GRAIN-SIZE IMPLICATIONS ON INFRARED SPECTROSCOPY OF COMPOSITE PLANETARY SIMULANTS: ALTERATION BY SURFACE PRESSURE.

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Introduction: Mineral mixtures that replicate the expected geochemical composition of rocky planetary surfaces (hereinafter referred as “simulants”) are important materials for the laboratory analysis of simulated space weathering. Chemically and size-different heterogeneous regolith, typical for surfaces of atmosphere-less celestial bodies, is formed by the constant bombardment of meteoroids and cosmic particles that decompose the surface rock. In addition to the released heat, which can cause thermal alteration of the rock, considerable mechanical forces break down the soil. The induced pressures can be estimated by the shock values such as those found in meteorites: average values of 200-430 MPa for stony and iron-type meteorites [1,2]. This leads to a broad grain size distribution, while such complex mixtures are commonly assumed to have an average composition that corresponds to the relative abundances of the elements from which the different hard minerals are formed. Often simulants are made with a chemical composition that can explain observed optical and thermal properties of the celestial body of interest, such as infrared reflectance (IR) and emission spectra from orbital and flyby measurements. To simulate weathering by meteoritic impacts, solid samples are typically prepared by processing powder into pellets of representative mineral grains under low pressure (compared to the mean impact). Therefore, the influence of such a preparation procedure on conventional analytics in space research, including IR spectroscopy, is expected to be negligible.

We show in this work that additional destruction of the original grains in compositions, containing minerals with a wide range of hardness, can cause an alteration of the mid-IR spectra expressed in relative enhancement of particular phases according to their hardness.

Phobos simulants: We studied Phobos surface simulants, proposed for laboratory studies supporting the Martian Moon eXploration mission (JAXA), which “chemically” and mineralogically represent two main possible scenarios for Phobos origin: the disintegrating of the parent planet under a giant impact (PGI) and gravitational capture of an asteroid (PCA) [3]. The minerals in these simulants cover a wide range of hardness on the Mohs scale: from 1.0 to 7.0.

Natural minerals and coal from the [1]Institut für Planetologie collection [4] were used to prepare the simulants. For the powdered samples, the original solids were crushed and sieved to select the fractions within 63 µm to 125 µm, in the same size range like in the study of the Phobos surface simulants in visible and near-infrared wavelength ranges [4]. The PGI-1 simulant consists of phyllosilicates (ID707/vermiculite $(Mg,Fe^{2+},Fe^{3+})_3$ $[(Al,Si)_4O_{10}]$ $(OH)_2{\cdot}4H_2O$, the Mohs scale hardness ~**1.5-2.0**) at 35.3 wt%; olivine (ID249/forsterite $(Mg_x,Fe_{1-x})_2SiO_4$ ~ **7**) at 29.8 wt%; pyroxene (ID53/enstatite $(Mg,Fe)_2[Si_2O_6]$ ~ **5-6**) at 17.2 wt%; magnetite (ID591/$Fe^{2+}Fe^{3+}{}_2O_4$ ~ **5.5-6.5**) at 7.7 wt%; pyrite (ID710/FeS_2 ~ **6.0-6.5**) at 3.7 wt%; epsomite (ID709/$MgSO_4{\cdot}7H_2O$ ~ **2.0-2.5**) at 3.4 wt%; carbon (~**1.0-2.0**) at 2.9 Wt%. Mechanically stable pellets were prepared from these powders using a P/O Weber hydraulic press maintained at ~20 kPa for 15 min. Their shape after removal from the press is an approximately 1 mm high cylinder with a diameter of 6 mm.

Infrared Spectroscopy: The mid-IR reflection spectra were recorded using Bruker Vertex 70, 80v Fourier Transform Spectrometers in specular reflection (bi-conic) mode. The choice of the spectral range was motivated by the modern R&D in technology and space qualification of mid-infrared detectors, which allows a significant improvement in the accuracy of mineral identification using the thermal infrared range, which covers distinctive spectral features of minerals, such as Reststrahlen bands (strong reflectance) and the Christiansen feature(s) (minimum reflectance) [4]. The spot size on the sample was varied between 2 and 2.5 mm. The spectral resolution was set to 4 cm^{-1}. The spectra were recorded in the (extended “thermal”) mid-infrared range of 2-18 µm, which corresponds to the infrared spectrometers for both the past and the planned future missions.

Complementary Raman spectroscopy mapping of the sample surface in the visible wavelength range of the Stokes shifted light was performed by a WITec α300 Raman microscope to acquire spatial distribution of mineral phases after the pressing of the pellets. The confocal geometry of the microscope enables a spatial resolution of about 1.5 µm; the maps were taken with different step sizes down to 10 µm.

Fig. 1. shows the mid-IR spectra of the minerals and carbon phases used for the Phobos surface simulant with the sample ID 712, which is similar in composition to the PGI-1 (“Phobos giant impact”) simulant [4]. The spectra exhibit distinct spectral features: high reflectance due to Si–O stretching (~900-1100 cm^{-1}) bands of silicates in the wavelength range 8-13 µm, and dips in the high-frequency bands (bands around 1600 cm^{-1} and 3300-3600 cm^{-1}) due to OH-vibrations.

