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MID-INFRARED REFLECTANCE SPECTROSCOPY OF SYNTHETIC GLASS ANALOGS FOR MERCURY SURFACE STUDIES

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Abstract

We have synthesized and analysed silicate glasses that are representative for the glasses on the surface of Mercury by mid-infrared reflectance spectroscopy, based on high-pressure laboratory experiments and the resulting compositions of the glass phase. The spectra are of interest for investigating the surface of Mercury using the MERTIS (Mercury Radiometer and Thermal Infrared Spectrometer) instrument on board of the ESA/JAXA BepiColombo mission.

Both powdered fractions and polished blocks have been analyzed. Powdered size fractions of 0-25 μm , 25-63 μm , 63-125 μm , and 125-250 μm were measured in reflectance in the thermal infrared (2-20 μm). Spectra for powdered bulk glasses (1.6 wt% - 19.0 wt% MgO) show a single, dominating Reststrahlenband (RB, 9.3 - 9.8 μm), a Christiansen Feature (CF; 7.6 μm - 8.1 μm), and a size dependent Transparency Feature (TF; 11.6 - 11.9 μm). Micro-FTIR analyses of polished blocks of glasses (3.4 – 26.5 wt% MgO) have characteristic bands at 7.8 - 8.2 μm (CF), and 9.3 - 9.9 μm (RB). Only few olivine crystalline features were observed.

Spectral features correlate with compositional characteristics, e.g. SiO_2 content or SCFM ($\text{SiO}_2/(\text{SiO}_2+\text{CaO}+\text{FeO}+\text{MgO})$ index). The strongest correlation between band features CF and the strong RB are with Mg/Si. No simple mixture of glass spectra from this study is able to reproduce the entire ground based spectrum of the surface of Mercury. However Mg-rich glasses reproduce identified features at 8.5 μm , 9.9 μm and 12.4 μm .

1. Introduction

Given the lack of meteorites or samples from the surface of Mercury (e.g., Weber et al. 2016), our current knowledge of its surface chemical composition is primarily based on chemical measurements by X-ray (Schlemm et al., 2007), as well as gamma-ray and neutron (Goldsten et al., 2007) spectrometers onboard the MESSENGER spacecraft. Based on major element ratios from these observations, several different terranes with characteristic chemical compositions have been identified (Nittler et al., 2011; Peplowski et al., 2015; Weider et al., 2015; vander Kaaden et al., 2016; Peplowski and Stockstill-Cahill, 2019). In a refined model using multivariate statistics, Peplowski and Stockstill-Cahill (2019) identified seven terranes. **Characterized by their Mg contents are following terranes:** The High-Mg (*HMg*) region, a Northern High-Mg region (*N-HMg*), and the Rachmaninoff-Basin (*RB*). Units with lower Mg abundances include the Northern Low-Mg (*N-LMg*) terrane and a region that is also Al-rich (*LMg-HAl* region), which occurs mostly in the Caloris basin. A last unit characterized by its high Al is the High-Al (*HAl*) terrane. Defined by its K content is the High-K (*IHK*) terrane. Based on the chemistry, the rock types of these different terranes can broadly be described as komatiitic, boninitic, and andesitic (e.g., Weider et al., 2015; Peplowski and Stockstill-Cahill, 2019).

The chemical data provided by MESSENGER were the basis for the identification of the surface mineralogy and petrology of Mercury. One way is to model the mineral composition from the chemistry, (e.g., Cross et al., 1902; van der Kaaden et al., 2016; Solomon et al., 2018; Peplowski and Stockstill-Cahill, 2019). A further way to study the petrology of Mercury are laboratory experiments. High pressure experiments that studied phase equilibria of peridotite and partial melt compositions under hermean mantle conditions were performed by Charlier et al., 2013; Namur et al., 2016 and Namur and Charlier, 2017. These techniques suggested that the hermean surface mineralogy should be dominated by variable abundances of plagioclase, forsterite, diopside, and enstatite, with unconstrained proportions of silicate glasses.

For Mercury, mid-infrared spectroscopy has only previously been undertaken using terrestrial telescopic observations. Studies that cover larger surface regions (Donaldson-Hanna et al., 2007; Sprague et al., 1994, 1997, 2000, 2002, 2007; Sprague and Roush, 1998; Emery et al., 1998; Cooper et al., 2001) show some surface variation, with a mineralogy dominated by plagioclase and some pyroxene. Glassy silicate materials are difficult to identify in the mid-infrared owing to their rather featureless spectra. Usually, only a single, broad band is visible in the region around 10 μm (e.g., Speck et al., 2010; Morlok et al., 2020a.) Earlier successful utilization of the thermal infrared wavelength range in planetary remote sensing covered the lunar surface (e.g., Sprague et al., 1992) and the Martian regolith (e.g., Bishop et al., 1995; Christensen et al., 2004).

This study focuses on the spectral properties of glasses relevant to Mercury's surface, which could have been formed by three major processes. First, explosive volcanism in the form of pyroclastic eruption-style volcanic activity occurred locally until about one billion years ago as evidenced by pyroclastic deposits (Goudge et al., 2014; Thomas et al., 2014; Murchie et al., 2015). Second, the surface of Mercury is dominated by lava flows. Magma quenching is very efficient in the hermean environment owing to the generally cold temperatures at the surface and at shallow depths. Therefore, it is conceivable that the surface contains a significant portion of quenched glasses with a range of compositions (e.g., Weitz et al., 1997; Kerber et al., 2011; Byrne et al., 2013; Charlier et al., 2013; Denevi et al., 2013; Namur et al., 2016; Namur and Charlier, 2017). Third, rapid melting and quenching of rocks occurred during high velocity impacts also central to the formation of the planet's surface. Mercury's regolith is therefore expected to contain high amounts of impact derived glass (e.g., Hörz and Cintala, 1997; Warrell et al., 2010; Murchie et al., 2015). A further process that can produce a glass component on planetary surfaces is space weathering, which can amorphize the surfaces of mineral phases (e.g., Brunetto et al. 2014; Weber et al., 2020; Stojic et al., 2020). Warell et al. (2010) estimated a glass content of 20 – 45 % for the hermean regolith based on spectral modelling of hermean surface data.

