



# Mercury Laboratory Workshop

## 2024

### Abstract Booklet

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Institute of Planetary Research, DLR, Berlin Germany



Session I

# **Probing Mercury's materials**

## Petrology experiments to produce the best Mercury analogues

C. Cartier<sup>1\*</sup>, O. Namur<sup>2</sup>, M. Lecaille<sup>3</sup>, L. Llado<sup>3</sup> and B. Charlier<sup>3</sup>

\*camille.cartier@univ-lorraine.fr, <sup>1</sup>Université de Lorraine, CNRS, CRPG, Nancy, France, <sup>2</sup>Department of Earth and Environmental Sciences, KU Leuven, Heverlee, Belgium, <sup>3</sup>Department of Geology, University of Liège, Sart Tilman, Belgium.

Mercury's crust, made of volcanic products, formed under very specific conditions, notably a very reduced redox (very low oxygen fugacity,  $fO_2$ ) and volatile-rich environment [1]. Thus, the mineralogy at Mercury's surface includes Na-rich plagioclase, FeO-free silicates (enstatite, diopside, forsterite), and Na-Si-rich volatile-bearing volcanic glass, whose proportion is unknown [2]. Mercury's crust also contains a sulfide component of approximately 5 wt%, which could either consist of a variety of exotic sulfide minerals (FeS, CaS, MgS, TiS<sub>2</sub>), or be dissolved as sulfide species in the glass [1-5]. Finally, Mercury's crust may contain moderate to large quantities of graphite [6], and possibly unusual minerals such as Fe-Si alloys, carbides, and silicides [7].

Therefore, analogs of Mercury's surface, in terms of mineralogical and elemental compositions, are not available as natural samples on Earth. Some meteorites are more similar, in particular aubrites formed under the same redox and S-rich conditions as Mercury. Their mineralogy is largely dominated by FeO-free enstatite, followed by Na-rich plagioclase, FeO-free forsterite and diopside [8]. Aubrites also contain up to 2 wt% exotic sulfides (FeS, CaS, MnS, etc.). Because of their mineralogy very similar to that of Mercury, aubrites are considered as the best natural analogs for Mercury's crust [9,10]. However, the difference in mineral proportions between Mercury's crust and aubrites, and in particular the presence of FeO-free volatile-bearing glass in Mercury lavas and not in aubrites, means that the latter are imperfect analogs.

In this contribution, we illustrate how various experimental techniques can advance our understanding of Mercury and assist in calibrating BepiColombo's geochemical and spectroscopic instruments. Low-pressure experiments using gas-mixing furnaces can produce large quantities (up to several grams) of glassy or crystal-bearing glass analogue material under relevant  $fO_2$  conditions. This method also permits the production of large quantities of pure FeO-free silicate minerals (forsterite and enstatite). A limitation of this method is however the vaporization of volatile elements, in particular sulfur, which prevents their dissolution in silicate melts or the synthesis of sulfides. To retain volatiles and maintain appropriate  $fO_2$ , methods at low pressure (evacuated silica tubes, i.e., 1 atm) or high pressure (piston cylinder, multi-anvil press) can be used. These methods, however, produce only small quantities of material (milligrams to gram maximum for evacuated silica tube experiments). While these amounts may suffice for in situ mid-infrared measurements (e.g. [11]), they are insufficient for high-temperature emissivity measurements or MIXS detector calibration. One solution is to repeat the experiments until the necessary quantities of material are obtained. Thus, these techniques make it possible to produce volatile-bearing glass with exact chemical composition of Mercury target terranes, as well as synthesizing the variety of exotic minerals that might be present at Mercury's surface.

[1] Cartier & Wood (2019) *Elements*. [2] Namur & Charlier (2017) *Nat. Geosci.* [3] Namur et al. (2016) *Earth Planet. Sci. Lett.* [4] McCubbin et al. (2017). [5] Vander Kaaden et al. (2017) *Icarus*. [6] McCoy et al. (2018) *Mercury - The view after MESSENGER*. [7] McCubbin et al. (2017) *J. Geophys. Res. Planets*. [8] Keil (2010) *Chemie der Erde*. [9] Morlok et al. (2020) *Meteorit. Planet. Sci.* [10] Wilbur et al. (2022) *Meteorit. Planet. Sci.* [11] Morlok et al. (2023) *Icarus*.

## Synthetic crystalline samples of MESSENGER compositions as Mercury analogues

Barry, T.L.<sup>1</sup>, Fox, A.R.D.<sup>1</sup>, Cartwright, J.A.<sup>1</sup>, Martindale, A.<sup>1</sup>, Yoshino, T.<sup>2</sup>, Charlier, B.<sup>3</sup>, Bunce, E.<sup>1</sup>

<sup>1</sup> University of Leicester, Leicester, UK. <sup>2</sup>Institute for Planetary Materials, University of Okayama, Japan.

<sup>3</sup>University of Liege, Liege, Belgium.

As we know from NASA's MESSENGER data, the surface of Mercury has a chemical composition unlike anything on Earth. The planet's surface is highly reduced (IW -6) with incredibly low FeO content (<~2 wt % compared to Earth's <14 wt %), despite an Fe-core that makes up ~85% of the planet. Surface compositions of Mercury can be divided into at least 7 distinct terranes, that, although similar to mafic and ultramafic rocks on Earth, have some clear differences.

