EXPERIMENTAL AND MODELLED MID-INFRARED SPECTRA OF OLIVINE: SIMULATIONS OF EXTREME TEMPERATURE CONDITIONS ON MERCURY SURFACE.

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Introduction: Spectral signatures of minerals are intimately related to the crystal structure; therefore, they may represent a remote sensing model to determine surface composition of planetary bodies, analyzing their spectral reflectance and emission. For planetary surfaces, which are influenced by extreme environmental conditions as Mercury, which is the closest planet to the Sun, data interpretation must take into account changes in spectral characteristics induced by the high temperatures conditions [1].

State of Art: Recently we modelled high-temperature mid-IR spectra, by means of HF/DFT calculations to predict the changes in spectral features due to the increase of temperature, with promising results [2]. The approach was first tested modelling forsterite Mg_2SiO_4. The results were compared with the experiments on a natural olivine (Fo#89). The outcomes are shown in Figure 1. As shown the main changes in spectral characteristics due to temperature are successfully reproduced. This first attempt reveals that the computational approach employed can reliably be used to predict band shifts due to temperature: a significant good agreement between measurements and simulated data is shown, especially within the spectral range of 1200-600 cm^{-1}, where the agreement with the experiments is found to be exceptionally good.

Aims: However, some discrepancies between calculated and experimental spectra are evident, mostly because with this approach it is not possible to model the bands shape due to grain sizes or potential preferential orientation in a granular sample. Moreover it is known that for some silicates the spectral features due to the iron content overlap with the effects of temperature [3]. In this study, we take into account The effects of temperature, composition and grain sizes on emissivity bands investigating experimentally natural samples of olivine. The aim is refine and better constrain future modellings.

Methodology: The measurements have been carried out at the Planetary Spectroscopy Laboratory (PSL) in the Institute for Planetary Research, Deutschen Zentrums für Luft und Raumfahrt (DLR). 11 different olivine samples (most of them for a fine and broader fraction) within the forsterite-fayalite series have been studied, measuring their thermal emissivity up to 900 K as well as IR reflectance at room temperature. On these 11 samples, 5 of them have been measured on two different grain sizes (4 samples 125-250 µm and 0-25 µm, 1 sample 300-500 µm and 38-68 µm), according to the availability of sample. The thermal emissivity measurements have been performed at different temperatures, from 320K up to 900K, with intermediate temperature steps at 500K and 700K, in order to simulate the typical diurnal equatorial temperature variation of the surface of Mercury. The IR bi-directional reflectance measurements have been performed for each sample (and when available on each grain size) on the fresh and on the heated sample. The spectral region covered in both emissivity and reflectance measurement is between 50 and 1400 cm-1, which is the fundamental range for distinguish spectral absorption features of silicate [4]. To collect our laboratory spectra we employed two detectors: a liquid nitrogen cooled HgCdTe detector plus a KBr beamsplitter to cover the 1 to 16 µm spectral range, and a DTGS detector plus a Mylar multilayer beamsplitter from 16 to 200 µm.

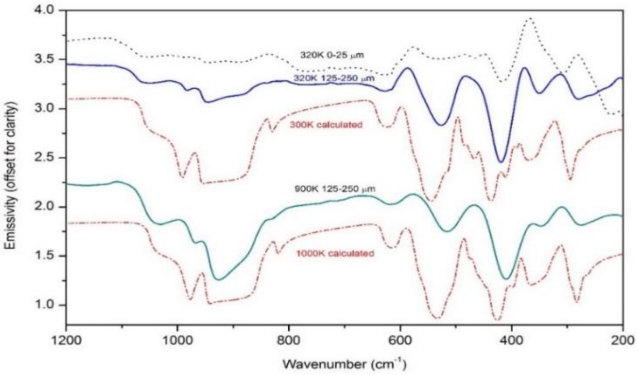

Figure 1: Comparison between calculated 1-R mid IR spectra and experimental emissivity measurements. Solid line: experimental thermal emissivity spectra of an Mg-rich olivine (Fo_{89}) measured at 320K and 900K.

Preliminary results and outlooks: The results complement the modelling of emissivity spectra already performed with HF/DFT modelling, which, at the present state, successfully predict the bands shift due to temperature and composition [1]. Preliminary results show a consistent good agreement with calculations; by means of this approach we calculate and predict with a good level of accuracy band minima shift as a function of temperature and, consequently, it is possible to reliably predict which modes are particularly sensitive to temperature variations. The post processing of data is still ongoing, and it will be focused on overcoming the volume scattering issues due to the grain size.

Acknowledgements: The measurements at Institute of Planetary Research, Deutschen Zentrums für Luft und Raumfahrt (DLR), Planetary Spectroscopy Laboratory (PSL), have been possible within the project Europlanet 2020 RI-TA.

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