We present mid-infrared laboratory reflectance spectra of synthetic glasses. These laboratory spectra are needed for the accurate interpretation of future remote sensing spectra from the joint ESA/JAXA BepiColombo space probe, which will arrive at Mercury in 2025, and start investigating the innermost planet with a wide range of instruments in 2026 (e.g., Benkhoff et al., 2010, Hiesinger et al., 2010 and 2020; Rothery et al., 2020). Among the instruments is, for the first time, a mid-infrared spectrometer, MERTIS (Mercury Radiometer and Thermal Infrared Spectrometer). It will map the surface of the planet in the 7-14 μm spectral range, with a pixel scale of at minimum ~ 500 meters or even lower, depending on the orbit (Hiesinger et al., 2010, 2020). These mid-infrared emission features will permit the detection of Mercury's surface mineralogy in much more detail than with earlier instruments (e.g., Hiesinger et al., 2020).

The aim of this study is to provide spectra of synthetic glasses covering a representative range of compositions that are to be expected for regolith that formed by petrological processes under appropriate conditions for Mercury. This is in contrast to earlier studies (Morlok et al., 2017b and 2020a) which are based on quenched melts with the average chemical composition of the whole terranes and thus representative of larger averaged areas. These glasses will also be used for future studies, where we will mix these glasses with crystalline phases to create synthetic bulk analog mixtures similar to the hermean regolith for additional spectral studies.

2. Samples and Techniques

2.1. In Situ Glasses and Composition of Bulk Glasses

The glassy areas studied using micro-FTIR in run products from earlier high pressure laboratory experiments (Namur and Charlier, 2017) are in the following referred to as *in situ* samples. In these experiments, melts with starting compositions of the various geochemical terranes on Mercury were

equilibrated under different temperatures (1100 – 1480 °C), high pressure (0.1 GPa), varying oxidation fugacities relative to the iron-wuestite buffer (ΔIW) from ΔIW -7.2 to -4.7, and run times of 4 to 108 h (Namur and Charlier, 2017). The resulting run products (Table1) showed a wide range in modal abundance of forsterite, diopside, plagioclase, enstatite, and quartz. The abundance of the glass component varied from samples consisting entirely of glass to minimum contents of 21 wt%.

The second group of glasses studied are referred to as *bulk glasses*. For the synthetic bulk glasses, we used glass compositions based on the experimental runs in Namur and Charlier (2017) (for a list see Table 2), which are based on the starting compositions of the high-Mg and low Mg northern volcanic plains (*HMg-NVP* and *LMg-NVP*, respectively), Smooth Plains (*SP*), Inter crater Plain and Heavily Cratered Terrains (*ICP-HCT*), and the High-Mg Province (*HMg*). The intention is to cover a compositional range expected for glasses on Mercury. The modeled compositions (sources see Table 2) used to prepare the bulk glasses were for the low Mg endmember glass *159 Low-Mg C* an MgO content of 1.8 wt% and 72.3 wt SiO₂. Glass *158 Low-Mg B* has 5.1 wt% MgO and 66 wt% SiO₂. The ‘intermediate’ sample with an MgO content of 10.7 wt% and SiO₂ at 61.3 wt% is *174 Low-Mg A II*. The high-Mg composition end member is a glass with a calculated starting composition of 55.9 wt% SiO₂ and 21.8 wt% MgO (*181 High-Mg II*). The comparison of the in situ glass spectra with the powdered bulk glasses from this study will serve as a quality control. We expect the spectral features of glass phases synthesized for this study to be similar to the glasses from the run products from the high pressure petrological experiments.

Since the FTIR measurements have to emulate the porous and fine-grained surface conditions on Mercury, sieved and powdered fractions (several grams) are needed, much more than the few mg available from the run products of the elaborate high pressure laboratory experiments producing the in situ samples (Namur and Charlier, 2017).

2.2 Synthesis of Bulk Glasses

The bulk glasses were synthesized from reagent grade oxides (SiO_2 , TiO_2 , Al_2O_3 , Fe_2O_3 , and MgO) and carbonates (CaCO_3 , MnCO_3 , Na_2CO_3 , and K_2CO_3). The mixtures were decarbonated at 1000 °C for two hours and subsequently melted in air at 1450 °C for six hours. The obtained oxidized glasses were crushed to a fine powder. The synthetic bulk glasses were reduced at the graphite-CO buffer, which is at IW-6.7 at 1450 °C. Specifically, the oxidized glass powders were pressed into graphite crucibles with a diameter of 3 cm and heights of 5 cm and suspended on W-Re wires in a gas-mixing furnace. The glasses were reduced at 1450°C in pure CO-gas for 24 hours.

