EPSC Abstracts
Vol. 12, EPSC2018-714, 2018
European Planetary Science Congress 2018


# Experimental and modelled mid-infrared spectra of olivine: simulations of extreme temperature conditions

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## Abstract

The effects of temperature, composition and grain sizes on emissivity bands have been investigated experimentally on natural samples of olivine. The measurements have been carried out at the Institute of Planetary Research, Deutschen Zentrums für Luft und Raumfahrt (DLR), at the Planetary Spectroscopy Laboratory (PSL), where 11 different olivine samples within the forsterite-fayalite series have been studied, measuring their thermal emissivity up to 900 K and IR reflectance.
The outcomes implement the modelling of emissivity spectra with *ab initio* modelling, which, at the present state, successfully foresee the bands shift due to temperature and composition [1], but do not take into accounts the bands shape due to grain sizes. Moreover, we point out the main spectral features due to the composition and temperature, since the spectra features due to the iron content in the samples overlap with the effects due to temperature [2].

## 1. Introduction

Planetary bodies may be influenced by extreme temperature conditions (e.g. Mercury), thus data interpretation must take into account changes in spectral characteristics induced by temperatures effects [3]. Recently we modelled high-temperature mid-IR spectra, by means of *ab initio* methods to predict the changes in spectral features due to the increase of temperature, with promising results [1]. However, some discrepancies between calculated and experimental spectra are evident.
In this study we take into account the effects on spectral features due to the composition and the grain size of different olivine samples, in order to better constrain future modelling.

## 2. Preliminary results

The approach was first tested on the modelling of forsterite. The results were compared with the experiments on a natural olivine ($Fo_{89}$). The outcomes are shown in Figure 1.
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 exceptionally good.

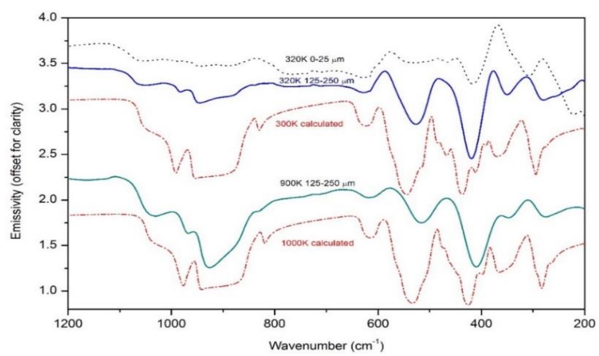


Figure 1: Comparison between calculated 1-R mid IR spectra and experimental emissivity measurements. Solid line: experimental thermal emissivity spectra of an Mg-rich olivine ($Fo_{89}$) measured at 320K and 900K.

## 3. Methodology

In this study, 11 samples of olivine with different compositions, within the series forsterite-fayalite have been measured. 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

Mercury surface. The IR 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 detected for both emissivity and reflectance measurements are between 50 and 1400 $cm^{-1}$, which is the fundamental range for distinguish spectral absorption features of silicate [4]. To do so 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.

# 4. Summary and Conclusions

Preliminary results show a consistent good agreement with calculations; by means of this approach we calculate and foresee 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.

Europlanet 2020 RI has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 654208.

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