Here, we have attempted to produce larger volume (<20g) synthetic glass bead and crystalline samples of the 7 terranes, to find suitable methodologies for replicating major element ratios, analogous to MESSENGER data. One set of crystalline samples were allowed to cool slowly until the encasing graphite crucible had completely combusted (Figure 1), whereas another set were allowed to cool slowly at temperature, to facilitate crystal growth, before quenching.

The samples will be analysed by XRF and SEM to quantitatively demonstrate similarities to target compositions, and the information will be used to produce further refined samples. In the future, samples will be treated in a gas-mixing furnace to generate reduced conditions, more akin to Mercury, and sample compositions will include carbon to help test hypotheses for high carbon content in Mercury's low reflectance medium.

Both oxidized and reduced synthetic samples will be used to characterise mineralogy and physical properties, to ground-test instrument operations ahead of the orbiter mission, particularly for the MIXS instrumentation. Samples are available for further tests, and can be shared with the instrument teams preparing for the 2025 BepiColombo mission.



**Figure 1:** Crystalline synthetic analog sample of High-Mg Region major-element composition.



## **Production of Mercury's surface analogues by experimental petrology: an overview of the evacuated silica tube technique**

Laurie Llado<sup>1</sup> and Bernard Charlier<sup>1</sup>.

<sup>1</sup> *University of Liege.*

Evacuated silica tube experiments are designed to investigate multi-phase interactions within a closed system, operating under low pressure (below 1 bar), high temperature (up to 1400°C), and controlled oxygen fugacity (ranging from  $\sim\text{IW}+2$  to  $\text{IW}-6$ ). The experimental setup comprises a crucible containing a sample and a solid buffer within an evacuated silica tube that enables gas-melt-solid interaction under controlled temperature. Complete or partial melting of the sample enhances evaporation of volatile elements and the production of a vapor in thermodynamic equilibrium with the silicate glass. This technique is particularly valuable for replicating natural systems involving gaseous components, magmatic melts, and crystals, and allows the investigation of a wide range of magmatic processes such as the solubility of moderately volatile elements, crystallization sequences, element partitioning, diffusion, or degassing processes. Various magmatic environments can be reproduced, ranging from the formation of chondrules in the protoplanetary disk to Mercury's surface magmatism processes (e.g. degassing, volatile-rock interaction, sulfidation). While this technique is highly adaptable and offers versatility, it comes with experimental limitations including challenges in determining gas speciation and their partial pressures, the impact of partial pressure of volatile species on the C-CO buffer equilibrium, and the temperature limitation due to the softening point of silica ( $\sim 1400^\circ\text{C}$ ). We provide an overview of this technique along with the applications conducted in our laboratory, encompassing the behavior of elements, elemental speciation in reduced magma, S isotope fractionation, smelting and sulfidation processes, as well as the production of Mercury's surface analogues.

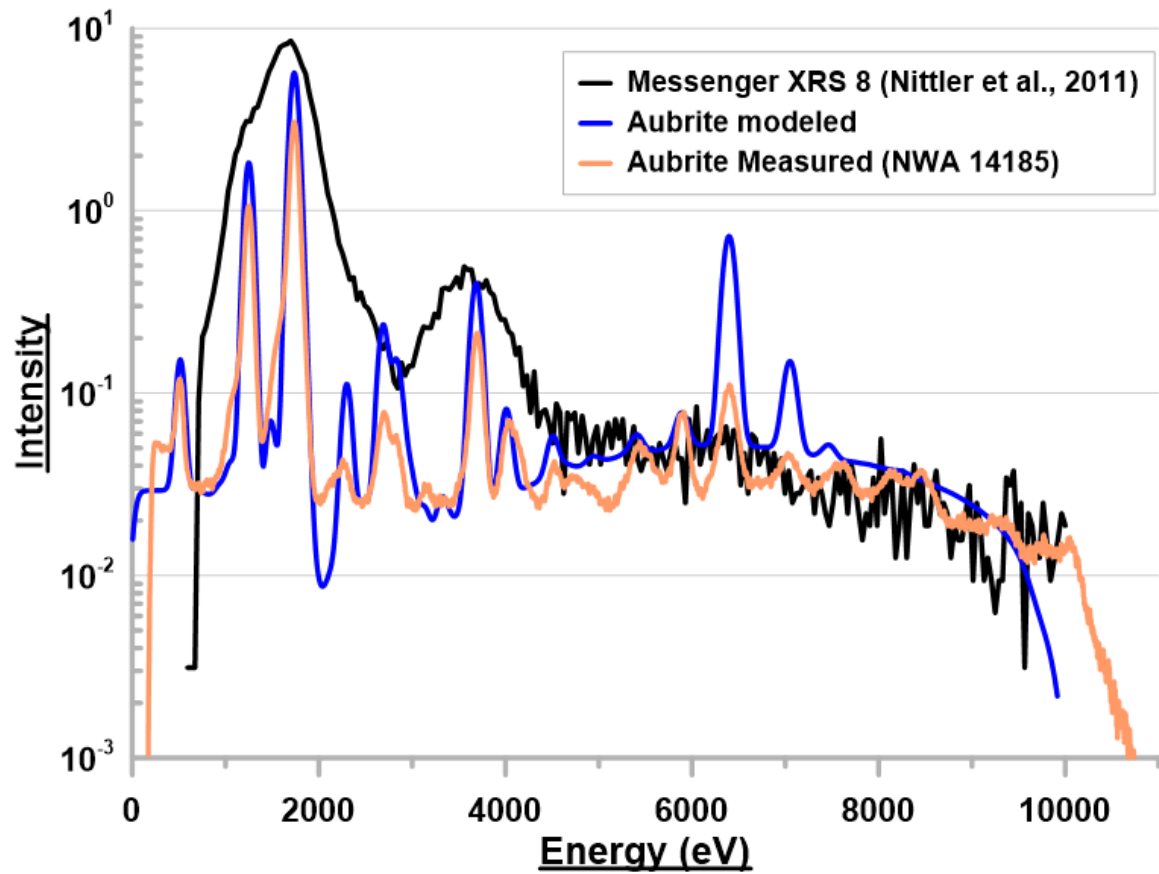
## Exploring Mercury's Diverse Surface Compositions Using the Ground Reference Facility (GREF)