2.4. Sample characterization

Polished blocks of in situ samples and thin sections of aliquots of the bulk samples were first examined in transmission and reflectance using optical microscopy (Figs.A1,1;2). The samples were then characterized using a JEOL JXA-8530F Hyperprobe electron probe micro analyzer (EPMA) (Institut für Mineralogie, Münster) at a voltage of 15 kV, using a beam current of 15 nA (Fig.3; Table 2). Glasses were analyzed using a defocused beam of 5 μm diameter. Matrix corrections were made using the $\Phi\rho(z)$ procedure. Natural and synthetic minerals were used as standards: Jadeite (Na_2O), SanCarlos olivine (MgO), disthene (Al_2O_3), hypersthene (SiO_2), sanidine (K_2O), diopside (CaO), fayalite (FeO), rutile (TiO_2), Cr_2O_3 , and rhodonite (MnO).

Back-Scattered Electron (BSE) images were taken with a JSM-6610 Series Scanning Electron Microscope. The images were taken at an acceleration voltage of 20 kV and a working distance of 10 mm.

Raman measurements were made with an Ocean Optics IDR-Micro Raman system (IRIS laboratory, Münster) using an OneFocus optical system with a 40 x objective (Fig.4). The laser excitation

was 532 nm at a spectral resolution of $\sim 7 \text{ cm}^{-1}$ and a spot size of $\sim 2 \text{ }\mu\text{m}$. Spectra were obtained at a laser power of 1.8 mW ($0.6 \text{ mW}/\mu\text{m}^2$ on the sample surface). Since the spectrometer used is not a confocal instrument, for each spectrum, 4 measurements and only 3 seconds acquisition time were accumulated. The final results were background- and baseline-subtracted using a standard optimized routine of the Ocean Optics software.

2.5. Infrared Spectroscopy

2.5.1. Micro-FTIR Studies of in situ Samples

To test the spectral homogeneity of the bulk glasses in the spectral range of the MERTIS instrument (7-14 μm), we conducted micro-FTIR analyses using the ATR (Attenuated Total Reflectance) at the Institute for Geology in Bern. A line of spots was measured across the sample, with a spot size of approximately 5 μm (Fig.4).

In situ FTIR microscope analyses were conducted on polished glass samples using a Bruker Hyperion 1000/2000 System at the Hochschule Emden/Leer. We used a $250 \text{ }\mu\text{m} \times 250 \text{ }\mu\text{m}$ sized aperture (Fig.5). For analyses requiring higher spatial resolution, a Perkin-Elmer Spotlight-400 FTIR spectrometer at the University of Manchester was used to map samples using an adjoining Focal Plane Array (FPA) mapping unit with a resolution of $6.25 \text{ }\mu\text{m} \times 6.25 \text{ }\mu\text{m}$ in the reflectance mode (Fig.5). Spectra for the glass phases were extracted from the mapped area by [Principal Component Analysis \(PCA\)](#) (Martin et al., 2017). One of the spectral features of interest in the spectral range of from 7 – 14 μm is the Christiansen Feature (CF), a reflectance low (or emission high). This feature is important since it is usually observable even in data with low signal to noise ratio. In addition, it is a good proxy for the bulk composition, since the band position shifts with the SiO_2 content of the material (Cooper et al., 2002). The Reststrahlen Bands (RB) is the vibrational mode of the structure, characteristically for each mineral and glass phase.

The Transparency Feature (TF) occurs in spectra of the finest grain size fraction (below 60 μm) and is thus a very good indicator for grain sizes in remote sensing spectra (e.g., Salisbury et al. 1993).

2.5.2. Diffuse Reflectance of Powdered Bulk Glasses

For the FTIR diffuse reflectance analyses of the bulk glasses, size fractions smaller 25 μm , 25 μm to 63 μm , 63 μm to 125 μm , and 125 μm to 250 μm of the powdered bulk glass material were measured. For diffuse reflectance analyses in the range from 2 μm to 20 μm we used a Bruker Vertex 70v infrared system with a MCT detector at the IRIS (Infrared and Raman for Interplanetary Spectroscopy) laboratory at the Institut für Planetologie in Münster. Analyses were conducted under low pressure ($3 \cdot 10^{-3}$ bar) (Fig. 5 and 6). For each analysis, 512 scans were integrated to obtain a high signal to noise ratio. To emulate variations in orbital geometry, we obtained spectra with a A513 variable mirror stage. The results in this study were measured used a geometry of 20° incidence and 30° emergence angle in order to avoid specular reflectance. The laboratory spectra will be archived in the IRIS laboratory (Hiesinger et al., 2020), and also be available after publication on Mendeley Data under doi: 10.17632/tkcn436c4z.1.

3. Results

3.1. Characterization

Optical images of particular glass rich samples from Namur and Charlier (2017; list of used samples see Table 1) show mostly homogeneous, glassy patches with only a few crystallization products in the low-Mg glasses (Fig.A1). A few in situ samples (*Y124_HMg*, *Y126_HMg*, and *Y131HMg*) were highly crystalline, so we were using mapping modes for the FTIR analyses to extract the spectral properties of the glass (Fig.1).

Optical images of all bulk glass samples in backscattered electron (BSE) mode (Fig. 2a-d) show generally a homogenous, glassy material. However, fine iron particles in schlieren-like formations occur as a minor component. Additional SEM studies of the bulk glass samples also shows small, usually sub- μm sized particles identified as Fe metal by EDX. They occur also in schlieren-like concentrations, with abundances increasing from the iron poor *181 High-Mg II* samples to the iron-rich *159 Low-Mg C* sample. Fe solubility is a function of $f\text{O}_2$. With decreasing $f\text{O}_2$, the solubility of Fe decreases and such metal nuggets form.

