MODELING VNIR SIGNATURES OF SPACE WEATHERING USING THE MULTIPLE SPHERE T-MATRIX MODEL: COMPARISONS TO OBSERVATIONS AND PREVIOUS MODELS. C. Legett IV[1], T. D. Glotch[1] and P. G. Lucey[2], [1]Geosciences Department, Stony Brook University 255 ESS Building, Stony Brook, NY 11794-2100 carey.legett@stonybrook.edu, [2]Planetary Geosciences/SOEST, University of Hawaii.

Introduction.

Previous Work. Nanophase iron ($npFe^0$) bearing rims on lunar regolith particles have been identified as the product of space weathering processes, including solar wind sputtering/implantation and micrometeoroid bombardment [1]. The spectral effects due to $npFe^0$ appear to be dependent on the size of the $npFe^0$ particles [2,3]. Laboratory work with lunar soils and analog materials has shown that if the $npFe^0$ is less than approximately 50 nm in size, the overall effect will be to both redden and darken the spectra whereas larger $npFe^0$ particles lead to only darkening without reddening (Figure 1) [4].

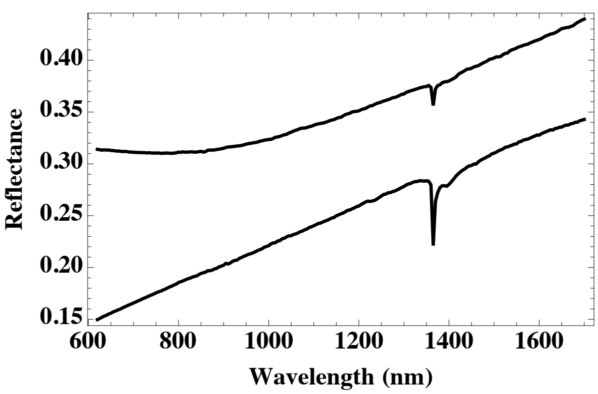

Figure 1. Spectra of silica gels impregnated with $npFe^0$. Samples contain similar amounts of $npFe^0$ but the top spectrum contains larger $npFe^0$ particles. The absorption features at 1365 nm are due to water adsorbed onto the silica gels.

Recent modeling efforts based on Mie theory and Hapke's radiative transfer model [5] have been successful at reproducing laboratory spectra using Maxwell-Garnett effective medium theory with empirical corrections [2]. These modeling efforts have not yet fully reproduced the transition from darkening and reddening to only darkening with the $npFe^0$ grain sizes indicated by laboratory work. In the models, the transition occurs at approximately 300 nm instead of 50 nm [3].

Multiple Sphere T-Matrix Model. We are investigating the use of the Multiple Sphere T-Matrix (MSTM) model in an attempt to replicate the success of the previous Mie-Hapke models and to resolve the $npFe^0$ grain size discrepancy. The MSTM model is a first-principles, direct simulation method for calculating an exact analytical solution to the time-harmonic Maxwell's equations for multiple sphere systems [6]. This method improves on Mie theory based methods by allowing multiple spheres to be in close proximity. The tradeoff is that MSTM calculations are much more computationally intensive and require either a very large number of processors or extremely long runtimes. Work being presented at this conference shows that the MSTM/Hapke approach improves the modeled spectra of fine particles over Mie/Hapke methods [7].

The model is passed a list of sphere positions and sizes with associated optical constants and then calculates the scattering, extinction, and absorption efficiencies, the asymmetry parameters, and the scattering matrix elements for either a fixed or random (averaged) orientation using either plane wave or Gaussian beam illumination. The latest version of the model is designed to take advantage of modern distributed-memory cluster computers. The results of our first test cases show reasonable reflectance spectra except when modeled particles are very small and effectively transparent.

Methods.

Model and Theory. The space weathered analog materials in [4] are silica gel particles with varying pore sizes that have been exposed to an iron containing solution to form $npFe^0$ in and on the silica particles. We are investigating several different approaches to modeling the silica particles and $npFe^0$. The first approach is to model the silica gels as collections of nanoscale silica spheres with a packing density roughly equivalent to the porosities indicated in laboratory work. A second approach is to generate a single large sphere to represent the silica gel, apply effective bulk optical constants given the porosity, and populate it with $npFe^0$ particles to reach the desired iron content.