J. A. Cartwright<sup>1,2</sup>, S. T. Lindsay<sup>2</sup>, T. L. Barry<sup>3</sup>, G. Hall<sup>2</sup>, A. R. D. Fox<sup>2</sup>, A. Martindale<sup>2</sup>, and E. J. Bunce<sup>1,2</sup>.

<sup>1</sup>*Institute for Space, University of Leicester, Leicester, UK;* <sup>2</sup>*School of Physics and Astronomy, University of Leicester, Leicester, UK;* <sup>3</sup>*School of Geography, Geology and the Environment, University of Leicester, UK.*

As the least explored (and smallest) rocky planet in the Solar System, Mercury's surface composition is not well characterised, while its apparent complex history is of great importance for understanding planet formation and planetary migration models. NASA's MESSENGER mission (2011-2015) revealed unexpected surface compositional variability, with evidence for distinct geologic terranes, unusual regions enriched in moderately volatile elements and clues to reducing formation conditions in the form of low iron concentrations coupled with high sulphur and carbon contents (e.g., Peplowski et al., 2019 JGR; McCoy et al., 2018 Mercury: The View after MESSENGER, *book*). The ESA/JAXA BepiColombo Mission, scheduled to arrive at Mercury in 2025, has the potential to obtain improved compositional data for the surface. Specifically, the Mercury Imaging X-ray Spectrometer (MIXS), designed and built at the University of Leicester (UoL), has the capability to acquire higher resolution surface elemental composition data (max. achievable resolution ~ 10 km vs. ~ 200 km non-imaging field of view for MESSENGER). MIXS uses X-Ray Fluorescence (XRF), generated by interaction of solar-coronal X-rays and charged particles with the Mercurian regolith, releasing X-rays characteristic of elemental compositions (Bunce et al., 2020, SSR). Importantly, the MIXS instrument features new technology including optics and a novel detector (e.g., Bunce et al., 2020, SSR). To gain the highest science output, ground-truthing the spectra gathered by MIXS with those gathered *in the lab* will allow for the best interpretation of Mercurian terranes and features.

We are using the MIXS Ground Reference Facility (GREF), which is equipped with flight-like MIXS instrumentation including a detector identical to the flight model, and is based at UoL (Space Park Leicester). With GREF, we are applying XRF to Mercurian analogues including meteorites (e.g., aubrites, enstatite chondrites), terrestrial samples (e.g., boninites, komatiites) alongside synthesised materials that share properties with Mercury, to establish a sample library to allow for direct comparison with incoming mission data from MIXS. In particular, we are looking to explore the volatile enrichments on the surface, while also establishing the effects of topography and space weathering. We will introduce the facility, present our preliminary results, and compare with modelled spectral data for expected compositions. We will also discuss our plans to further investigate compositional and textural features on Mercury.



**Figure 1:** Plot showing diagnostic X-ray energy vs. Intensity. Example MESSENGER data (Nittler et al., 2011, Science), Aubrite modelled data based on overall compositions (Keil et al., 2010, Geochemistry) on GREF, Aubrite measured for Northwest Africa (NWA) 14185 on GREF.

## The hyperspectral remote sensing laboratory at CRPG Nancy, France

Jessica Flahaut<sup>1</sup>, Clarisse Peignaux<sup>1</sup>, Marie Barthez<sup>1</sup>, Gen Ito<sup>1</sup>, Mélissa Martinot<sup>1</sup>

<sup>1</sup> Centre de Recherches Péetrographiques et Géoehimiques (CRPG), UMR7358, CNRS/Université de Lorraine, 15 rue Notre-Dame des Pauvres, 54500 Vandœuvre-lès-Nancy, France.

Equipped with a point spectrometer (ASD Fieldspec 4) and two hyperspectral cameras (Hyspex VNIR 3000N & SWIR 640) spanning the visible near-infrared (VNIR) and short wavelength infrared (SWIR) ranges, the CRPG hyperspectral remote sensing laboratory is dedicated to reflectance spectroscopy analyses (<https://crpg.univ-lorraine.fr/en/hyperspectral-remote-sensing-en/>). Whereas the Fieldspec 4 provides single spectrum at a spectral resolution of 3-10 nm between 350 and 2500 nm, the Hyspex cameras cover the 400-1000 nm and 960-2500 nm ranges at 2 nm and 4.38 nm/channel respectively. With an adjustable set of lenses/fields of view, these instruments can be used both in the field and in the laboratory, where the high spatial resolutions of the cameras (up to 15 microns/px in the VNIR, 32 microns/px in the SWIR) allow for detailed grain to grain mineralogical analyses.