The bulk samples also exhibit schlieren of fine, dark particles in the optical transmission images (Fig. 2a-d). These are expected contamination from the carbon crucibles used to synthesize the glasses. For quality control, the fine dark particles were analyzed using micro-Raman (Fig. 4). The particles were identified as carbon, characterized by typical bands at 1580 cm^{-1} as the single Raman active mode of graphite. This corresponds to the mode in the middle of the Brillouin zone with an E_{2g} -symmetrie (Debus, 2012). To investigate if the carbon grains affect the spectral properties of the samples, several spots on the surface of a polished sample were analyzed using the surface sensitive ATR (Attenuated Transmission and Reflectance) technique (Fig. 4). Despite variations in the distribution of the metal and carbon grains, the spectra of each spot are identical, overall variation intensities of the strong silicate feature at $10.7\text{ }\mu\text{m}$ is below 1% absorbance.

Compositional EMPA analyses of the glasses in the in situ samples are listed in Table 1 and illustrated in Fig. 3. Compositions range for SiO_2 from 54.7 wt% (*Y122_ICP*) to 68.1 wt% (*Y144_SP*). MgO ranges from 3.4 wt% (*Y144_SP*) to 26.5 wt% (*Y121_HMg*). Among the bulk glasses (Table 2; Fig.3), sample *159 Low-Mg C* is the MgO-poorest end member (1.6 wt %), and has a SiO_2 content of 75.7 wt%. Glass *158 Low Mg-B* has a slightly higher MgO with 4.7 wt%, and a SiO_2 content of 67.3 wt %. Sample *174 Low-Mg A II* covers an intermediate compositional MgO range with 9 wt% and SiO_2 at 64.3 wt%. Al_2O_3 shows comparatively little variation in this Mg-poor group (14.3 wt% - 15.4 wt%), as does Na_2O (4.8 wt% - 6.1 wt%). CaO shows more variation, 1.9 – 6.8 wt%. The *181 High-Mg Glass II* is the Mg rich endmember

with 19.0 wt% MgO, and low SiO₂ (59.3 wt%) and Al₂O₃ (11 wt%). All other elements are below 1 wt%. Differences to the model starting compositions (Table 2) were difficult to avoid due to the production process, but all samples cover the intended range.

3.2.1. Micro-FTIR Reflectance Studies of in situ Samples

The in situ reflectance spectra obtained from glassy spots with micro-FTIR mostly show only a dominating, single RB in the range from 9.3 μm to 9.9 μm (Fig.5; Table3a). This results from the ‘classic’ Si-O stretching of silicate-rich glass (King et al., 2004; Speck et al., 2011; Zeng et al., 2019). The other main feature, the CF, falls between 7.8 μm and 8.2 μm. Only a few spectra show more spectral bands: Sample *Y124_HMg* has additional (weak) bands at 10.1 μm, 10.5 μm, 12.6 μm, and 13.2 μm. Spectra for *Y126_HMg* have similar features at 10.1 μm, and 10.5 μm. These are typical forsterite features, indicating incipient crystallization (Lane et al., 2011).

3.2.2. FTIR Diffuse Reflectance Studies of Bulk Glasses

All four bulk glass samples exhibit the typical simple spectra of amorphous materials, i.e., one strong RB in the 6 μm to 18 μm range in the size fractions over 25 μm (Fig. 6; Table 3b). Band intensities increase with increasing grain size. At shorter wavelengths (below 7 μm), weak volatile features occur, mostly in the finer size fractions. Typical are water and CH₄ bands (e.g., King et al., 2004) at 2.8-2.9 μm, 3.4 μm, 3.5 μm, and 5.8 μm (not shown in figure). Low Mg end member *159 Low-Mg C* (1.6 wt% MgO) has the RB at 9.2 -9.3 μm, and the CF at 7.6 – 7.7 μm. The finest size fraction (0-25 μm) has the characteristic TF at 11.6 μm. Sample *158 Low-Mg B* also exhibits low Mg contents (4.7 wt% MgO). Its CF is at 7.8 μm, the single RB is at 9.4 μm. The TF in the 0 – 25 μm size fraction is at 11.7 μm.

Intermediate sample *174 Low Mg A II* (9 wt% MgO) has the characteristic features shifted slightly to longer wavelengths: the CF is at 7.9 μm , the RB at 9.6 μm , and the TF is at 11.8 μm . The Mg-rich endmember *181 High-Mg II* (19.0 wt% MgO) still shows only bands of amorphous material: the CF is at 8.1 μm and the broad RB is at 9.8 μm . The comparatively weak TF is at 11.9 μm .

4. Discussion

4.1. General Chemical Composition and CF

Of particular interest are correlations between chemical aspects of the glass and the fundamental spectral features, i.e. the CF and the dominating RB. Since it is difficult to extract quantitative chemical abundances from remote sensing data, it is easier to use elemental ratios (weight %; Fig. 3), e.g., relative to wt% Si (Table 1, 2). For the CF, strongest Coefficient of Determination (r^2) is found for Mg/Si with $r^2=0.77$. Ca/Si only has a moderate correlation of $r^2=0.33$. K/Si show good correlation with $r^2=0.55$. All other elements only have a weak correlation.

4.2. Bulk and Micro-FTIR Spectra

Here, we compare the glasses obtained from high pressure laboratory experiments (Namur and Charlier, 2017) analyzed in situ with micro-FTIR with the results of the largest size fraction (125 – 250 μm) of the bulk glasses, arranged by increasing Mg content from top to bottom (Fig. 5). The spectra of the four powdered bulk glasses agree very well with trends defined by the spectra from micro-FTIR analyses, both regarding the positions of the CFs and the dominating RB, which both shift to longer wavelengths with increasing Mg content. The changes of the band shapes (broadening with increasing Mg) are also very similar.

