

UNMIXING OF LABORATORY IR SPECTRAL REFLECTANCE MEASUREMENTS OF LABRADORITE-ENSTATITE-GLASS MINERAL MIXTURES. K. E. Bauch¹, A. Morlok¹, H. Hiesinger¹, M. P. Reitze¹, N. Schmedemann¹, A. N. Stojic, I. Weber¹, M. D'Amore², J. Helbert², A. Maturilli², I. Varatharajan², K. Wohlfarth³, C. Wöhler³, ¹Institut für Planetologie (IfP), Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany (karinbauch@uni-muenster.de), ²DLR-Institute for Planetary Research, Rutherfordstrasse 2, 12489 Berlin, Germany, ³Image Analysis Group, TU Dortmund University, Otto-Hahn-Str. 4, 44227 Dortmund, Germany.

Introduction: The Mercury Radiometer and Thermal Infrared Spectrometer (MERTIS) is part of the payload of ESA/JAXA's BepiColombo mission, launched in October 2018 [1,2,3]. MERTIS consists of an IR-spectrometer and radiometer, operating in the wavelength range of 7-14 μm and 7-40 μm , respectively. This range covers several spectral features, such as the Christiansen feature, Reststrahlen bands, and Transparency feature, which allows the determination of Mercury's surface mineralogy.

During its cruise to Mercury, the spacecraft will perform a total of nine swing-by maneuvers at Earth (1x), Venus (2x), and Mercury (6x), during which MERTIS will be switched on and take measurements [4]. During the first swing-by maneuver in April 2020, MERTIS acquired thermal infrared spectra of the lunar surface and thus was the first opportunity to test the instrument under 'real' planetary observation conditions [5].

At the IRIS (Infrared and Raman for Interplanetary Spectroscopy) laboratory of the Institut für Planetologie at the Westfälische Wilhelms-Universität Münster we study a wide range of natural minerals, rock samples including impact rocks and meteorites, synthetic analogs and glasses [6]. Additionally, we measure spectra of mineral mixtures, which are used to perform unmixing studies [7,8]. The results of these investigations contribute in generating a mid-IR reflectance database. This database enables the qualitative, but also quantitative interpretation of MERTIS spectra.

A first preliminary comparison of MERTIS data and laboratory spectra after geometry [9] and thermal corrections [10] does not reveal the typical diagnostic features of common lunar minerals [6]. Mean emissivity spectra of highlands and mare appear very similar [5,10,11]. However, due to the large distance between spacecraft and the Moon, the footprint of MERTIS was relatively large (>500 km). [6] calculated reflectance spectra using Kirchhoff's law (1-emissivity) of specific regions, namely the central Imbrium mare region and the Abenezra region in the southern central highlands, by averaging over 18 pixels each. Current investigations study also the possibility of a very thin uppermost layer of the regolith, formed by extensive space-weathering dominated by a glassy component [11].

Here we present results of an unmixing model to quantify abundances in mineral mixtures [7,8]. As

planetary surfaces are composed of a variety of different minerals, such mixing is also reflected in the obtained spectral data. In order to quantify the mineral abundances we use a non-linear unmixing model, based on the Hapke reflectance model [12,13]. The intrinsic reflectivity of an average single surface is described by the "single-scattering albedo" [12]. Incidence and emission angle govern multiple scattering within a surface, which also depends non-linearly on the single-scattering albedo. A "single-particle scattering function" describes the scattering behavior of an individual particle. For the full set of equations, the reader is referred to [12].

The model applied here has previously been used for spectral unmixing of NASA RELAB data [14], lunar analog materials [15], and IRIS laboratory olivine-pyroxene and grain-size mixtures [7,8].

Based on first MERTIS results, we focused on plagioclase-orthopyroxene-glass mixtures for this analysis.

IR spectroscopy: At the IRIS laboratory, samples are sieved in grain size fractions of <25 μm , 25-63 μm , 63-125 μm , and >125 μm . For the mineral mixing analysis presented here, we focused on the 63-125 μm fraction. Samples are placed in aluminum cups and analyzed by a Bruker Vertex 70v spectrometer with an A513 variable mirror reflectance stage under the following specular geometries: 20° incidence (i)/30° emergence (e), and 30°(i)/30°(e) angles. After background calibration using a commercial diffuse gold standard (INFRAGOLD™) a total of 512 scans were generated to ensure high signal-to-noise ratios.

Samples: For the present study we used ID2 labradorite from an unknown location in Scotland, and ID 53 enstatite from Bamble, Norway. IDs refer to the position in our database. These samples were investigated in previous studies at the IRIS laboratory [16-18]. Furthermore, synthetic lunar analogs were used. These glasses are based on the bulk composition of lunar highlands (ID59) and mare (ID57) [6]. From the endmembers, we derived different mineral mixtures, which were analyzed by the unmixing model.