Although these instruments have numerous possible applications, at the CRPG they are mainly used for planetary analogue studies (ground-truthing of remote sensing data in the field, building new reference spectral libraries for Mars, the Moon & Mercury). Rock slabs, cores, soils, thin sections, powders have all been measured using various setups and accessories in ambient T conditions. Acquired rock and powder spectra are processed with state-of-the-art, dedicated software (ENVI, BREEZE/EVINCE, Mineral Recognizer). Two calculation servers and 150 TB of allocated storage are available for associated data processing and archiving. In addition, acquired spectra are publicly shared on the CRPG database, Mirabelle, hosted on S-SHADE (<https://www.sshade.eu/db/mirabelle>).

The present contribution will give an overview of the available instrumentation and of previous/ongoing applications for various projects, e.g., the ESA-ESRIC lunar resource challenge (<https://www.spaceresourceschallenge.esa.int/>), the Mars-Spec ANR project (<https://crpg.univ-lorraine.fr/en/anr-mars-spec-en/>).



**Figure 1:** The hyperspectral remote sensing laboratory at CRPG Nancy.

## High-*PT* experimental facilities for planetary materials

Sieber, M. J.<sup>1,2</sup>, Morgenroth, W.<sup>1</sup> and Wilke, M.<sup>1</sup>

<sup>1</sup> *Institute of Geosciences, University of Potsdam*, <sup>2</sup> *GFZ German Research Centre for Geosciences*

The high-pressure and high-temperature (high-*PT*) experimental facilities at the University of Potsdam, Institute of Geosciences, are suitable to advance the understanding of Mercury's structure, geology, magnetosphere, and exosphere, particularly by constraining properties of related materials. By replicating extreme environments characteristic of this planet, our facilities enable the simulation and exploration of specific planetary conditions and processes. Our high-*PT* laboratories are equipped with a 1-atm gas mixing furnace, internally heated gas-pressure vessels, and laser-heated diamond anvil cells and are complemented by facilities at the GFZ Potsdam in a collaborative manner. We further utilize synchrotron radiation for in-situ investigations in large-volume presses and in diamond anvil cells at DESY, Hamburg and ESRF, Grenoble.

We conduct comprehensive investigations of the physical and chemical conditions of various materials, including crystalline solids, melts, fluids, and gases, and their interactions under both ambient and extreme pressure conditions. These studies are crucial for deciphering the dynamic processes and conditions prevalent during planetary formation and evolution.

For instance, experiments at 1 atmosphere under controlled oxygen fugacity allow us to examine the behavior of multivalent elements, such as tellurium, during evaporation processes. These conditions provide insights into the condensation and volatilization cycles that influence volatile element distribution in magmatic and hydrothermal systems on rocky planets. Additionally, we determine melting conditions, trace element distributions, and melt (glass) structures.

We also investigate the Fe-spin transition as a function of pressure, a critical phenomenon that impacts the physical and chemical properties of planetary cores and mantles. Constraining the conditions of this transition aids in modeling the internal structure and evolution of Mercury and similar planetary bodies.

Moreover, we are able to synthesize reference materials and standards essential for accurate and reproducible scientific measurements. By producing these materials under controlled high-*PT* and chemical conditions, we ensure the reliability of experimental data and enhance the precision of many analytical techniques that rely on calibration to reference samples.

Overall, our high-*PT* experimental facilities provide an invaluable platform for studying the complex processes that govern planetary formation and evolution. Through meticulous control of experimental parameters and advanced analytical capabilities, we may contribute to a deeper understanding of Mercury and other rocky planets, shedding light on the complex interplay between solid, liquid, and gaseous phases under extreme conditions.

## **The Spectral Characterization of the Ribbeck Aubrite as Mercury Analog : The Effect of Heating in Preparation for MERTIS Flyby 5.**

A. Van den Neucker<sup>1</sup>, J. Helbert<sup>1</sup>, O. Barraud<sup>1</sup>, M. D'Amore<sup>1</sup>, N. Verma<sup>1</sup>, S. Adeli<sup>1</sup>, G. Alemanno<sup>1</sup>, A. Maturilli<sup>1</sup>, C. Hamann<sup>2</sup>, L. Hecht<sup>2</sup>, A. Greshake<sup>2</sup>, H. Hiesinger<sup>3</sup>

<sup>1</sup>German Aerospace Center (DLR) – Institute of Planetary Research, Rutherfordstrasse 2, 12489 Berlin, Germany.

<sup>2</sup>Museum für Naturkunde - Invalidenstraße 43, 10115 Berlin, Germany.

<sup>3</sup>Institut für Planetologie (IfP), Universität Münster, Wilhelm-KlemmStr. 10, 48149 Münster, Germany.