4.3. Comparison with Earlier Studies

4.3.1. CF and SiO₂ content

Previous studies showed that the chemical composition and spectral parameters are correlated with the bulk SiO₂ content and the position of the CF (Fig.7a). By its nature as a reflectance minimum (or emission maximum), the CF is relatively easily identified even in weak or noisy data, and thus is very useful in remote sensing. The powdered bulk glasses from this study follow the typical linear trend observed by earlier studies (Cooper et al., 2002), and also overlap with synthetic glasses with similar compositions from earlier studies (Morlok et al., 2016b; 2017b; 2020a). Glasses from the in situ samples also follow the general trend well and overlap with the synthetic glasses from our earlier studies (Fig.7a).

4.3.2. RB and SiO₂ Content

The correlation between glass SiO₂ content and the dominating RB has been shown to be strong for glasses (e.g., Morlok et al., 2017b, 2020a). Similar to the CF, such a single, strong spectral feature is relatively easy to identify in most spectra. Glasses with high and intermediate SiO₂ contents follow a linear trend line from 100 to 50 wt% SiO₂ that splits at lower SiO₂ (Fig.7b). At lower SiO₂ contents, two potential trends are recognizable. A shallow one depicts glass from conventional melting processes. A steeper trend was observed in glasses that underwent vaporization processes (Morlok et al., 2020a and b). The powdered bulk glasses as well as spectra from micro-FTIR from this study fall into the intermediate range and follow the trend established by earlier studies of synthetic glass very well. In a remote sensing context, this would make distinguishing glassy material from magmatic processes from glasses formed in other processes difficult.

4.3.3. CF and Polymerization

The interconnection of the SiO_4 tetrahedrons is a way to describe the degree of polymerization of the phases. This can be done in the form of the SCFM index, which is calculated as $\text{SiO}_2/(\text{SiO}_2+\text{CaO}+\text{FeO}+\text{MgO})$ (Walter and Salisbury, 1989; Salisbury et al., 1997; Cloutis et al., 2002; Cooper et al., 2002) (Fig.7c). While high SiO_2 glasses fall near the trend line for earlier, usually crystalline phases (Cooper et al., 2002), samples with intermediate and basaltic compositions plot slightly off the trend line for crystalline terrestrial rocks (Cooper et al., 2002). The results from the micro-FTIR are very similar to those of synthetic glasses from earlier studies (Morlok et al., 2020a and b; Zeng et al., 2019). This indicates a similarity of the synthetic glasses and that the material from the high pressure experiments is generally structurally similar to natural materials.

4.4. Comparison with the Surface of Mercury

In this part, we will compare the results from this study with available mid-infrared data from the surface of Mercury. This is an entirely qualitative comparison between band features, in order to see if there is any direct sign of glassy material in the surface spectrum.

Only a few mid-infrared ground-based spectra of Mercury are available (Donaldson-Hanna et al., 2007; Sprague et al., 1994, 1997, 2000, 2002, 2007; Sprague and Roush, 1998; Emery et al., 1998; Cooper et al., 2001). The spectra cover larger surface regions of up to 10^6 km^2 . Due to observational limitations, terrestrial spectra of Mercury have only weak spectral contrast and low signal to noise ratio (e.g. Sprague et al., 2007). Therefore, we limit our comparison of the results from this study to a hermean spectrum showing a high signal to noise ratio by the Mid-Infrared Camera (MIRAC) at the Kitt Peak Observatory of a region at about $210\text{--}250^\circ$ longitude (Sprague et al., 2000). The spectrum for the hermean surface

(Fig.8; top) was recalculated from reflectance form emissivity and baseline subtracted. It exhibits significant RBs at 9.3 μm , 9.9 μm , and 11 μm , a CF is at 8.5 μm , and a (potential) TF occurs at 12.4 μm .

Of the samples synthesized for in this study, only the Mg-rich (SiO_2 poor) glasses have a CF near that of the spectrum of the surface of Mercury (8.5 μm), such as samples *Y121_ICP-1* (8.2 μm) and *181 High-Mg II* (8-8.1 μm). Regarding the band position of the dominating RB in the glass spectra, *181 High-Mg II* and high MgO in situ samples, are similar to the 9.9 μm feature in the hermean surface spectrum with band positions between 9.8 and 9.9 μm . The single, dominating RB of *159 Low-Mg C* at 9.2-9.3 μm has similarities to the 9.3 μm band in the hermean spectrum. The TF closest to the 12.4 μm band in the Mercury spectrum is that of *181 High-Mg II* (11.9 μm). Thus no individual glass spectrum from this study would reproduce the astronomical spectrum of Mercury. Particularly, crystalline phases are needed in order to provide the strong RB features.

5. Summary and Conclusions

We synthesized and characterized size fractions of synthetic analog glasses based on high pressure laboratory studies of the hermean mantle and surface analog rocks. These samples were studied as powders in the mid-infrared (2-20 μm). In addition, a series of glassy areas from high pressure petrological laboratory experiments in situ using micro-FTIR (Fig.5).

Results for the powdered bulk glasses with very low MgO (1.6 wt% to 19.0 wt%) show simple spectra typical for glassy materials: A single, dominant RB between 9.2 μm and 9.8 μm , and a CF between 7.6 μm and 8.1 μm . The TF is located between 11.6 μm and 11.9 μm (Fig.6). Features for the in situ glass samples with 3.4 – 26.5 wt% MgO range from 7.8 μm to 8.2 μm for the CF, and 9.3 μm to 9.9 μm for the RB. Minor crystalline features were found in rare cases at 10.1 μm , 10.5 μm , and 12.6 - 12.8 μm (Fig.5), recording the crystallization of forsterite.

