n, k FOR MARS REMOTE SENSING AND MSTM MODELING K. M. Pitman[1,2], M. J. Wolff[2], E. A. Cloutis[3]. P. Mann[3], M. Cuddy[3], D. Applin[3], and A. Chanou[3], [1]Planetary Science Institute, 1700 E. Fort Lowell Road, Ste. 106, Tucson, AZ 85719 USA <pitman@psi.edu; pitman@spacescience.org>, [2]Space Science Institute, 4750 Walnut St., Ste. 205, Boulder, CO 80301 USA, [3]Dept. of Geography, Univ. Winnipeg, Winnipeg, MB, Canada, R3B 2E9.

Introduction: When spacecraft data are interpreted with analytic radiative transfer models for light scattering in planetary surfaces, it is generally assumed that minerals do not form clusters and that individual, isolated or well separated spherical particles dominate the spectral signature. However, this "far-field" assumption has been challenged [1-3]: groups of particles may actually be the constituent scatterers. If true, then this is a problem for interpreting Mars, since its soils and atmospheric dust are prone to forming clusters.

We study the changes in light scattering properties (e.g., the 4 x 4 F_{ij} scattering matrix which describes the interaction of a mineral with light) when particles are packed in close proximity in various clusters. In particular, we explore how the scattering phase function changes if the constituent scatterer is not spherical but instead has corners or edges, which is more realistic for Mars minerals. Changing the scatterer shape from a sphere, which is the default for many radiative transfer models, to a cube breaks the strong resonance features present in clusters composed of large spheres, particularly at larger size parameters [4-5]. Here we further construct "gypsum" rectangular prisms, with length-to-width ratios as estimated from SEM imaging of real gypsum grains, to approach realistic particle shapes for gypsum and include new Mars analog minerals in our shape exploration.

Methodology: We use the publicly available multisphere T-matrix (MSTM) code, versions 2.2 and 3.0 [6], cross-checked with the discrete dipole approximation code DDSCAT version 7.2 [7-8]. The MSTM code can accurately compute the scattering properties of a collection of particles, based on a rigorous solution of the Maxwell equations, and accounts for all near- and far-field effects. This paradigm is currently one of the best available numerical methods to compute light scattering in densely packed planetary surfaces [9-11]; we invoke the finite element approach (DDSCAT) to better represent true edge effects.

Thus far, we have tested several different shapes of subvolumes (sphere, cube, prolate vs. oblate rectangular prism) composed of smaller spheres to determine the constituent scattering unit shape (Fig. 1). The deep minima in the Fig. 2 phase functions are artifacts of using groups of modestly-sized spheres to approximate these shapes. Nevertheless, this approximate approach demonstrates the significant differences in scattering properties that can occur when the constituent scatterer is nonspherical.

Laboratory methods. Models shown in Fig. 1-2 are for gypsum, but we are also testing additional Mars-relevant species. Each of these minerals is characterized at the University of Winnipeg's Planetary Spectroscopy Facility after [12], both compositionally (e.g., via X-ray fluorescence, microprobe, light element analysis) and structurally (X-ray diffraction, scanning electron microscopy), then prepared as powders in several size fractions (c.f. Fig. 3). Using diffuse bidirectional VNIR+FTIR reflectance spectra acquired at λ = 0.35-25 μm and viewing geometries of i=30°, e=0°, we derive imaginary index of refraction $k(\lambda)$ using the method of [13], in which k is derived from hemispherical albedo as a function of real index of refraction in the visible, porosity and optical path length in the sample, and transmission and reflectance coefficients. Initial estimates of average particle diameters are obtained from the median sieve size and from optical and SEM microscopy images. We will present reflectance spectra and optical constants for minerals definitively or potentially identified in Mars spectra (e.g., polyhalite, datolite, prehnite, thenardite), from models of Mars dust (marcasite, lizardite), and from martian meteorites (siderite, pyrrhotite). Fig. 3 shows an example of estimated optical constants for the last case.

Significance: This work will improve our understanding of Mars in the areas of identifying, mapping the distributions, and quantifying the abundances for minerals by adding new laboratory and optical constants data on Mars-relevant minerals and addressing long-standing questions on fundamental physics in the martian surface. The ultimate goal is to clearly identify and characterize the regimes where near-field or clustering effects will fundamentally change the way that Mars spectral and photometric observations are changed. Such models help quantify how much the single scattering albedo lowers and the phase function changes in real Mars dust minerals.

