Modelling of Thermal-IR spectra of Forsterite: Application on Remote Densing for Mercury

C. Stangarone[1], J. Helbert[1], A. Maturilli[1], M. Tribaudino[2], M. Prencipe[3]

[1] *Institute for Planetary Research, Deutschen Zentrums für Luft- und Raumfahrt, Berlin, Germany*
E-mail: claudia.stangarone@dlr.de
[2] *Department of Physics and Earth Science, University of Parma, Italy*
[3] *Department of Earth Sciences, University of Torino, Italy*

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]. The approach was first used on olivine [2], 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 [3]. 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 have been then simulated using the Hybrid HF/DFT Hamiltonian WC1LYP [4, 5], by means of the CRYSTAL code [6]. 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} as shown in Figure 1.

The 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 and on board of the ESA/JAXA mission, BepiColombo Mercury Planetary Orbiter (MPO) [7].

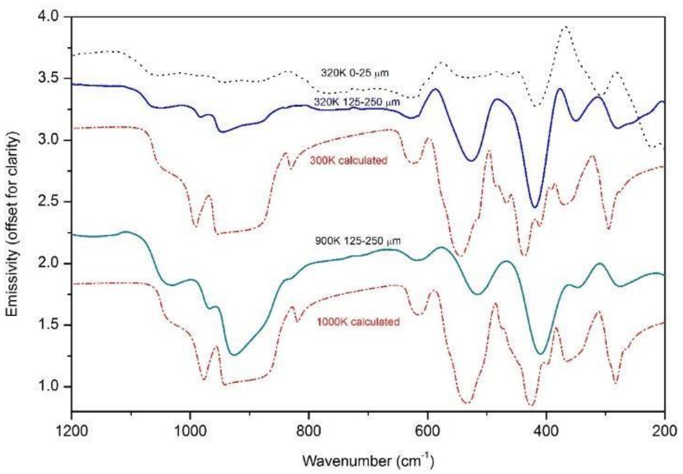

Figure1: Comparison between calculated 1-Rmid IR spectra and experimental emissivity measurements.
Solid line: experimental thermal emissivity spectra of an Mg-rich olivine (Fo89) measured at 320K and 900K (extreme situations).
Dotted lines: calculated IR reflectance (inverted 1-R) bands of an Mg_2SiO_4endmember. Spectra are offset for clarity

References:

[1] Helbert, J., Nestola, F., Ferrari, S., Maturilli, A., Massironi, M., Redhammer, G. J., Capria M. T., Carli C., Bruno, M.: Olivine thermal emissivity under extreme temperature ranges: Implication for Mercury surface, Earth and Planetary Science Letters, Vol. 371, pp. 252-257, 2013.

[2] Sprague, A. L., Hanna, K. D., Kozlowski, R. W. H., Helbert, J., Maturilli, A., Warell, J. B., & Hora, J. L.: Spectral emissivity measurements of Mercury's surface indicate Mg-and Ca-rich mineralogy, K-spar, Na-rich plagioclase, rutile, with possible perovskite, and garnet, Planetary and Space Science, Vol. 57(3), 364-383, 2009.

[3] Maturilli, A., & Helbert, J.: The Planetary Spectroscopy Laboratory (PSL): Spectral Measurements of Planetary Analogues from UV to FIR, Lunar and Planetary Science Conference, 21-25 March 2016, The woodlands, Texas, USA, 2016

[4] Wu, Z., & Cohen, R. E.: More accurate generalized gradient approximation for solids, Physical Review B, Vol. 73(23), 235116, 2006.

[5] Lee, C., Yang, W., & Parr, R. G.: Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. Physical review B, Vol. 37(2), 785, 1988

[6] Dovesi, R., Saunders, V. R., Roetti, C., Orlando, R., Zicovich-Wilson, C. M., Pascale, F., Civalleri B, Doll K, Harrison N. M., Bush I. J., D'Arco Ph., Llunell M., Causà M., Noël Y.: CRYSTAL14 user's manual. University of Torino, Torino 2014.

[7] Helbert, J., Hiesinger, H., Walter, I., Säuberlich, T., Maturilli, A., D'Amore, M., Knollenberg J., Lorenz E., Peter G., Arnold, G. E.: MERTIS: understanding Mercury's surface composition from mid-infrared spectroscopy, SPIE Optical Engineering Applications, International Society for Optics and Photonics, 1-5 August 2010, San Diego, California, USA