Spectra from powdered bulk glasses and in situ samples are very similar regarding band position and band shape. Furthermore, the synthetic materials from this study show very similar behavior in comparison with earlier studies, when spectral features (CF, RB) are compared to compositional characteristics (SiO₂ content, SCFM index) (Fig.7a-c).

The strongest correlation between the CF or the dominant RB in a spectrum is with Mg/Si ratios. Contamination by carbon from the sample cups during sample synthesis as well as metallic iron nuggets probably have no recognizable impact on the spectral properties, since both phases are very minor, and do not exhibit detectable features in the mid-infrared region.

Mid-infrared spectra of large areas of the hermean surface show similarities only to some bands of glass investigated here and hermean surface data. This implies that further components will be needed to reproduce the known spectral data from Mercury in a quantitative way. The hermean regolith has up to 80% crystalline phases (Warrell et al., 2010). So for detailed, quantitative modeling of the hermean surface, further, crystalline components will have to be taken into account (e.g., Martin et al., 2017). The same applies to the following MERTIS related studies, where we will mix the glassy material from this study with crystalline phases in order to emulate the composition of the hermean surface regolith. Such mixtures will allow us to obtain spectra of the hermean surface much closer to those expected from MERTIS on BepiColombo. **The suitability of the glass synthesized and studied in this work for both spectral comparison with the surface of Mercury as well as for future mixing experiments is confirmed by the similarity to results from earlier studies, and the internal consistency of the data set.**

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574 **Figure Captions**

575 **Figure Appendix A1.** Optical images of polished blocks from the in situ samples used in the Micro-FTIR
576 studies (white rectangle = 256 μm $\times$ 250 μm). The samples are ordered by decreasing Mg content of the
577 glass (Table 1). Most areas analyzed are homogeneous glass areas, with brighter inclusions being
578 crystallized phases. *SP*=Smooth Plains, *HMg*=High Mg-Region, *HMg-NVP*=High-Mg Northern Volcanic
579 Plains, *IcP*=Inter Crater Plains.

580 **Figure 1** Samples used for micro-FTIR studies. Here whole areas were scanned (red boxes) and the
581 spectral properties extracted (marked in the colored spectral map). *SP*=Smooth Plains, *HMg*=High Mg-
582 Region, *HMg-NVP*=High-Mg Northern Volcanic Plains, *IcP*=Inter Crater Plains.

583 **Figure 2.** Optical images of polished blocks from the samples used for the powdered bulk glass studies.
584 **(left)** optical transmission images. The silicate part of the material is very homogeneous glass with no
585 larger crystals. However small particles are visible, presumably carbon bits of the sample containers.
586 **(center and right)** Backscattered electron images. Bright particles are metallic iron, enlarged image in the
587 center show areas of higher density of these grains. Abundances of the metal grains decreases with with
588 increasing Mg contents (top to bottom),

589 **Figure 3.** Chemical composition of synthetic glasses used in this study (Electron Microprobe Data,
590 weight%). **Circles:** In situ samples, **Crosses:** Bulk Samples, **Squares:** Data for composition of geochemical
591 terranes on Mercury (vander Kaaden et al., 2017).

592 **Figure 4** (left)Optical image of test sample with high abundance of fine-grained carbon particles from the
593 containments. Insert shows Raman spectrum of representative particles, confirming them as graphite.
594 **(right)** Optical image of polished block from sample 174 *Low-Mg A II*. White circles show spots from
595 which ATR spectra were taken (left to right, top to bottom), which are shown as insert. Despite varying
596 abundance of fine-grained graphite particles, the spectra show only very minor variations in intensity.

Figure 5: Comparison of spectra from glassy spots in in situ sample measurements with micro-FTIR (black spectra) to the 125 – 250 μm fraction of the bulk glass powder spectra (grey). Spectra are off-set by a constant value, and for a better comparison of data from different techniques, normalized to the same intensity based on the CF (lowest reflectance) and the strongest RB (point of maximum reflectance). Vertical lines show the position of the Christiansen Feature (CF) and Reststrahlen Band (RB). Samples are ordered with increasing Mg content from top to bottom. *SP*=Smooth Plains, *HMg*=High Mg-Region, *HMg-NVP*=High-Mg Northern Volcanic Plains, *IcP*=Inter Crater Plains.

Figure 6: Reflectance spectra of powdered bulk glass size fractions 0-25 μm , 25-63 μm , 63-125 μm , and 125-250 μm (in μm). CF = Christiansen Feature, a reflectance low, RB=Reststrahlenband, TF = Transparencies Feature characteristic for the finest size fraction. All features show a shift to longer wavelengths with increasing Mg content.

Figure 7(a): Comparison of SiO_2 contents and the position of the CF. Results of earlier studies fall on a linear trend line, confirming the observation of Cooper et al. (2002). Results of this study also plot along the trend line. **(b)** Comparison of SiO_2 content with the position of the single RB of the glasses. Results from earlier studies show a basically linear trend from high SiO_2 contents to ~50 wt% SiO_2 . At lower SiO_2 two possible trends are forming, one continuing the trend line, the other following a shallower trend. The results for glasses in this study follow the main trend line. **(c)** Comparison of the SCFM index ($\text{SiO}_2/(\text{SiO}_2+\text{CaO}+\text{FeO}+\text{MgO})$) (Walter and Salisbury, 1989; Salisbury et al., 1997; Cooper et al., 2002; Cloutis et al., 2002) to the CF band position. With increasing mafic composition, glasses tend to diverge slightly from the trend line for terrestrial rocks (Cooper et al., 2002). Again, the result for the synthetic glasses from this study follow earlier trends very well.