### **Introduction**

The MErcury Radiometer and Thermal Infrared Spectrometer (MERTIS) of the BepiColombo mission aims to characterize Mercury's surface mineralogy by measuring its spectral emissivity with a spatial resolution of at least 500 meters per pixel. On the 2nd of December 2024, the spacecraft will perform its 5th FlyBy along Mercury, allowing MERTIS to operate and perform surface measurements on a large area of the planet. To prepare for the upcoming remote sensing measurements of MERTIS, analogue materials to simulate the expected mineralogy within our observed region were selected and analyzed in laboratory. For this study Aubrite samples of the recent January 21st 2024 meteorite fall BX-1 "Ribbeck" was chosen as analogue material, as this enstatite-rich material is highly reduced such as expected for Mercury. Microscopical XRF measurements and reflectance bulk spectra were acquired before and after heating Ribbeck at Mercury temperatures (450 °C) to see the effect of heating on this material. These results will be used as a baseline for interpreting the lab and remote sensing emissivity spectra once the BepiColombo spacecraft reaches Mercury and MERTIS can operate.

### **Results**

Point-localized and bulk IR reflectance measurements on the Ribbeck hand-specimen (Fig.1) revealed distinct absorption features around 2.7 and 5  $\mu\text{m}$  and emission bands between 8-13  $\mu\text{m}$ . The data showed that the absorption bands in the MIR are significantly attenuated in the fusion crust compared to the freshly exposed interior, including the strong reduction of the OH-stretching band. The reduced mineralogy of nearly FeO-free primary minerals (e.g. enstatite), and abundance in exotic sulfides (e.g. alabandite) characteristic of the Ribbeck aubrite meteorite, can be expected on other planetary bodies such as Mercury. The XRF geochemical maps revealed that the heated sample shows an overall reduction in sulfides, suggesting that some wt% of S might be outgassed during the heating process.

The MERTIS instrument is designed to measure Mercury's surface composition over a wavelength range of 7 - 14  $\mu\text{m}$ . Most of the absorption features of the meteorite Ribbeck fall into the MERTIS spectral range, including that the low iron content of Mercury will not be an issue for MERTIS to map the planet's surface mineralogy. MERTIS will therefore help us to clarify the possible link between the composition and geochemistry of Mercury and the Aubrites.



**Figure 1:** Ribbeck meteorite sample with exposed interior that was used for the non-destructive laboratory measurements.

## **Phobos' Origin: A Ground-Truthing Investigation through Laboratory Analysis of Analogues and Meteorites.**

E. Branagan-Harris<sup>1,2</sup>, N. E. Bowles<sup>2</sup>, A. J. King<sup>1</sup>, K. A. Shirley<sup>2</sup>, H. C. Bates<sup>1</sup>, S. S. Russell<sup>1</sup>

<sup>1</sup>*Natural History Museum, London, UK*, <sup>2</sup>*Atmospheric, Oceanic and Planetary Physics, University of Oxford, Oxford, UK*.

**Introduction:** The origin of Mars' moon Phobos is unknown. Two theories prevail: Phobos is a by-product of a collision between an asteroid and Mars, which resulted in ejected material forming Phobos. Alternatively, Phobos is a captured asteroid. JAXA's Martian Moons eXploration (MMX) mission is set to visit Phobos and then return samples from the surface to Earth in 2031. The characterisation of these samples will determine the origin of Phobos.

To ground-truth remote observations of Phobos, we have used X-ray diffraction (XRD) and Fourier transform infrared (FTIR) reflectance spectroscopy to characterise the bulk mineralogy and IR spectral properties of an analogue and carbonaceous chondrites, the composition of which could be indicative of a captured asteroid, and shock darkened ordinary chondrites that could represent a collisional formation. By acquiring XRD and IR data from the same material, mineral abundances can be directly correlated with features in reflectance spectra. When MMX reaches Phobos, meteorite data collected in the laboratory will play a crucial role in interpreting the mineralogy and composition of its surface materials.

**Methods:** We have characterised the mineralogy and spectral properties of 15 meteorites including Tarda (C2-ung), and a Tagish Lake (C2-ung) based analogue created by the University of Tokyo, known as UTPS-TB.

Diffuse reflectance spectra (1.7 - 50  $\mu\text{m}$ ) of powdered sample were collected using a Bruker VERTEX 70V FTIR spectrometer. The samples were measured under a vacuum to reduce terrestrial atmospheric contributions.

XRD patterns of the same powders were collected using an INEL X-ray diffractometer with a position-sensitive detector. Powdered samples were measured, and measurements of standard minerals were collected and compared with sample patterns to identify minerals and quantify their abundance in the sample (e.g. Cressey et al. (1996), *Powder diffraction*).

**Results & Discussion:** Ordinary chondrites have a higher reflectance than carbonaceous chondrites in the near infrared. Their reflectance spectra show a 3  $\mu\text{m}$  band related to OH/H<sub>2</sub>O, more pronounced in carbonaceous chondrites. Carbonaceous chondrites also display a 6  $\mu\text{m}$  feature from carbonates, especially in the analogue UTPS-TB, which is brighter with stronger features. The Christiansen and transparency features vary with composition: in carbonaceous chondrites, they relate to phyllosilicates; in ordinary chondrites, to olivine and pyroxene. Overall, carbonaceous chondrites exhibit phyllosilicate and carbonate features, while ordinary chondrites show olivine and pyroxene features. Phobos' spectrum resembles Tagish Lake and carbonaceous chondrites, with Tarda and carbonaceous chondrites matching Phobos' near-IR spectra (e.g. Fraeman et al. (2014), *Icarus*).