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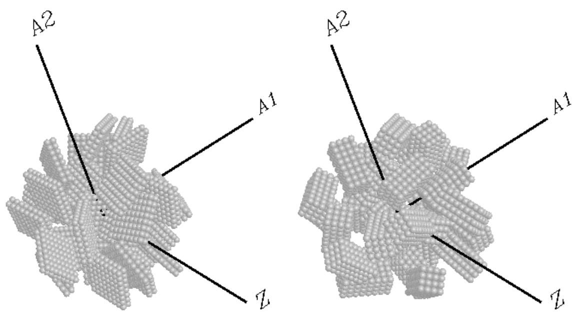

Fig. 1: Gypsum equivalent volume rectangular prisms of different aspect ratios (oblate, prolate) composed of smaller spheres used in MSTM code calculations to explore shape effects on phase function and albedo. Each sphere in the prism has a diameter such that $2\pi(\text{diameter})/\lambda = 1$. Packing fraction = 21.1%.

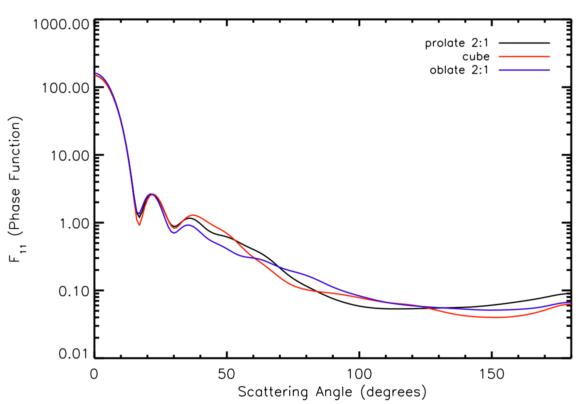

Fig. 2: MSTM single-scattering phase functions as a function of scattering angle for Fig. 1 geometries and clusters of cubes. The significant changes in amplitude in magnitude and slope highlight the importance of including reasonable particle shapes in the accurate numerical treatment of surface reflectance problems.

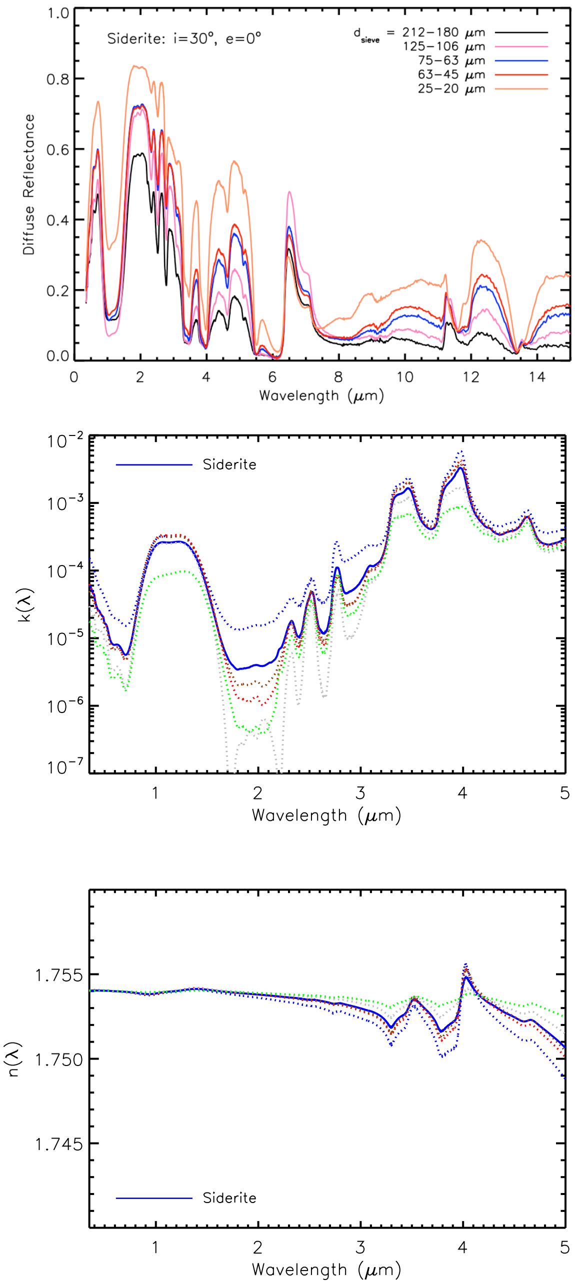

Fig. 3: Example of laboratory diffuse reflectance spectra and optical constants (imaginary and real indices of refraction *k* and *n*) to be shown at LPSC 2015. Pictured: siderite, $FeCO_3$, a mineral identified in martian meteorites (Nahklites). Top panel shows full wavelength range available; middle and bottom panels focus on MRO CRISM-relevant wavelength range. Solid blue line in middle and bottom panels indicate average optical constants.