Figure 8. Comparison of a ground-based, base-lined spectrum of the surface of Mercury (Sprague et al., 2000) to the most similar spectra from this study (in μm). Spectra are off-set by a constant value, and for a better comparison of data from different techniques, normalized to the same intensity based on the CF

(lowest reflectance) and the strongest RB (point of maximum reflectance). The large grain fraction (125-250 μm) of Mg-poor end member *159 Low-Mg C* (1.6 wt% MgO) has a RB similar to the 9.3 μm feature on the hermean surface. The 125-250 μm fraction of Mg-rich *181 High-Mg II* (19.0 wt% MgO) has a feature similar to the 9.9 μm band in the astronomical spectrum Both CF and TF show clear differences.

	Y144_SP	Y143_SP	Y131_HMg	Y131_LMg-NVP	Y140_HMg-NVP	Y140_SP	Y121_LMg-NVP	Y133_SP	Y126_ICP
SiO₂	68.09	66.12	66.14	65.94	65.25	62.06	62.25	59.22	58.40
TiO₂	0.51	0.02	0.35	0.26	0.04	0.09	0.38	0.38	0.33
Al₂O₃	15.72	15.48	15.57	15.67	15.21	17.09	14.13	15.91	16.33
FeO	0.13	0.06	0.25	0.19	0.03	0.10	0.14	0.14	0.08
MnO	0.20	0.04	0.13	0.19	0.07	0.00	0.20	0.00	0.07
MgO	3.37	5.17	5.22	5.35	6.68	7.27	10.18	11.12	12.18
CaO	3.65	5.69	5.30	5.27	6.64	7.46	5.69	7.51	7.27
Na₂O	7.45	7.50	6.72	7.16	5.87	5.24	6.17	5.31	4.88
K₂O	0.20	0.16	0.22	0.21	0.14	0.09	0.16	0.11	0.09
	99.32	100.24	99.90	100.24	99.93	99.40	99.30	99.70	99.63
T(°C)	1170	1210	1220	1220	1250	1250	1480	1360	1320
P (GPa)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Time (h)	108	96	72	72	69	69	4	48	70
ΔIW	-6.2	-5.6	-5.7	-5.9	-5.0	-4.9	-4.8	-	-5.6
Glass	0.42	0.54	0.42	0.87	0.73	0.91	1	1	0.79
Unit	Smooth Plains	Smooth Plains	High-Mg Province	Low-Mg Northern Volc. Plains	High-Mg Northern Volc. Plains	Smooth Plains	Low-Mg Northern Volc. Plains	Smooth Plains	Inter Crater Plains

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	C580_NVP	Y126_HMg	Y133_HMg-NVP	Y124_HMg	Y123_ICP	Y123_HMg	Y121_ICP	Y122_ICP	Y121_HMg
SiO₂	57.47	59.96	60.13	59.51	56.44	57.45	55.53	54.69	55.22
TiO₂	0.40	0.56	0.62	0.45	0.29	0.48	0.25	0.27	0.39
Al₂O₃	14.28	10.56	12.52	9.87	14.40	9.00	12.37	12.66	6.97
FeO	0.01	0.18	0.14	0.15	0.06	0.05	0.23	0.07	0.15
MnO	0.13	0.24	0.21	0.20	0.03	0.24	0.09	0.10	0.25
MgO	12.90	14.44	15.41	16.33	17.74	20.34	21.51	21.73	26.51
CaO	5.87	10.30	6.54	9.19	5.87	8.86	5.40	5.75	7.06
Na₂O	7.01	3.60	3.99	3.97	4.74	3.40	4.14	4.02	3.16
K₂O	0.17	0.11	0.11	0.10	0.08	0.07	0.05	0.07	0.07
	98.24	99.95	99.67	99.77	99.65	99.89	99.57	99.36	99.78
T(°C)	1450	1320	1360	1360	1400	1400	1480	1440	1480
P (GPa)	0.15	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Time (h)	6	70	48	45	52	52	4	26	4
ΔIW	-6.4	-5.4	-	-5.6	-5.8	-6.1	-4.8	-4.8	-4.7
Glass	0.98	0.71	0.97	0.75	0.90	0.83	1	1	1
Unit	Northern Volcanic Plains	High-Mg Province	High-Mg Northern Volc. Plains	High-Mg Province	Inter Crater Plains	High-Mg Province	Inter Crater Plains	Inter Crater Plains	High-Mg Province

642

643 **Table 1:** Chemical composition (in wt%) of the glass phases analyzed in situ samples using micro-FTIR.
644 SP=Smooth Plains, HMg=High Mg-Region, HMg-NVP=High-Mg Northern Volcanic Plains, ICP=Inter Crater
645 Plains, LMg-NVP=Low Mg Northern Volcanic Plains. Source: Namur and Charlier, 2017. [R1-1]