## **Spectroscopic and minero-petrological investigation of boninites from Cyprus as potential analogues of Mercury lavas**

Landi, A.I.<sup>1,4</sup>, Carli, C.<sup>2</sup>, Capaccioni, F.<sup>2</sup>, Maturilli, A.<sup>3</sup>, Helbert, J.<sup>3</sup>, Alemanno, G.<sup>3</sup> and Pratesi, G.<sup>4</sup>

<sup>1</sup>*Università degli Studi di Trento, Via Sommarive, 14, 38123 Trento, Italy*

<sup>2</sup>*INAF-IAPS Via del Fosso del Cavaliere, 100, Tor Vergata 00133 Roma, Italy*

<sup>3</sup>*German Aerospace Center (DLR), Rutherfordstraße 2, 12489 Berlin, Germany*

<sup>4</sup>*Dipartimento di Scienze della Terra, Università degli Studi di Firenze, Via G. La Pira, 4, 50121 Firenze, Italy*

Although the formation conditions differ significantly in terms of oxygen fugacity, water contribution, and iron abundance in the source region, terrestrial boninites and komatiites are considered promising analogues for Mercury's lavas based on data from the MESSENGER Mission. The aim of this study is to compare terrestrial boninites with Mercury lavas, considering spectroscopic, petrological, and mineralogical characteristics.

We are studying samples coming from three distinct locations within the Troodos massif, Cyprus island. We selected representative samples for each locality and performed X-ray Fluorescence (XRF), scanning electron microscopy (SEM), electron microprobe (EPMA) analysis and reflectance spectroscopy in the spectral ranges covered by the VIHI imaging spectrometer (0.4-2.0  $\mu\text{m}$ ) and the MERTIS spectrometer (7-14  $\mu\text{m}$ ) onboard the ESA's BepiColombo mission.

XRF bulk composition analysis provided average values of major elements that closely match the average compositions of Mercury's geochemical terranes; the only major difference is the higher FeO content, as expected. The spectroscopic and compositional differences observed between the samples reflect their different mineralogy. VNIR spectra show the main absorption band at  $\sim 1 \mu\text{m}$  which is associated with olivine and pyroxene and some samples show also smaller but clear absorption features due to hydrated alteration phases.

Taking into account the differences in the acquisition methods and in the objects under investigation, we conducted a preliminary comparison between laboratory reflectance spectra of boninite samples and MASCS/MESSENGER Mercury data. The comparison will be improved with ongoing measurements including VNIR reflectance analysis at various acquisition angles and on various grain sizes and TIR emittance spectroscopy studies. These new data, together with minero-petrologic characterization, could also support future comparisons with mineralogical data expected from SIMBIO-SYS/VIHI and MERTIS spectrometers. Moreover, it would be interesting to go deeper into the analysis of the samples with analytical techniques similar to the instruments (MIXS and MGNS) on board BepiColombo mission which will measure elemental abundances on Mercury's surface. That could help understanding how to correlate the reflectance and emittance spectroscopy information with the information from X-ray and gamma-ray and neutron spectrometers.

## Basaltic glasses in the lower mantle: trace elements as markers of local structure changes

Kovalskii, G.<sup>1</sup>, Rosa, A.D.<sup>2</sup>, Mathon, O.<sup>2</sup>, Morgenroth, W.<sup>1</sup>, Morard, G.<sup>3</sup>, Pennacchioni, L.<sup>1</sup>, Wilke, M.<sup>1</sup>

<sup>1</sup> *Institut für Geowissenschaften, Universität Potsdam, 14476 Potsdam, Potsdam, Germany.* <sup>2</sup> *European Synchrotron Radiation Facility, ESRF, Grenoble France.* <sup>3</sup> *Insitut de Minéralogie, de Physique, des Matériaux, et de Cosmochinie, IMPMC, Paris, 75005, France.*

The geological structures of Earth and Earth-group planets (Mercury, Venus, Mars) share many similarities, such as solid surfaces and internal structures, consisting of a crust, mantle, and a core primarily composed of iron and nickel. Understanding the internal structures helps us grasping planetary evolution and geological processes in the solar system. Silicate melts in these planets contribute to regulating global changes in heat and material over geological timescales and insight on magmas is crucial for modeling chemical differentiation, cooling history, petrogenesis, and ore genesis. Defining the conditions under which silicate melts form and how distribution of elements works at extreme pressure and temperature aids in understanding processes in the deeper parts of planetary bodies, where direct access is unavailable. (Elkins-Tanton LT (2012), AREPS).

An experimental study was conducted to understand the local structure of minor cations in silicate glasses and melts under extreme conditions of the lower mantle. This experiment was the first to use the newly installed laser-heating setup dedicated to x-ray absorption spectroscopy (EXAFS and XANES) at extreme conditions at ID24 (ESRF). A series of spectra was collected for yttrium in fluorescence mode for a simplified synthetic Ab-Di glass compressed in a diamond anvil cell (Krstulović M et al. (2021), Chemical Geology) up to 117 GPa (2500 km).

