MID-IR OPTICAL CONSTANTS OF ANISOTROPIC MINERALS. J. A. Arnold[1] and T. D. Glotch[1], [1]Dept. of Geosciences, Stony Brook University, Stony Brook, NY 11794-2100, jaarnold@ic.sunysb.edu

Introduction: The complex index of refraction (ñ=n+ik) as a function of wavelength is an essential input into scattering models of planetary surfaces [1]. Hence, the optical constants n and k for a variety of minerals are needed to obtain estimates of planetary surface compositions. While minerals of orthorhombic and higher symmetry are well-covered, optical constants have been evaluated for only a few monoclinic and triclinic materials [2,3]. The monoclinic system includes many geologically important materials such as feldspars, pyroxenes and sulfates.

Background: Optical constants can be determined for minerals of orthorhombic symmetry and higher using the approach of [4]. Displacements of atomic dipoles within a crystal are modeled as Lorentzian damped harmonic oscillators.

$$(n+ik)^2 = \epsilon = \epsilon^{\infty} + \sum_{k=1}^{N} \frac{4\pi\rho_k\nu_k^2}{1-i\gamma_k(\frac{\nu}{\nu_k^2})-(\frac{\nu}{\nu_k})^2}$$

The resonant frequencies of these oscillators (ν_k) are due to the interaction of the incoming E field with bound electrons. The parameters ρ_k, γ_k and ε^{∞} are the oscillator strength, dampening coefficient and infinite frequency dielectric constant respectively. For the orthorhombic case, we can assume that these oscillations occur parallel to the crystal axes. Reflectance spectra need to be acquired for each of the three principal axes with the polarization parallel to each axis. Reflectance, given by

$$R = \frac{(n-1)^2+k^2}{(n+1)^2+k^2}$$

for normal incidence, is iteratively fit with estimated values of the oscillator parameters as input [4].

When a mineral is biaxial and the axes are not orthogonal, the oscillators cannot be assumed to be parallel with the crystal axes[5]. In a monoclinic material, the index of refraction parallel to the b-axis can be determined in the same manner as the orthorhombic case[2]. To determine the other two indices, it is necessary to make measurements at at different angles (φ) with respect to the crystal axes in monoclinic plane (⊥ to b). The complex indices of refraction are the eigenvalues of the dielectric tensor, which can be calculated as follows[2].

$$\epsilon = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xz} \\ \epsilon_{xz} & \epsilon_{zz} \end{pmatrix} =$$

$$\epsilon^{\infty} + \sum_{k=1}^{N} \begin{pmatrix} cos^2(\theta_k-\phi) & cos(\theta_k-\phi)sin(\theta_k-\phi) \\ cos(\theta_k-\phi)sin(\theta_k-\phi) & sin^2(\theta_k-\phi) \end{pmatrix} L_k$$

$$\text{where } \epsilon^{\infty} = \begin{pmatrix} cos\phi & sin\phi \\ -sin\phi & cos\phi \end{pmatrix} \begin{pmatrix} \epsilon_{xx}^{\infty} & \epsilon_{xz}^{\infty} \\ \epsilon_{xz}^{\infty} & \epsilon_{zz}^{\infty} \end{pmatrix} \begin{pmatrix} cos\phi & -sin\phi \\ sin\phi & cos\phi \end{pmatrix}$$

$$\text{and } L_k = \frac{S_k}{1+i\gamma_k(\frac{\nu}{\nu_k})-(\frac{\nu}{\nu_k})^2} .$$

The angle between each oscillator and the a-axis is denoted θ_k. Three reflectance spectra are fit simultaneously. The reflectance coefficients depend on the elements of the dielectric tensor. Although the incidence angle is oblique (30°), normal incidence is assumed. This appears to be a reasonable approximation.

Methods: The optical constants for gypsum have been previously determined by [2]. We chose this mineral as a starting point, given the opportunity for direct comparison. The sample needs to be cut so that one surface contains the ac plane and the other surface is parallel to the b-axis. In the case of gypsum, we were able to cleave the crystal along the naturally occurring (010) plane and a surface was cut perpendicular to this. We rotated the sample with respect to the incident polarization to measure reflectance at varying values of φ. Reflectance spectra can be fitted simultaneously with the non-linear fitting function lsqcurvefit, available in Matlab. While it is possible to estimate the oscillator parameters from the reflectance spectra, for gypsum we were able to use values from [2] as initial estimates. We then calculated optical constants from the resulting refined parameters.

Results and future work: Figure 1 shows measured reflectance spectra of gypsum and fits for φ = 0, 45 and 90. Figure 2 gives n and k for the optic axes parallel to the monoclinic plane. The absorption index (k) agrees with previously published results. We will apply this method to minerals belonging to the monoclinic system for which there are no published values.

References: [1] Moersch J. E. and Christensen P. R. (1995) *JGR, 100,* 7465–7477. [2] Aronson J. R. et al. (1983) *Applied Optics, 22, 24,* 4093-4098. [3] Aronson J. R. (1985) *Spect. Acta, 24A, 2/3,* 187-190. [4] Spitzer W. G. and Kleinman D. A. (1960) *Phys. Rev., 121, 5,* 1324-1335. [5] Belousov M. V. and Pavinich V. F. (1978) *Opt. Spectrok., 45,* 920-926.

Fig 1: Modeled and observed reflectance of the monoclinic plane of gypsum

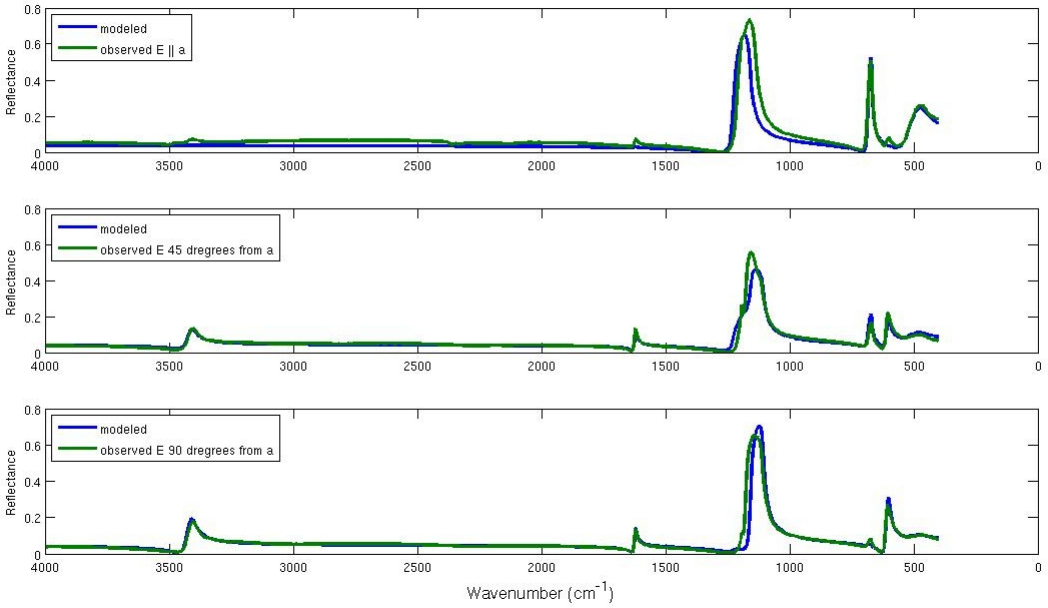

Fig 2: Optical constants for the monoclinic plane of gypsum