181 High Mg II				174-Low Mg A II			158 Low- Mg B			159 Low- Mg C		
Model	Glass	Std		Model	Glass	Std	Model	Glass	Std	Model	Glass	Std
SiO ₂	55.91	59.29	±0.37	61.25	64.26	±0.63	66.03	67.26	±0.73	72.30	75.66	±0.45
TiO ₂	0.36	0.41	±0.12	0.44	0.46	±0.04	0.18	0.23	±0.12	0.21	0.26	±0.12
Al ₂ O ₃	10.54	10.95	±0.20	14.18	14.30	±0.21	15.84	15.41	±0.16	15.36	15.04	±0.42
FeO	0.12	0.05	±0.06	0.13	0.05	±0.17	0.18	0.18	±0.27	0.25	0.35	±0.09
MnO	0.16	0.17	±0.04	0.17	0.16	±0.05	0.09	0.09	±0.05	0.04	0.04	±0.05
MgO	21.74	19.00	±0.22	10.68	8.97	±0.25	5.06	4.69	±0.25	1.76	1.63	±0.24
CaO	6.98	7.16	±0.19	6.96	6.81	±0.16	5.39	5.77	±0.30	1.77	1.88	±0.25
Na ₂ O	3.72	3.29	±0.15	5.54	4.81	±0.23	6.93	6.00	±0.18	7.14	6.14	±0.26
K ₂ O	0.07	0.11	±0.04	0.14	0.19	±0.06	0.17	0.23	±0.05	0.29	0.35	±0.05
	99.60	100.07		99.48	100.01		99.86	99.87		99.11	101.37	
T(°C)		1450			1450			1450			1450	
P (GPa)		10⁻⁴			10⁻⁴			10⁻⁴			10⁻⁴	
Time (h)		24			24			24			24	
ΔIW		-6.7			-6.7			-6.7			-6.7	
Glass												
Based on Samples in [1]	Y121_ICP, Y122_ICP, Y122_HMg, Y123_HMg			Y121_LMg-NVP, Y123_LMg-NVP, Y124_LMg-NVP, Y126_LMg-NVP, Y139_HMg-NVP, Y134_SP, Y133_SP, Y128_HMg			Y131_LMg-NVP, Y143_HMg-NVP, Y143_SP, Y131_ICP, Y131_HMg, Y132_HMg			Y172_LMg-NVP, Y173_HMg-NVP, Y146_ICP, Y146_HMg		

Table 2: Chemical composition in wt% of the synthetic bulk glasses used for the size fractions of the powder studies, arranged by increasing SiO₂ content. In wt%. Model: Composition calculated for the starting mixture based on results from **Namur and Charlier (2017)** [1]. Glass: Chemical composition of the synthesized glass (in wt%). Std: Standard Deviation. SP=Smooth Plains, HMg=High Mg-Region, HMg-NVP=High-Mg Northern Volcanic Plains, ICP=Inter Crater Plains, LMg-NVP=Low Mg Northern Volcanic Plains. Source: Namur and Charlier, 2017

Sample	CF		RB				
	μm	μm	μm	μm	μm	μm	μm
Y144_SP	7.76		9.47				
Y143_SP	7.79		9.61				
Y131_HMg	7.96		9.45				
Y131_HMg	7.87		9.33			12.66	
Y131_LMg	7.91		9.62				
Y131_LMg	7.89		9.62				
Y140_HMg-NVP	7.91		9.69				
Y140_SP	7.8		9.53				
Y121_LMg-NVP	7.94		9.71				
Y133_SP	7.99		9.81				
Y126_ICP	7.93		9.79				
C580A_NVP	8.05		9.81				
Y126_HMg	8.02		9.8		10.51	12.83	
Y126_HMg	8		9.76	10.1	10.51		
Y133_HMg-NVP	8.06		9.86				
Y124_HMg	7.97	9.69	9.84	10.12	10.53	12.63	13.23
Y123_ICP	8.03		9.81				
Y123_HMg	8.1		9.88				
Y121_ICP	8.23		9.93				
Y122_ICP	8.12		9.94				
Y121_HMg	8.1		9.94				

Table 3a: Band positions (in μm) of glasses in situ samples on polished blocks. CF = Christiansen Feature; RB = Strongest Reststrahlenband; TF = Transparency Feature. *SP*=Smooth Plains, *HMg*=High Mg-Region, *HMg-NVP*=High-Mg Northern Volcanic Plains, *ICP*=Inter Crater Plains.

Sample						CF	RB	TF
181 High Mg II	μm	μm	μm	μm	μm	μm	μm	μm
0-25 μm	2.95	3.38	3.42	3.5		8.07	9.81	11.91
25-63 μm	2.95	3.38	3.41	3.5		8.07	9.8	
63-125 μm	2.94	3.38	3.41	3.5		8.06	9.78	
125-250 μm	2.93	3.38	3.41			8.03	9.8	
174 Low-Mg A II								
0-25 μm	2.95	3.37	3.41	3.5		7.89	9.58	11.77
25-63 μm	2.94	3.37	3.41			7.87	9.57	
63-125 μm	2.93	3.38	3.41			7.91	9.57	
125-250 μm	2.93	3.37	3.41			7.9	9.57	
158 Low-Mg B								
0-25 μm	2.9	3.37	3.41	3.49	3.98	7.82	9.41	11.68
25-63 μm	2.8	3.37	3.41			7.78	9.43	
63-125 μm	2.79					7.75	9.42	
125-250 μm	2.79					7.77	9.43	
159 Low-Mg C								
0-25 μm	2.82	3.37	3.41	3.5	5.76	7.66	9.25	11.55
25-63 μm	2.81	3.37	3.41	3.5	5.8	7.64	9.24	
63-125 μm	2.8	3.37	3.41	3.5	5.81	7.63	9.25	
125-250 μm	2.8	3.37	3.41			7.62	9.25	

Table 3b: Band positions of the powdered bulk glass size fractions (in μm). CF = Christiansen Feature; RB = Strongest Reststrahlenband; TF = Transparency Feature. Features below 6 μm are volatile bands.

Figure 1

Figure 2

Figure 3

Figure 3

Figure 4

[Click here to access/download;Figure;FIG_4.pdf](#)

Figure 4

Figure 5

Figure 5

Figure 6

Figure 7a

Figure 7b

Figure 7c

Figure 8

Figure **Appendix 1**