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Modelling of thermal-IR spectra of forsterite: application on remote sensing for Mercury

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Abstract

In this work, we study experimental thermal emissivity spectra with an innovative approach: we calculate IR spectra, with ab initio methods, of the main mineral families that presumably compose the surface of Mercury and we compare them with high temperature laboratory measurements. The measurements are carried out at the Institute of Planetary Research, Deutschen Zentrums für Luft und Raumfahrt (DLR) Planetary Spectroscopy Laboratory (PSL). The laboratory has the unique capability to obtain emissivity measurement of samples at temperature up to 1000K, by means of a planetary emissivity chamber. This allows measuring samples at realistic temperature conditions for the surface of Mercury. The goal is to interpret the high temperature infrared (HT-IR) emissivity spectra that will be collected by the Mercury Radiometer and Thermal infrared Imaging Spectrometer (MERTIS), the spectrometer developed by DLR that will be on board of the ESA BepiColombo Mercury Planetary Orbiter (MPO) [1].

1. 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, analysing 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 [2].

2. Methodology

The approach was firstly used on olivine [3], one of the possible major phases in the surface of Mercury. A natural sample of olivine (Fo#89) has been studied at Planetary Spectroscopy Laboratory [4]. The emissivity of the sample has been measured at different steps of temperature by means of a planetary simulation chamber that has the unique capability to heat samples to temperatures up to 1000K. IR reflectance spectra of forsterite has been then simulated using the Hybrid HF/DFT Hamiltonian WC1LYP [5, 6], by means of the CRYSTAL code [7]. IR vibrational frequencies at high temperature are calculated evaluating the vibrational frequencies at the Γ point of first BZ of the unit cell at different volumes corresponding to increasingly higher temperatures. Thus, in order to simulate extreme environmental conditions, IR frequencies and intensity has been calculated for volumes estimated at 0, 300 and 1000K (taking into account zero point effects). The comparison with the experiment reveals that such computational approach 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 1200-600 cm^{-1}.

3. Figure

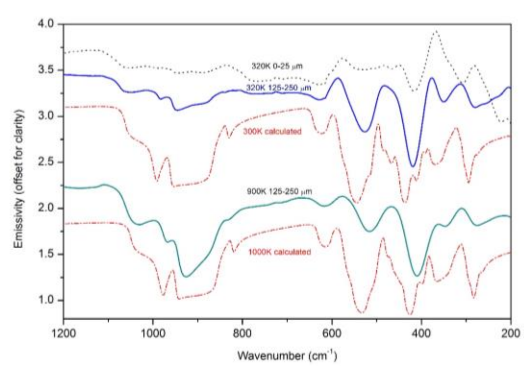

figure 1: Comparison between calculated 1-R mid IR spectra and experimental emissivity measurements. Solid line: experimental thermal emissivity spectra of an Mg-rich olivine (Fo89) measured at 320K and 900K

(extreme situations). Dotted lines: calculated IR reflectance (inverted 1-R) bands of an Mg_2SiO_4 endmember. Spectra are offset for clarity.

4. Summary and Conclusions

This study aims to enhance the knowledge of spectroscopic techniques applied to remote sensing and it might occur on two levels.

The first one concerns the IR frequencies that are influenced by temperature and occur during the insolation of the surface and which not and which structural feature are involved. These temperatures changes must be taken into account since they induce variation not only on the bond distances and on angles of minerals, but also on the density of rocks that compose the surfaces of a planetary body. The temperature factor also affects the interpretation of thermal emissivity spectra, which appear extremely challenging to unravel, due to the broadening of the bands, which is observed especially at high temperature.

At a higher level, results will be useful to create a theoretical background to interpret high temperature infrared (HT-IR) emissivity spectra that will be collected by the Mercury Radiometer and Thermal infrared Imaging Spectrometer (MERTIS), the spectrometer developed by DLR that will be on board of the ESA BepiColombo Mercury Planetary Orbiter (MPO).

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