Results: Minerals and their mixtures were investigated with the Vertex 70v spectrometer. Spectra of the endmembers and their mixtures are shown in Figures 1 and 2 for highland and mare spectra, respectively. Additionally, we plotted the mean MERTIS spectra of the

central Imbrium mare region and the Abenezra region as derived by [6]. The ID2 labradorite and ID53 enstatite spectra show characteristic Christiansen features and Reststrahlen bands, while both glass spectra are relatively flat. General intensity decreases with increasing observation angles.

Results of the spectral unmixing procedure of the mixtures are summarized in Table 1.

Table 1: Spectral unmixing results of labradorite-enstatite-glass mixtures under different geometries. Actual fractions of the mixtures are written in italics.

	ID2 Labradorite	ID53 Enstatite	ID57 Mare Glass	ID59 High- land Glass
<i>ID245</i>	87.6%	5.5%	-	6.9%
<i>i20/e30</i>	91.42%	3.37%		5.21%
<i>i30/e30</i>	90.27%	5.11%		4.61%
<i>ID246</i>	79.2%	14.9%	-	5.9%
<i>i20/e30</i>	79.43%	13.74%		6.82%
<i>i30/e30</i>	81.11%	11.02%		7.86%
<i>ID247</i>	35.8%	53.3%	10.9%	-
<i>i20/e30</i>	31.57%	53.42%	15.02%	
<i>i30/e30</i>	30.63%	53.52%	15.85%	

Summary & Conclusions: First quantitative results of spectral unmixing of glass mixtures show good overall agreement with the actual proportions. For the highland mixtures, the labradorite component is overestimated, however, the largest deviation is less than 5%. At the same time, the enstatite component is slightly underestimated. For the mare mixture, the estimated enstatite component is in very good agreement with the actual amount. For these mixtures, the glass component is overestimated by ~5%.

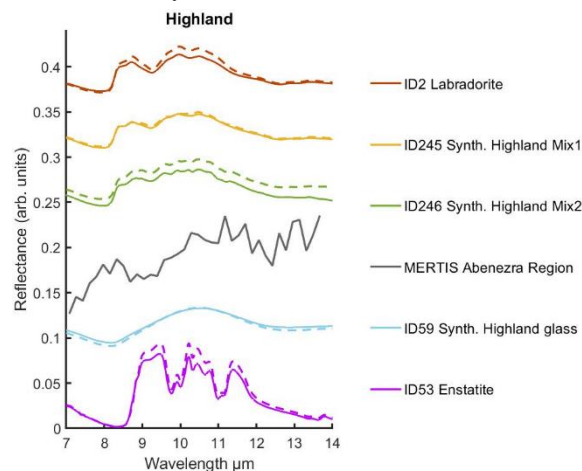


Fig. 2: IR reflectance spectra of endmembers and synthetic highland mixtures in the MERTIS-relevant wavelength range between 7-14 μm . Dashed lines correspond to $20^\circ(i)/30^\circ(e)$, while solid lines correspond to $30^\circ(i)/30^\circ(e)$ angles. Plotted in gray is a mean MERTIS spectrum of the Abenezra region in the southern central highlands [6].

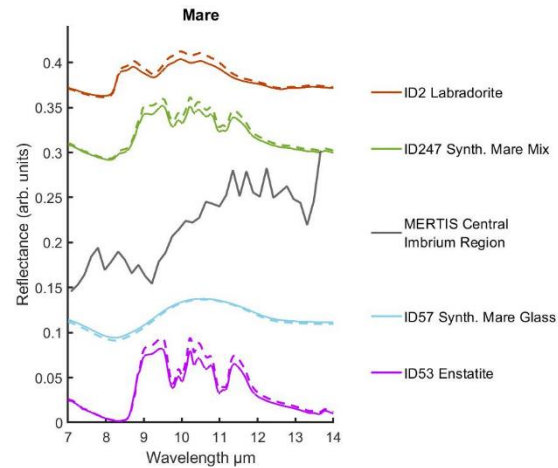


Fig. 1 IR reflectance spectra of endmembers and synthetic mare mixture in the MERTIS-relevant wavelength range between 7-14 μm . Dashed lines correspond to $20^\circ(i)/30^\circ(e)$, while solid lines correspond to $30^\circ(i)/30^\circ(e)$ angles, respectively. Plotted in gray is a mean MERTIS spectrum of the central Imbrium mare region [6].

As [6] has shown, further minerals have to be taken into account when interpreting MERTIS lunar spectra, obtained during the swing-by maneuver. This also requires further unmixing analysis of mineral mixtures with more components. We will also take into account the possibility of an epi-regolith, dominated by a glassy component [11].

With further calibration, the unmixing routine can also be applied to MERTIS data, in order to quantitatively interpret the spectra from further fly-by maneuvers and finally orbital measurements.

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