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The interaction between multiple nanophase iron particles changes the slope of lunar reflectance spectra

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1 Introduction

The current understanding of space-weathering is that spectral changes of space-weathered airless planetary bodies are mainly caused by the gradual formation of submicroscopic-sized iron particles (smFe^0) in the upper layer of the regolith. The resulting spectral changes include the darkening and reddening of the spectrum as well as the obstruction of diagnostic features [1,2,3]. Previous research also indicates that very small particles (nanophase iron <10 nm) mainly account for reddening and larger iron particles cause spectral darkening without reddening [3]. This theory has been adopted in a variety of studies such as [3,4,5]. However, this interpretation does not come without issues. The estimated sizes of large particles may deviate from the experimental particle size [3]. Recently, Denevi et al. [6] suggested that agglutinates might be the main cause for substantial reddening even though they are abundant in large iron particles. We add another aspect to the discussion: Previous mathematical treatments of small iron particles implicitly assumed that the distances between particles are large and no interactions occur. However, TEM imagery of lunar soil and laser irradiated samples [1] suggests that cases exist in which the iron particles are close together and form layers or clusters. We apply advanced light scattering theory [7] to simulate clusters and layers of very small iron particles with varying geometries and densities. We find that interparticle interactions between nanophase iron particles can alter the spectral slope and counteract the reddening effect.

2 Methods

To investigate the spectral behaviour of nanophase iron particle layers or clusters, we carry out three steps.

(1) First, we define our baseline. We utilise Mie scattering to simulate the spectral effects that non-interacting smFe^0 (radius = 5nm) has on a fresh lunar soil spectrum as described by [4]. A fresh highland spectrum from calibrated data of the Moon-Mineralogy-Mapper (M^3) [https://pds-imaging.jpl.nasa.gov/volumes/m3.html] is converted to single scattering albedo via the Hapke model [8]. Mie modelling yields the single scattering albedo w, the phase function p(g) and the extinction/scattering efficiencies Q_{ext} and Q_{sca} of smFe^0 [9]. We use the optical constants of iron from [10]. The soil albedo and the iron albedo as well as the phase functions are combined via Hapke's mixing equation [8]. The resulting albedo $w_{soil,\ smFe0}$ is subsequently fed into the Hapke model to generate computationally space-weathered soil spectra.

(2) Secondly, we assume that not all iron particles are present in the form of single particles but many of them are somewhat closely packed and form layers. Now, we simulate these layers. The particle radii are drawn from a normal distribution with μ = 22nm and σ = 10nm and populate a box with dimensions 700nm x 700nm x 100nm (figure 1b). The dimensions of the box represent a small layer of particles that accumulate at the grain rim. The depth (100nm) is largely inspired by TEM imagery that suggest depths of roughly 10–100nm [1]. We utilise the T-matrix method [7] using the CELES framework [11] and compute the interaction between adjacent particles. Again, the resulting quantities (albedo, phase function, efficiencies) are fed into the Hapke model to simulate a computationally weathered spectrum.

(3) Finally, we compare the results of steps (1) and (2).

