MID-INFRARED OPTICAL CONSTANTS OF PHYLLOSILICATES FOR ANALYSIS OF OSIRIS-REX THERMAL EMISSION SPECTROMETER DATA. O. L. Koren[1], T. D. Glotch[1], and L. B. Breitenfeld[1], [1]Dept. of Geosciences, Stony Brook University, Stony Brook, NY, olivia.koren@stonybrook.edu.

Introduction: Primitive materials that inform us about processes that occurred in the early stages of the Solar System are found in CI and CM chondrite meteorites. NASA's OSIRIS-REx (Origins, Spectral Interpretation, Resource Identification, and Security–Regolith Explorer) spacecraft is returning a sample from the near-Earth asteroid Bennu that displays similar spectral properties to CI and CM chondrites. The remote sensing mission data and returned sample will help the planetary science community gain insight into how planets formed and, potentially, the origins of organic material in the Solar System [1]. In this work we derive the mid-infrared (MIR) optical constants of several mineral phases that will be critical inputs to a radiative transfer model that will be used to model spectra of Bennu using mineral abundances estimated from machine learning analyses [2]. These modeled spectra will help in the analysis of the data collected by the OSIRIS-REx Thermal Emission Spectrometer (OTES) to better constrain the composition of Bennu.

Background: Analysis of the MIR data indicates that Bennu is composed primarily of phyllosilicates, as also seen in CI and CM chondrites [3]. While it is difficult to quantify mineral abundances of finely particulate planetary surfaces in the MIR due to nonlinear mixing effects, machine learning models were developed to tackle this problem and aid in composition predictions of Bennu [2]. These machine learning models estimate that the average composition of Bennu is 78% phyllosilicates, with smaller abundances of olivine, carbonate, and magnetite [2]. To further understand the composition of Bennu and improve the accuracy of the machine learning models, we can model the OTES spectra using the derived mineral composition through a radiative transfer model approach. The first step is to ensure that we have adequate optical constants of all relevant phases for this task.

Methods: To begin, reference spectra of minerals that match the predicted composition of Bennu are needed. We ground samples into fine particulates (<60 μm) and pressed them into pellets using a Pike press and anvil set. We acquired simulated asteroid environment (SAE) MIR emissivity spectra of each sample using Stony Brook University's Nicolet 6700 Fourier Transform Infrared (FTIR) spectrometer attached to the Planetary and Asteroid Regolith Spectroscopy Environmental Chamber (PARSEC). The samples were chosen because they are commonly found in CI and CM chondrite compositions, and include olivine, ferrihydrite, pyrrhotite, Mg-rich serpentine (antigorite), gypsum, magnetite, saponite, Fe-rich serpentine (cronstedtite), calcite, dolomite, and enstatite [2]. From these samples, we derived the real (n) and imaginary (k) refractive indices.

To find the n and k values, we use a dispersion theory model coupled with a Fresnel reflectance model while minimizing the difference between the measured and modeled spectra using a nonlinear least squares optimization. We convert the measured emissivity spectra to reflectance using Kirchhoff's Law ($\varepsilon = 1 - R - T$), assuming transmission (T) is zero. Oscillator parameters (center frequency of the oscillation (ν), the band strength ($4\pi\varrho$), width (γ), and the high frequency dielectric constant (ε_0)) were set at wavenumbers where spectral features are visible to model the spectra. Additional oscillators are added until the residual between the modeled and measured spectra is low. When the modeled spectra fit the measured spectra the optical constants are derived using the following relationships [5]:

$$n^2 - k^2 = \varepsilon_0 + \sum_j \frac{4\pi\rho_j\nu_j^2(\nu_j^2-\nu^2)}{(\nu_j^2-\nu^2)^2+(\gamma_j^2\nu_j^2\nu^2)} \quad (1)$$

$$nk = \sum_j \frac{4\pi\rho_j\nu_j^2(\gamma_j^2\nu_j^2\nu^2)}{(\nu_j^2-\nu^2)^2+(\gamma_j^2\nu_j^2\nu^2)} \quad (2)$$

This closely follows the method used by [4] for estimating the optical constants of phyllosilicates.

Results: The reflectance spectra were modeled from 1200 cm^{-1} to 300 cm^{-1}. The calcite and dolomite emissivity spectra have features associated with a thin layer of fines so their results have not been considered thus far. For the remaining pellets, using the dispersion theory model and the Fresnel equation, we found the optimal oscillation parameters and the best-fit modeled reflectance spectra. Most importantly, the n and k values of each sample were calculated and plotted. The biggest challenge in this process was finding the correct number of oscillators for each sample as it differs with each sample.

