A FORWARD AND INVERSE MODELING STUDY OF THE MAGNETITE REFLECTANCE. Luis F.A. Teodoro¹², Ted L. Roush¹, David T. Blewett³ and Joshua T.S. Cahill³. ¹NASA ARC, Moffett Field, CA 94035, USA (luis.f.teodoro@glasgow.ac.uk), ²BAERI, NASA ARC, Moffett Field, CA 94035, USA, ³Johns Hopkins University Applied Physics Laboratory, MS 200-W2320, 11100 Johns Hopkins Rd., Laurel, MD 20723 USA.

Introduction: Reflectance spectroscopy in the UV, visible and NIR wavelengths is an important means for remotely obtaining information concerning the composition and physical state of planetary surfaces. In Hapke's formulation [1], the bidirectional reflectance spectrum of a mixture is computed from single-scattering albedo spectra of the endmembers under consideration. Single-scattering albedo (SSA) is the probability that a photon incident on a particle will be scattered, and is a function of a grain's scattering behavior (e.g., degree of internal scattering) and absorption coefficient. The absorption coefficient is in turn governed by the material's complex index of refraction: \( m = n + jk \) (e.g., [2]), where \( n \) and \( k \) are the optical constants, or real and imaginary parts of the index of refraction, respectively, and \( j = \sqrt{-1} \). The optical constants are inherent properties of a material independent of particle shape, angle of incidence of the light, etc. The optical "constants" of a material vary with wavelength, and hence are a spectral quantity. The spectral features apparent in absorption and reflectance spectra of materials in the near-IR are dominated by variations of \( k \) [e.g. 3]. Here we present our efforts to model the reflectance of magnetite, a low-reflectance, opaque mineral.

Optical constants: Central to our research are the magnetite optical constant values as function of wavelength. The optical constant data can be classified into two distinct categories:

Derived Optical Constants. We applied legacy Fortran programs, using the Hapke (1981) [1] formulation in a reverse sense (LHR) converted to Python (PHR), to estimate the imaginary index of refraction from measured reflectance of two separate grain sizes of magnetite over the 0.4–2.5 \( \mu m \) region. Briefly, the measured reflectance is fit by adjusting the \( k \)-value, at each wavelength, until the differences between measured and calculated reflectances are minimized. The measured reflectances were obtained from the RELAB database [4] and are of a fine (0-45 \( \mu m \)) and coarser (45-90 \( \mu m \)) size fraction of the same sample observed with \( i = 0^\circ \) and \( e = 15^\circ \) and \( g = 15^\circ \). In our calculations, we assumed a particle size corresponding to the average of the reported sieve size range for each sample: 22.5 \( \mu m \) for the 0-45 \( \mu m \) separate and 67.5 \( \mu m \) for the 45-90 \( \mu m \) separate. The resulting \( k \)-values are shown in Fig. 1 (orange and purple lines).

Literature Optical Constants: Visible and near-infrared optical constants of magnetite have been previously published [5,6,7]. All of these studies used polished samples and measure the specular reflectance at near normal incidence. We also employed unpublished magnetite optical constants, attributable to A. Triaud, [8]. All of these values are shown in Fig.1 along with those estimated here from reflectance using the LHR approach. The Huffman (1977) [5] values have sparse spectral sampling at these wavelengths. The Triaud values [8] are provided with no description of the experimental approach while the Schlegel et al. (1979) [6] values were digitized from their Fig. 4. The Query (1985) values have good spectral sampling and adequate experimental description. However, as illustrated in Fig. 1, they are discordant from all other literature (and web) sources, particularly at wavelengths <0.6 \( \mu m \) for \( n \) and <1.5 \( \mu m \) for \( k \). Finally, despite all these issues, we use the Query refractive indices in the Fig. 2, where we attempt to model the measured laboratory reflectance with literature values. We believe our general conclusions will remain unchanged even given the discordant nature of the Query values compared to the other available

Figure 1 Magnetite optical constants from the literature and estimated here a) Imaginary index of refraction \( k \), b) Real index of refraction \( n \) (the assumed \( n \) for lab data is the same for both grain sizes).
2020


2020

the literature values. As an extension of the PHR, we

LHR approach are

literature refractive indices. As shown in the upper panel of Fig. 1 the k-values derived here using the LHR approach are \( \sim 3 \) orders of magnitude smaller than the literature values. As an extension of the PHR, we

have also implemented a Mie calculation of the SSA. This was achieved through re-writing the Bohren and Huffman (1983) [9] Mie algorithm to quantify the light scattering and extinction efficiencies in Python.

Using the LHR estimated OCs shown in Fig. 1, their reflectances were calculated using the new PHR. We make two observations. First, the “H+M” calculations shown in in the upper panel of Fig. 2 (violet and brown lines), which used LHR OCs, present a much higher reflectance than those in the lower panel of Fig. 2, which used the Querry OCs. This seems to suggest that the much larger imaginary part of the Querry OCs (see Fig. 1) is acting to decrease the overall reflectance. Furthermore, in the lower panel of Fig. 2, the ripple pattern in the Mie reflectance is not present. This also suggests that a disparity of two orders of magnitude in the imaginary part of the refractive index also regulates the smoothness (absence of small-scale ripples) in the reflectance curve. Second, use of the incorrect grain size in the calculation of the Hapke (PHF) reflectance leads to values, presented in the lower panel of Fig. 2 (brown and orange curves), which do not reproduce the measured reflectance of each grain-size sample (green and dark blue).

**Discussion and Conclusions**: To further explore the discrepancies described above, we also employed the simple model based on Fresnel reflectance (as suggested by [10] in their modeling of the meteoric assemblages) can reproduce the gross features of the magnetite spectra. However, the calculated magnetite SSA using such model reproduces the Hapke’s counterparts. Therefore, we conclude that such a model cannot explain the measured magnetite reflectances either.

**Acknowledgments**: T.L.R., D.T.B. and J.T.S.C. were supported by NASA PDA RT grant NNX16AG41G.