Initial analysis of XANES spectra at different pressures for yttrium showed a shift of the first EXAFS peak (17080 eV) to higher energies with increasing pressure, indicating a decrease in the Y-O distance. Starting from 45 GPa, an increase in pre-edge intensity indicates a change in coordination towards non-centrosymmetric symmetry. Further analyses by fitting the EXAFS revealed Y-O distances decreasing smoothly from 2.202 Å at 1.7 GPa to 2.096 Å at 117.5 GPa. The strongest changes in Y-O distance corresponded to the pressure-ranges from 16 to 45 GPa and from 75 to 100 GPa, supporting the qualitative assignment of structural changes based on inspection of XANES and pre-edge region. The pressure-induced densification, associated with a decrease in Y-O distance and an increase in coordination number likely impacts diffusivity of Y and its chemical distribution between melt and crystals.

In addition to cold-compression runs, initial attempts of in-situ high-pressure high-temperature XANES/EXAFS at the Sr K-edge using laser-heating were performed. Successful runs at 2, 5, and 9 GPa provided insight into structural differences for strontium between the glass at room temperature and the melt at 3500 K.

Session II

# **Mercury's volatiles**

## High-temperature Mercury experiments at MPS

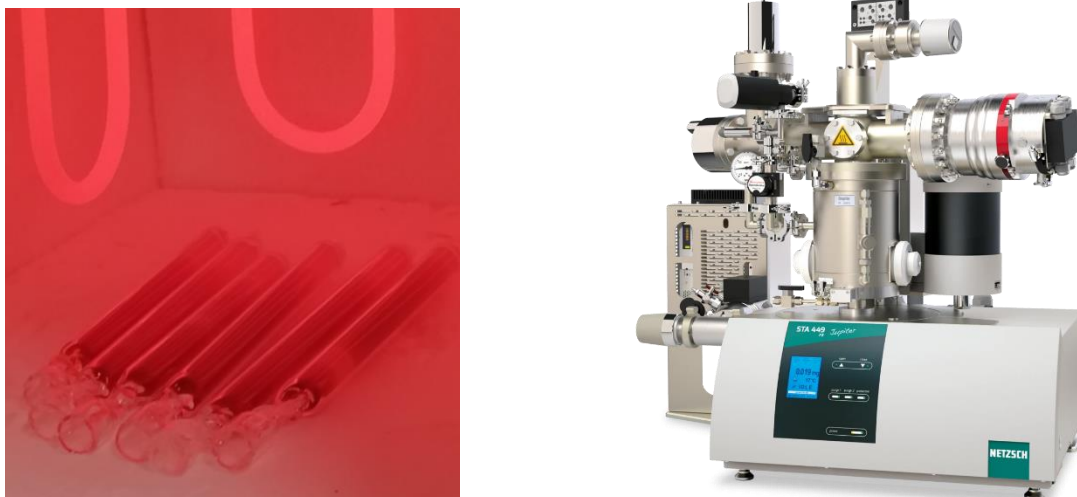
C. J. Renggli<sup>1</sup>, R. Erftemeijer<sup>1</sup>, M. Nieuwenhuis<sup>1</sup>, and T. Kleine<sup>1</sup>.

<sup>1</sup> Max Planck Institute for Solar System Research, Justus-von-Liebig-Weg 3, 37077 Göttingen, Germany

Mercury's surface has a high abundance of S with up to 4 wt.%. At highly reducing conditions S is proposed to occur in sulfides such as CaS (oldhamite) and MgS (ninningerite) [1]. The processes that resulted in the formation of these sulfides on Mercury remain debated and pose a key question for the BepiColombo mission [2,3]. A good understanding of these phases and detailed laboratory characterization is therefore an important experimental challenge. We use evacuated SiO<sub>2</sub> glass ampoules (Figure 1) to synthesize sulfides with controlled compositions for mineralogical and spectroscopic studies [e.g. 4,5]. Here, we will present the experimental approach and examples of sulfide investigation studies.

Hollows, currently active geological features on Mercury discovered by MESSENGER [6] will be an important target for investigation by BepiColombo. The formation of hollows may involve the loss or decomposition of volatile-bearing compounds such as sulfides [7]. At the Max Planck Institute for Solar System Research we are setting up a new experimental facility that will allow in-situ experiments on the phase stability of volatile-bearing compounds at Mercury dayside conditions (high vacuum, 430 °C). A NETZSCH F3 Jupiter scanning thermal analyzer with a graphite skimmer furnace and a coupled quadrupole mass spectrometer is expected to be delivered in October this year (Figure 1). With the capability to reach temperatures up to 2000 °C we further plan experiments on the Mercury magma ocean and the composition of the primordial atmosphere to better constrain the planets volatile inventory. In this presentation we will introduce the experimental possibilities to enable potential collaborations within the community.

[1] McCoy et al. (2018) Mercury, View after MESSENGER. [2] Namur et al. (2016) EPSL. [3] Renggli et al. (2022) EPSL. [4] Renggli et al. (2023) JGR Planets [5] Reitze et al. (2024) JGR Planets. [6] Thomas et al. (2014) Icarus. [7] Barraud et al. (2023) Sci. Adv.



**Figure 1:** High-temperature experiments in sealed and evacuated SiO<sub>2</sub>-glass ampoules (left). NETZSCH STA F3 Jupiter with skimmer furnace and coupled quadrupole mass spectrometer arriving at MPS in October 2024 for experiments in controlled atmosphere or at high vacuum at up to 2000 °C (right).

## Investigating Mercury from Core to Crust Through Multidisciplinary Approaches

Brendan A. Anzures<sup>1</sup>, Francis M. McCubbin<sup>2</sup>, Kayla Iacovino<sup>1</sup> and Megan D. Mouser<sup>1</sup>.