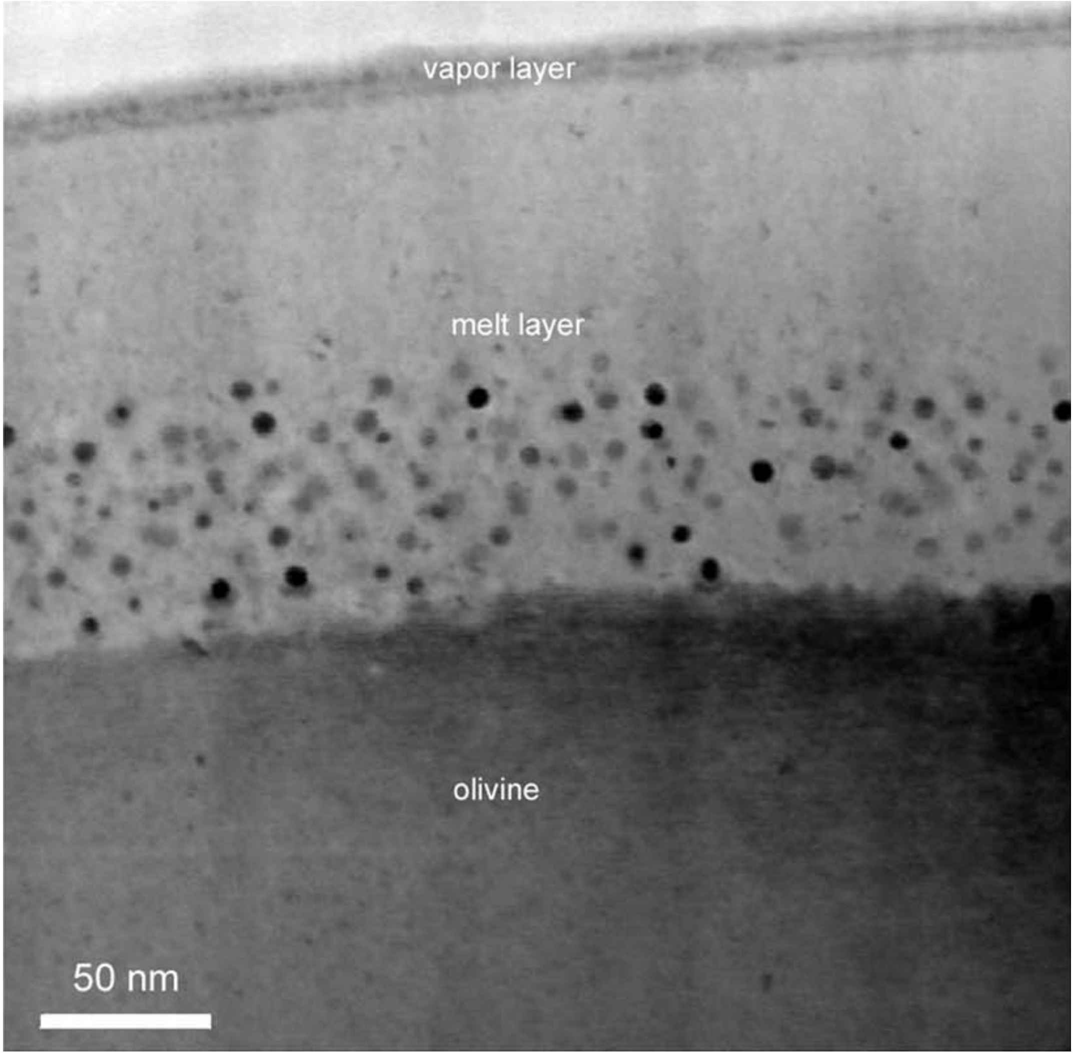

Figure 1a: TEM image of small iron particles (small dots) occurring in the melt and vapor phases of the soil grain (image from [1]).

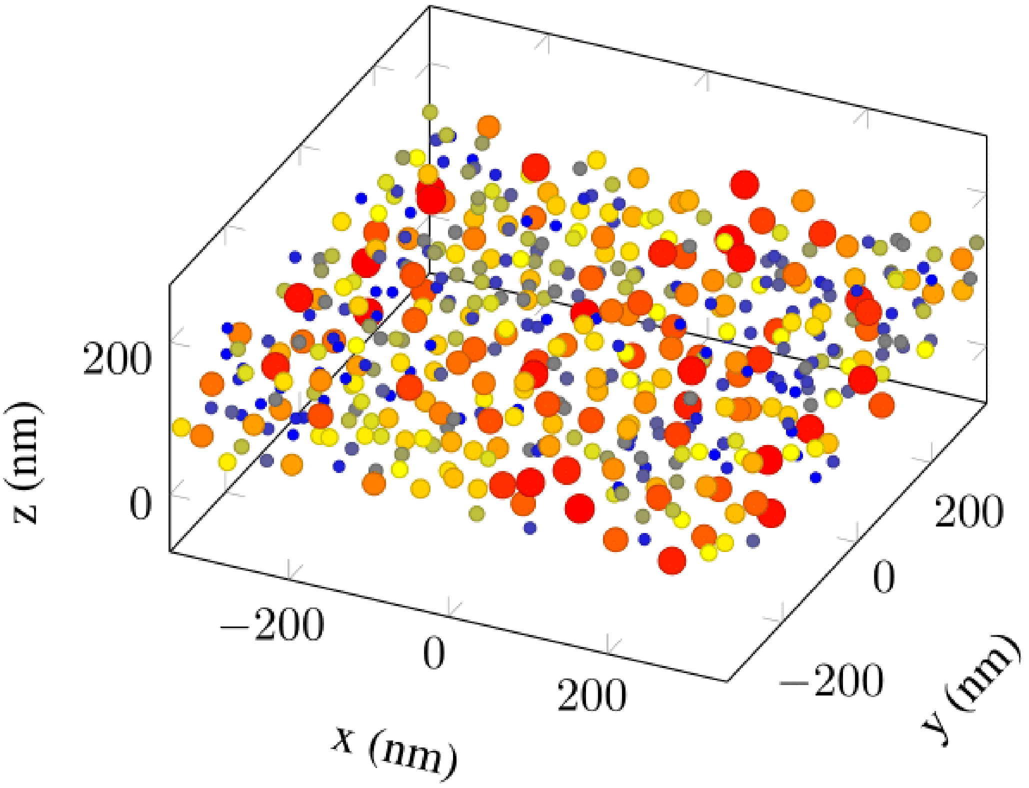

Figure 1b: Artificially created particle geometry with varying radius. The size is also colour coded with red particles being the largest, blue the smallest, and other sizes in between.