In the first approach, we generate a spherical volume containing several thousands of spheres using PackLSD molecular dynamics software [8,9]. The software generates a mono- or bidisperse collection of spheres with a specified packing density. The sphere positions output from PackLSD are reformatted into a format acceptable to the MSTM model, and an index of refraction (n) and extinction coefficient (k) are added to each sphere depending on the phase it is intended to represent and the wavelength we are modeling. If a monodisperse collection is used, the output from

PackLSD represents only the silica portion of each particle. Particles representing $npFe^0$ are added by a script written for the purpose and can be placed either entirely inside spheres representing silica particles, entirely outside spheres representing silica particles, or a random mix of the two. Due to limitations in the MSTM model, no two spheres may overlap, but one sphere can entirely contain another (or multiple) spheres. Wavelength-dependent optical constants for Fe^0 are taken from [9] while those for silica are from [10]. Where necessary, we apply a sixth order polynomial fit to interpolate between provided n and k values from the literature over our model spectrum range (620-1700 nm, 20 nm steps). The model is then run on the NASA Pleiades Supercomputer located at NASA Ames Research Center. Pleiades is a distributed-memory cluster with a total of 198,432 CPU cores and 616TB of memory (as of November 2014).

We take the output of the MSTM model at each wavelength analyzed and extract the scattering and extinction efficiencies (Q_{sca} and Q_{ext} respectively) and calculate single scattering albedo (w):

$$w = \frac{Q_{sca}}{Q_{ext}}$$

and use it to calculate the bidirectional reflectance via:

$$r(i,e) = \frac{w}{4\pi}\frac{\mu_0}{\mu_0+\mu}H(\gamma,\mu_0)H(\gamma,\mu)$$

where i is the angle of the incidence, e is the angle of the emergent ray (held constant at 0º and 30º respectively), $\gamma = \sqrt{1-w}$, $\mu = cos\,(e)$, $\mu_0 = cos\,(i)$, and $H(\gamma,x)=(1+2x)/(1+2\gamma x)$ [5].

First Model Tests. We started with two simplified test cases to troubleshoot the workflow and assess the degree of detail required to obtain reasonable results. For the first test case we built a 13x13x13 hexagonally close packed arrangement of 100 nm radius spheres, assigned n and k values for amorphous silica glass [10] and ran the MSTM model at 20 nm steps from 620-1700 nm wavelengths. The second test case took the same arrangement and added 20 nm radius spheres at the center of each 100 nm radius sphere. The new internal spheres were assigned n and k values for metallic iron [11]. The test cases were run on 960 processors on the Pleiades supercomputer using two threads per core for a total of 1920 parallel threads. The silica only run executed in 5.2 hours and the silica and iron run executed in just over 9.5 hours.

Results. The modeled spectra from the two test cases are presented in Figure 2. The output for the silica only test case yielded modeled reflectance values slightly greater than one at every wavelength. The silica and iron test case yields a reasonable reflectance curve with reflectance values from 0.17 (at 800 nm) to 0.51 (at 1700 nm) with a generally red slope.

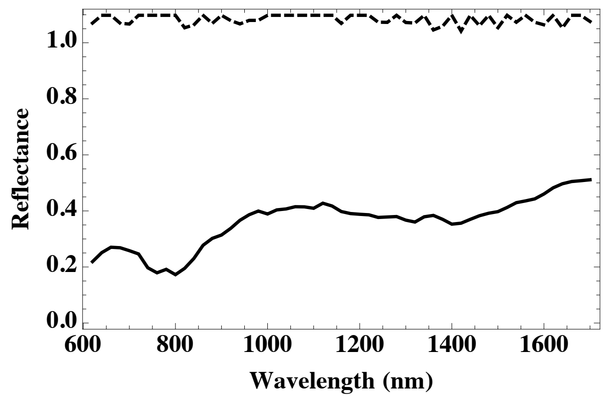

Figure2: Reflectance vs. Wavelength for silica only test case (dashed) and silica + iron test case (solid)

Discussion: Since there is no real physical meaning for the reflectance values greater than one, we can assume that the model is unable to accurately handle this case. We hypothesize that this is due to the extremely small k values at the given wavelengths (as small as $1x10^{-8}$) and the short light path through the simulated particle (~2.5µm). The results of these first tests are promising and larger particles (or more particles, resulting in a larger total volume) may result in more realistic reflectance values for a pure silica case.

Future work and Conclusions: We will be running future models that use one to two orders of magnitude more spheres in order to deal with the non-physical results of the simplified test case. We intend to iterate through the various pore sizes, iron contents, and iron particle sizes described in [4] and to detail any differences between the Mie-Hapke model of [3] and the MSTM model. We anticipate that this new approach may resolve the discrepancy in modeled vs. observed optical behavior due to $npFe^0$ particle size from previous works.

References:

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