The measured and modeled spectra of cronstedtite, their residual, and the modeled n and k values are shown in Figure 1. Figures 2 and 3 show equivalent data for the antigorite and saponite samples, respectively. These three minerals are of particular interest because they are phyllosilicates that are predicted to be a significant portion of Bennu's

composition [2, 3]. The cronstedtite sample required 14 oscillators, while 16 oscillators were used for the antigorite sample and 11 oscillators were used for saponite. The saponite sample required fewer oscillators because there are fewer noticeable features in its spectra.

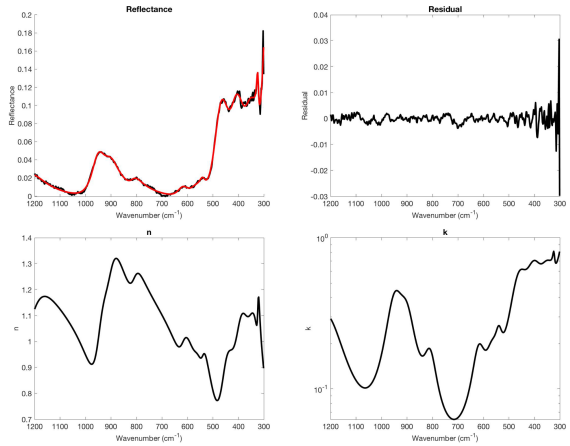

Figure 1: Optical constant data for the Fe-rich serpentine (cronstedtite) sample including (upper left) measured (black) and modeled (red) spectra of sample, (upper right) residual of the fit of the model (lower left) real index of refraction, and (lower right) imaginary index of refraction.

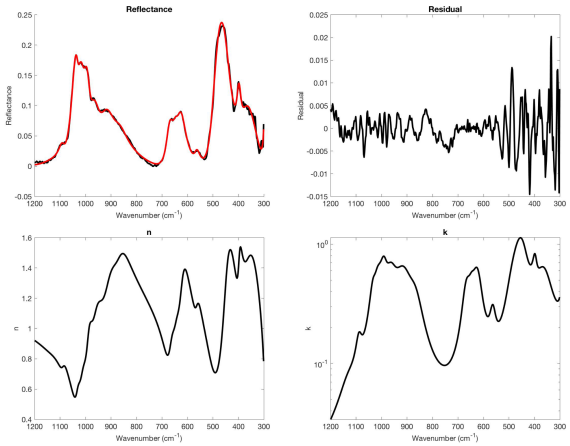

Figure 2: Optical constant data for the Mg-rich serpentine (antigorite) sample including (upper left) measured (black) and modeled (red) spectra of sample, (upper right) residual of the fit of the model, (lower left) real index of refraction, and (lower right) imaginary index of refraction.

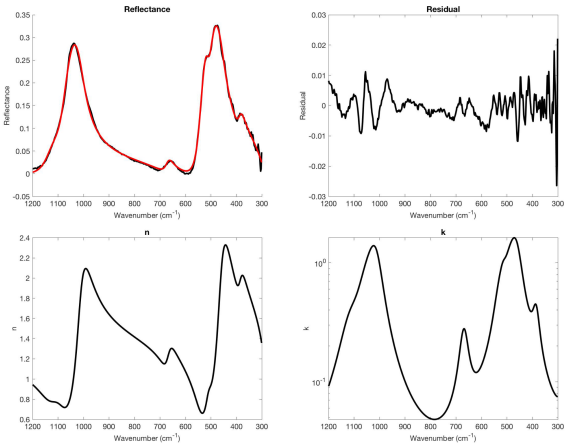

Figure 3: Optical constant data for the saponite sample including (upper left) measured (black) and modeled (red) spectra of sample, (upper right) residual of the fit of the model, (lower left) real index of refraction, and (lower right) imaginary index of refraction.

Conclusions and Future Work: We collected MIR SAE emissivity spectra of pressed pellets of fine particulates for 13 samples. For 11 of the samples, the reflectance spectra were modeled and the real and imaginary indices of refraction were calculated. These samples are all minerals detected on the asteroid Bennu or are commonly present in CI and/or CM chondrites. The development of the optical constant data calculated here lays the groundwork for additional modeling and can assist future OSIRIS-REx analyses.

Moving forward, the optical constants calculated serve as inputs to the Multiple Sphere T Matrix (MSTM) light scattering model. MSTM calculates the exact near field scattering properties of closely packed mineral grains in a cluster and outputs scattering parameters that can be used as inputs to a radiative transfer model to calculate reflectance or emissivity spectra. This method has been successfully used and discussed by [6]. The MSTM calculations will be run on the Seawulf cluster at Stony Brook University and the resulting spectra will be compared with the spectra measured by OTES to test and refine the machine learning model predictions from [2].

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