3 Results

To evaluate the influence of layered smFe^0, we chose a fresh highland spectrum near crater Krasovskiy [4], see figure 2a (blue solid line). The spectrum is red-sloped, has no strong features and a significant hydroxyl/water absorption band above 2.8µm. We simulate the spectral behaviour of single isolated iron particles according to (1) and obtain a spectrum with considerable reddening and some darkening (red line in figure 2a). If a mixture of single non-interacting particles and interacting layered particles is included, the spectral slope becomes flatter in the NIR region, i.e., exhibits less reddening as seen in figure 2a (black line). For the sake of comparison, we tuned the abundances of the components such that the weathered spectra have similar reflectance values near 2.5µm.

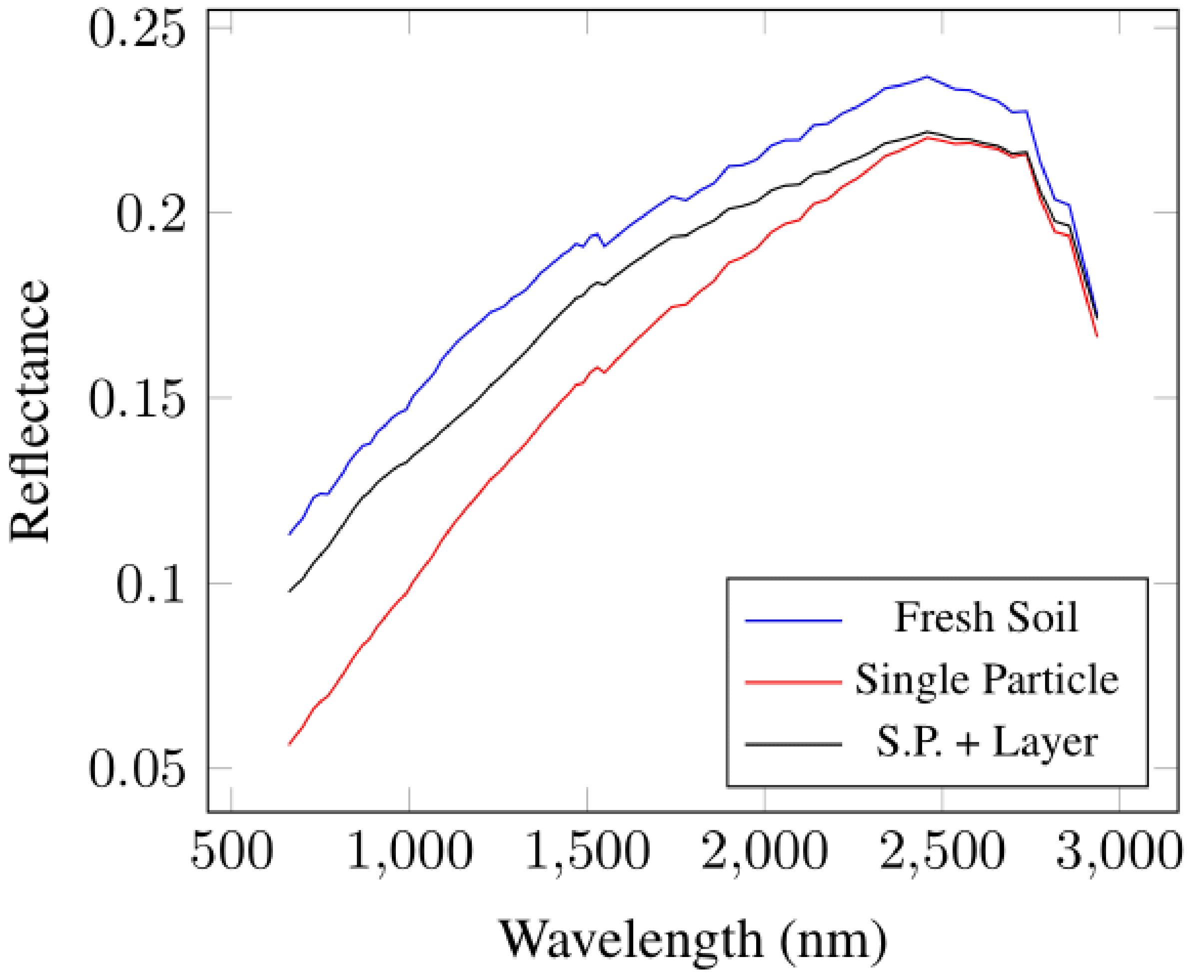

Figure 2a: Simulated spectra from the fresh spectrum (blue) using non-interacting particles (red) and layered particles (black)

