

SPACE WEATHERING SIMULATION OF INTERACTING NANOPHASE IRON PARTICLES IN THE THERMAL INFRARED REGION

Mirza Arnaut, Kay Wohlfarth, Christian Wöhler, Image Analysis Group TU Dortmund, Germany (mirza.arnaut@tu-dortmund.de, kay.wohlfarth@tu-dortmund.de, christian.woehler@tu-dortmund.de)

Introduction The spectral appearance of atmosphereless planetary surfaces that are subject to space-weathering is strongly influenced by the presence of sub-microscopic iron particles (smFe⁰). Most importantly, smFe⁰ causes the spectrum to darken and redden, and diagnostic absorption bands are obstructed. [1, 2, 3]. The work of [3] indicates that small ("nanophase") iron particles with diameters below 10 nm mainly induce reddening. In contrast, larger iron particles with some tens of nm diameter lead to spectral darkening but only weak reddening. Various subsequent studies have adopted this (e.g., [4, 5]), but it has issues. Previous physical models of small iron particles implanted into much larger soil grains assumed large distances between the iron particles so that the interaction between them could be neglected (e.g., [3], [4]). However, TEM studies of lunar soil grains and laser-irradiated samples [1, 6] indicate a distribution of the iron particles with small mutual distances so that they form layers or clusters. In our previous study, [7], we applied advanced light scattering theory [8] to simulate various configurations of clusters and layers of nanophase iron particles. We found that interparticle interactions between nanophase iron particles alter mineral reflectance spectra in the near-infrared (NIR) domain and may cause spectral darkening that has previously been associated only with larger microphase iron particles. This study extends our analysis to the thermal infrared (TIR) regime and simulates the spectral effects of interacting nanophase iron particles on an olivine spectrum. Further, we trace the influence of the assumption of a non-absorbing and an absorbing host medium.

Methods We extend the framework of [7] from NIR into the TIR range. In this spectral range, imaginary refractive indices have to be considered. Most minerals have a real-valued refractive index in the NIR with zero or negligible imaginary components. In the TIR region, silicate minerals exhibit an abrupt increase in the imaginary part of the refractive index k , which is also associated with an increase of the absorption coefficient $4\pi k/\lambda$, i.e., a measure of attenuation.

$$Q_{\text{sca}} = 2 \sum_{n=1}^{\infty} (2n+1) (|a_n| + |b_n|)^2 \frac{1}{|x|^2} \quad (1)$$

$$Q_{\text{ext}} = 2 \operatorname{Re} \left\{ \sum_{n=1}^{\infty} (2n+1) (a_n + b_n) \frac{1}{x^2} \right\}. \quad (2)$$

Because the Mie model [9] in our former implementation does not consider the imaginary part, we use the

equations of [10] for the extinction and scattering efficiencies that account for the imaginary part (equations 1 and 2). The Celes [11] framework that we use to compute the scattering of particle clusters accepts complex values as the refractive index of the medium by default. Still, the evaluation of the cross-sections is performed as described by Mishchenko [12]. A minor alteration to the placement of the medium's wavenumber k_1 in the cross-section equation from [12] has been done to obtain:

$$C_{\text{sca}} = \frac{1}{|E_{\text{inc}0}|^2} \sum_{n=1}^{\infty} \sum_{m=-n}^{\infty} \frac{|p_{mn}|^2 + |q_{mn}|^2}{|k_1|^2} \quad (3)$$

$$C_{\text{ext}} = \frac{-1}{|E_{\text{inc}0}|^2} \operatorname{Re} \left\{ \sum_{n=1}^{\infty} \sum_{m=-n}^{\infty} \frac{a_{mn} p_{mn}^* + b_{mn} q_{mn}^*}{k_1^2} \right\}. \quad (4)$$

The complex-valued refractive index k_1 of the medium has been taken into consideration in the computation of the spherical vector wave function expansion coefficients a_{mn} , b_{mn} , p_{mn} , and q_{mn} , and in the evaluation of the cross-sections C_{sca} and C_{ext} similar to the Mie scattering (equations 3 and 4, respectively).

Using the Hapke model [13], we obtain the albedo, efficiencies, and phase function from the olivine spectrum. This olivine spectrum was taken from [14] and does not show the effects of space-weathering. We use those quantities for the mixing procedure using the mentioned values of a single non-interacting particle and particle clusters. The single-particle parameters are modeled using the Mie model using the refractive index of iron [15]. The parameters of olivine and the single particle are then fed into Hapke's mixing equation and reflectance model [13] to obtain space-weathered spectra.

For the particle clusters, we used the CELES framework [11]. The geometric properties of the layer are as described in our previous work [7]. Using the T-Matrix method [12], we derive the needed parameters for the cluster and feed them into the mixture together with the olivine and single particle.