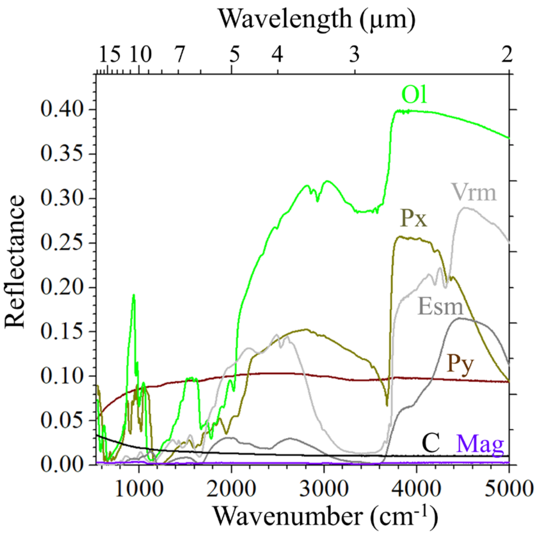

Fig. 1. Mid-IR reflectance spectra of the individual minerals and carbon phases, taken from the powders with grains of 65 µm to123 µm. The gray scale colors show the "softer" phases. The incident and collecting light angles are 13°, spot size on the sample ~ 2.5 mm.

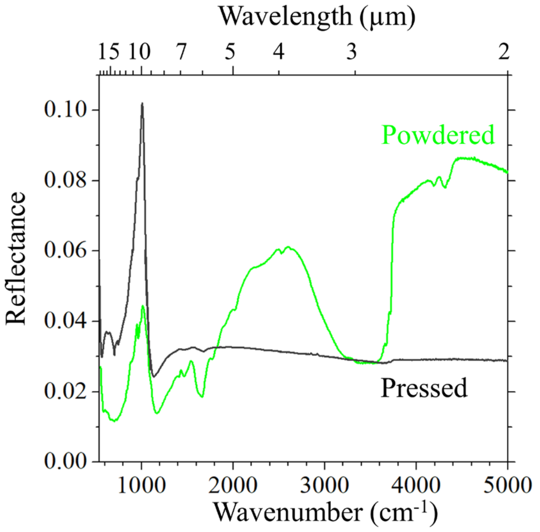

Fig. 2. Spectra of the Phobos surface simulant ID712, recorded as powder of the mixed minerals (63-125 µm grains) and later - after pressing into a pellet.

The powdered sample ID712 (Fig. 2) yields an IR spectrum that can be considered as a linear combination of the weighted contributions of the individual phases contained. The infrared reflection spectra become modified after the applied pressure: the Si-O stretching bands of silicates are relatively enhanced, while the high-frequency region is strongly masked, apparently due an enlarged distribution of carbon particles, whose absorption increases towards the near-IR. The similar alteration of the IR spectra was observed for the PCA-1 ("Phobos captured asteroid") type of the Phobos surface simulant. This is in contradiction with the usual observations of gradual decrease in band intensities with decreasing grain size [6]. The shifts of the Christiansen feature, e.g., from 8.81 µm to 8.54 µm, are large and of the order of magnitude observed in simulated space weathering of silicates [7].

The micro-Raman scans confirm that the softer (mineral) phases in the simulants: carbon, epsomite and vermiculate, appear to be largely distributed over the surface of the pressed samples than those of the harder minerals and thus "spatially unbalanced" compared to their abundances in the powders.

We suggest that such an increase in the density of spatial distribution of the softer phases (numbers on the Mohs hardness scale are 1.0-2.0) leads to such a specific spectral enhancement of the IR reflection signals acquired from the spots of a few mm in size. The applied pressure further crushes a portion of the original grains into smaller grains, as observed by optical microscopy. This indicates locally occurred compressing strengths exceeding the mechanical fracture of certain grains, while the reported ultimate compressive strengths for the Phobos simulants PGI-1: 1.7±0.4 MPa and PCA-1: 1.3±0.2 MPa [4]: The pressure cell used for the sample production was set to 5 kPa.

This suggests possible size-dependent mean values for different mineral phases, which follow the hardness of the individual minerals. Such a scenario should then be carefully evaluated when preparing planetary surface simulants, but also when analyzing infrared spectra returned from space observations.

The linear (i.e., proportional to the partial mineral abundances) contributions to the mid-IR reflectance spectra of complex mixtures are valid as long as the grains are much larger than the light wavelength, so that volume scattering (light can be refracted into the grain interior) remains insignificant when compared to surface scattering (light is reflected from the grain surfaces) [5]. As soon as the original distribution on particles size in complex mixtures is modified around the value of the wavelength of diagnostic light, changes in the reflectance spectra can become significant. Therefore, the regolith probably has a wider size distribution, which is considerably dependent on the hardness (soft = small, hard = larger) and the cleavage of the minerals.

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