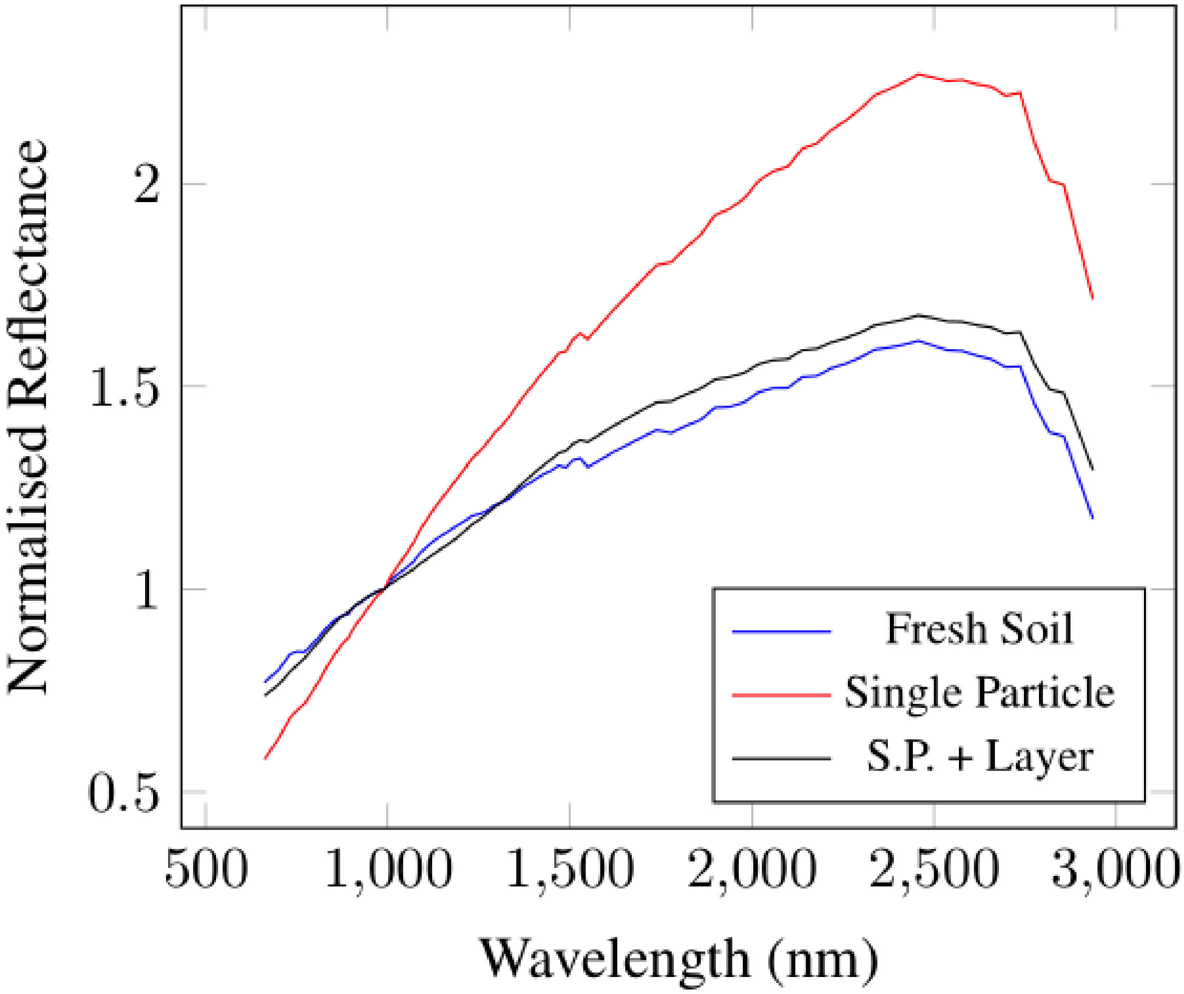

Figure 2b: Normalised spectra at 1µm

4 Conclusion

In figure 2a and 2b one can clearly see that interacting particles organised in layers counteract the reddening effect. Nanophase iron alone can thus mimic the behaviour of microphase iron which has previously been believed to be solely responsible for this effect [3,4]. This results in the following consequences: The distinction between nanophase iron and microphase iron become less clear. Not only the particle size matters but also the geometric alignment and the inter-particle interactions are important if the particles are somewhat dense. To arrive at a comprehensive understanding of space weathering and its spectral characteristics, the geometry, density, and distribution and interaction of smFe^0 should be taken into consideration. Further simulation campaigns are necessary to characterise the dependency of the spectral behaviour on these geometric parameters.

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