Results The olivine spectrum of [14] is the basis of our evaluation (solid black lines in figure 1 with a prominent Christiansen feature at about 9 μm). We perform the simulations with a non-absorbing (Figure 1a) and an absorbing host medium (Figure 1b). We start with the non-absorbing case: If we add single iron particles of a few nanometers size that do not interact, we observe an overall darkening of the spectrum (Figure 1a), similar to the finding of [14]. Mixing the olivine with a layer of

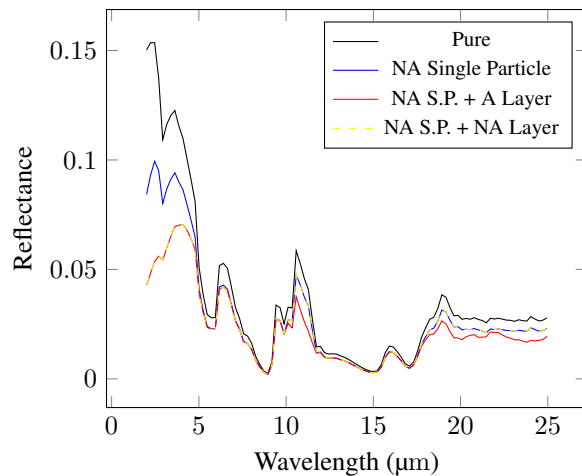


Figure 1 (a) Non-absorbing non-interacting particles.

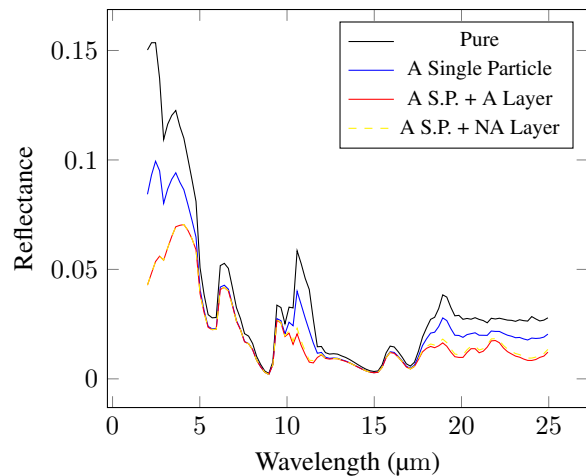


Figure 1 (b) Absorbing non-interacting particles.

Figure 1: Simulated spectra from the pure olivine spectrum (black) using non-interacting particles (blue) and single particles with particle clusters (red curve: absorbing medium; yellow: non-absorbing medium).

A: absorbing, NA: non-Absorbing

absorbing and interacting nanophase iron particles leads to a further decrease of the spectrum (Figure 1a red line). Note that the spectral slope significantly changes for up to 5 μm . From 5 μm onward, only darkening occurs, and the spectrum is close to the mixture with non-interacting single nanophase iron particles. We also simulated a non-absorbing layer of interacting nanophase iron particles (Figure 1a dashed curve). The spectral shape is similar to the previous case but follows the mixture with non-interacting single nanophase particles around 11.5 μm and from 18 μm onward. These wavelength regions coincide with the large imaginary part of the refractive index. The results are similar if we model an absorbing host medium (Figure 1b). However, the mixture of olivine, single iron particles, and a non-absorbing particle layer now aligns with the absorbing layer.

Conclusion The presence of submicroscopic iron particles or particle clusters alters the olivine spectrum in the TIR. From 5 μm onward, iron particles darken the mineral spectrum, regardless of the type of iron (single particle or cluster/layer). Up to 5 μm , we observe a transition zone. In this region, the particle cluster significantly darkens the mineral spectrum, compared to single non-interacting iron particles. The choice of absorbing or non-absorbing materials has only a minor impact on the spectral shape. This study is another step toward an integrated understanding of NIR and TIR effects of interacting and non-interacting sub-microscopic iron particles.

References: [1] Carle M. Pieters and Sarah K. Noble. In: *JGR: Planets* 121.10 (Oct. 2016), pp. 1865–1884. [2] Bruce Hapke. In: *JGR: Planets* 106.E5 (May 2001), pp. 10039–10073. [3] Paul G. Lucey and Miriam A. Riner. In: *Icarus* 212.2 (Apr. 2011), pp. 451–462. [4] Kay S. Wohlfarth et al. In: *Astron. J.* 158.2 (July 2019), p. 80. [5] Antti Penttilä et al. In: *Icarus* 345 (July 2020), p. 113727. [6] Yazhou Yang et al. In: *Astron. Astrophys.* 597 (Jan. 2017), A50. [7] Mirza Arnaut et al. In: *EPSC*. Vol. 15. July 2021. [8] Michael I. Mishchenko et al. Cambridge: Cambridge University Press, Jan. 2006. [9] Gustav Mie. In: *Annalen der Physik* 330.3 (Jan. 1908), pp. 377–445. [10] P Bruscaaglioni et al. In: *Waves Random Complex Media* 3.3 (July 1993), pp. 147–156. [11] Amos Egel et al. In: *JQSRT* (June 2017). [12] Michael I. Mishchenko. Cambridge: Cambridge University Press, Jan. 2002. [13] Bruce Hapke. Cambridge: Cambridge University Press, Jan. 2012. [14] Kay Wohlfarth et al. In: *EPSC*. Vol. 649. July 2018. [15] M. R. Querry. SAO/NASA Astrophysics Data System, Jan. 1985.