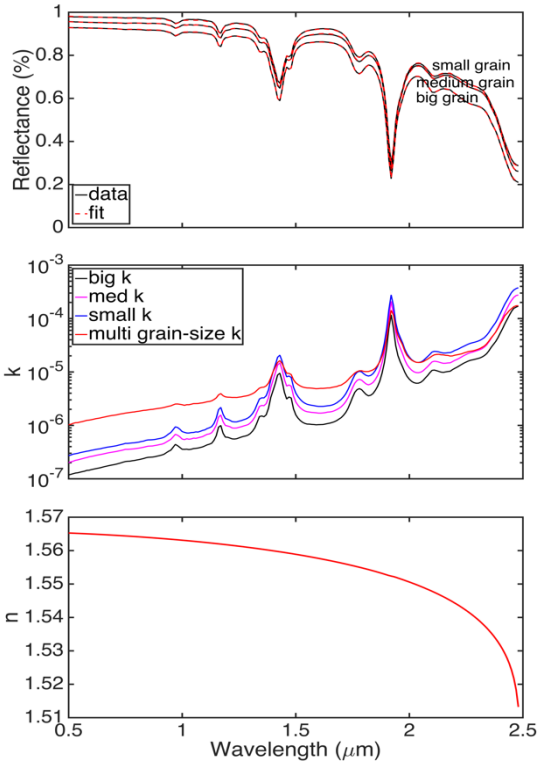

Figure 2. Fitting results and optical constants of bassanite. (Top) Reflectance from size-independent k overlying on laboratory data. (Middle) Imaginary index of refraction, k, for individual grain sizes and from multi grain size minimization. (Bottom) Real index of refraction, n.

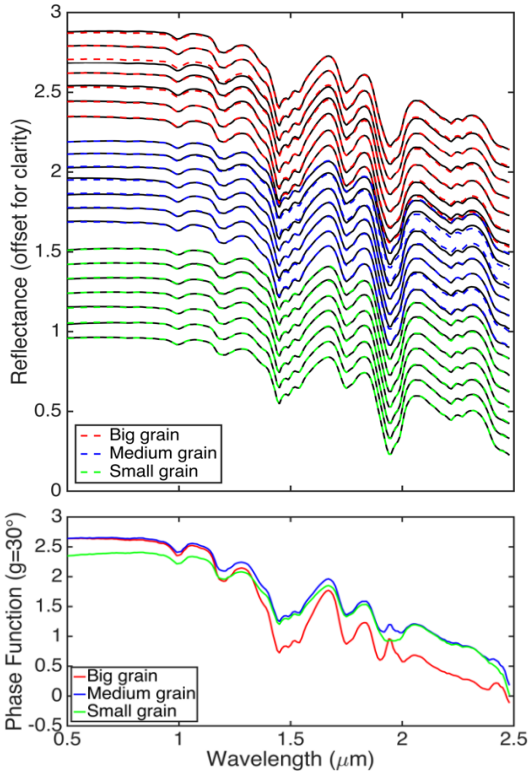

Figure 3. Phase function fitting results and determined phase function for gypsum. (Top) Calculated and measured reflectance for 3 sizes at 7 phase angles. (Bottom) Phase function at g=30º.

and phase angle error during the measurements are two big sources of error. Different values of porosity can change k substantially. Meanwhile, error from the phase angle should be considered carefully when taking spectral measurements and running the program.

Conclusion: Optical constants derived in this method are robust. This work expands the library of optical constants and can be used to compare with previous data from other methods. Optical constants presented here allow for the use of radiative transfer theory to extract the individual component from mixed spectra.

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References: [1] Langevin et al., (2005) *Science*, 307 (5715), 1581-1584. [2] Wray et al., (2010) *Icarus*, 209, 416-421. [3] Hapke, (1981) *J. Geophys. Res.*, 86(B4), 3039-3054. [4] Hapke, (2012) *Cambridge Univ. Press*, NY. [5] Sklute et al., (2015) *Am. Mineral.*, 100, 1100-1122.

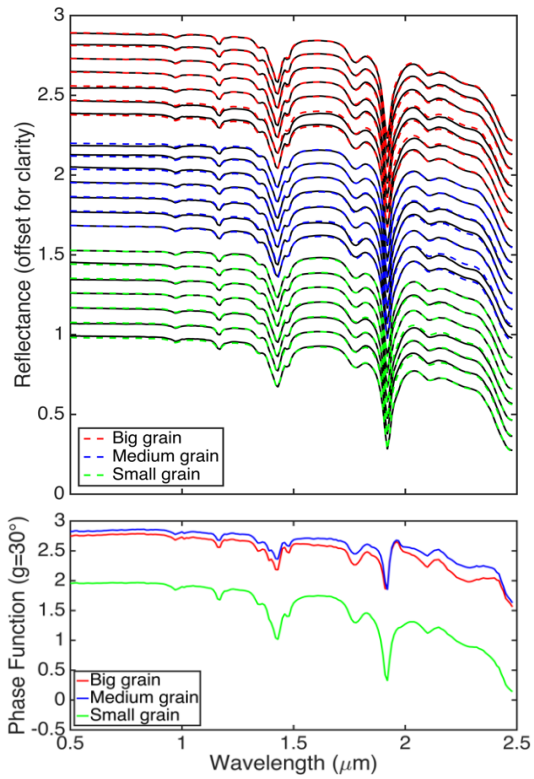

Figure 4. Phase function fitting results and determined phase function for bassanite. (Top) Calculated and measured reflectance for 3 sizes at 7 phase angles. (Bottom) Phase function at g=30º.