<sup>1</sup> *Jacobs, NASA Johnson Space Center.* <sup>2</sup> *ARES, NASA Johnson Space Center.*

At NASA Johnson Space Center (JSC), we have an experienced team and facilities that lead investigations into Mercury, exploring its deep interior to surface. We broadly explore Mercury's igneous processes through experimental, analytical, and modeling techniques, with projects ranging from magmatism, volcanism, differentiation, to space weathering. Specifically, we explore these processes through silicate melt speciation, metal-sulfide-silicate element partitioning, chemical detection limits through remote sensing reflectance/emissivity spectra, explosive volcanism experiments and modeling, and viscosity measurements. The central questions we work on are "What happens when a planet forms in an oxygen-poor and sulfur-rich environment?" and "Why do volcanoes erupt?"

Our team has abundant expertise in both producing experimental Mercury analogs and studying reduced meteorites including enstatite chondrites and aubrites, utilizing them all as analogs for Mercurian geochemistry and petrologic processes. One of the current projects is investigating the solubility of S, Cl, C, and Fe in Mercurian magmas which aims to explore differences in high- to low-pressure, and high-temperature outgassing and condensation reactions. This work would contribute to understanding Mercury's abundant pyroclastic deposits that will be measured by BepiColombo, providing important insights into the volcanic processes that occurred on Mercury.

Our experimental capabilities simulate Mercury's interior and surface evolution primarily through experimental petrology with evacuated silica tube experiments (gradient of 25 up to 1500°C), box furnaces (up to 1700°C), 4 1-bar gas mixing furnaces (fO<sub>2</sub>'s down to IW-2 and up to 1500°C), 3 QUICKpress piston cylinders (0.3-3 GPa and up to 1900°C), and a 880-ton Rockland Research multi-anvil (3-30 GPa and up to 2400°C). In addition, JSC can study dynamic processes such as impact cratering and shock metamorphism with three accelerators: the vertical gun, light gas gun, and flat plate accelerator. These accelerators operate under vacuum and can achieve dynamic stresses up to 7 km/s and over 70 GPa. Within the next year we will also have a laser levitation furnace (0.1 to 1 bar; up to 3000 °C) and sub-bar furnace (0.1 mbar to 1 bar; up to 1800 °C) with an RGA quadrupole mass spectrometer to measure 1-200 amu gas abundances. JSC also has state-of-the-art analytical equipment including EPMA, SEM, FIB, TEM, NanoSIMS, XRF, FTIR, XRD, Raman, LA-ICP-MS, and furnaces hooked up to RGA's along with next generation sample preparation instrumentation with an ion polishing system and a cryomill. These facilities enable coordinated experiments and analyses from the macro to nano-scale of Mercury analogs and processes.

## Insights into Mercury's melt structure from a multidimensional analytical approach

Emily L. Fischer<sup>1</sup>, Stephen W. Parman<sup>1</sup>, George D. Cody<sup>2</sup>, and Brendan A. Anzures<sup>3</sup>

<sup>1</sup>*Department of Earth, Environmental, and Planetary Sciences, Brown University, Providence, RI* <sup>2</sup>*Earth and Planets Laboratory, Carnegie Institution for Science, Washington, D.C.* <sup>3</sup>*Jacobs, NASA Johnson Space Center, Houston, TX*

Mercurian lavas have high sulfur contents due to their formation at low oxygen fugacities (Nittler et al., 2011, *Science*). The high sulfur contents decrease melt viscosity (Mouser et al., 2021, *JGR Planets*), though the mechanism for this is unclear. Recent NMR analyses (Pommier et al., 2023, *GCA*) indicates abundant S-Si bonds in reduced basaltic glasses, indicating that changes in the Si bonding environment could be responsible for the viscosity changes. To explore this further, a series of Mercurian glasses were synthesized at 1 GPa, with S contents ranging from 0-6 wt% and oxygen fugacities from IW-4 to IW-6. Experimental glasses were analyzed by Si K-edge X-ray Absorption Near Edge Structure (XANES) spectroscopy and <sup>29</sup>Si Nuclear Magnetic Resonance (NMR). Ongoing analyses will include Raman and Fourier Transform Infrared (FTIR).

The <sup>29</sup>Si NMR analyses suggest the presence of Si-S bonds in the melts, in agreement with the results of Pommier et al. (2023). The Si K-edge XANES spectra show a decrease in K-edge position of 0.4 to 0.6 eV from terrestrial basalts (at ~IW+3) to the experimental melts at IW-4 to IW-6. This shift suggests a moderate (<20 mole %) amount of Si has shifted to lower valence states. The melts contain 0-6 wt% S, so if the K-edge shifts are the results of Si-S bonding, it implies that the majority of the S in the melts is bonded to Si. However, S K-edge XANES analyses indicates that much of the S is also bonded with Mg and Ca at these low oxygen fugacities (Anzures et al, 2020, *GCA*). The overall implication is that non-bridging Si-S-(Mg,Ca) bonds are prevalent in the reduced melts, consistent with the decrease in viscosity of the melts being due to melt depolymerization.

Future analyses will explore a wider range of fO<sub>2</sub> and S contents. To explore possible correlations of melt structural changes with volatile contents, the experimental glasses will also be analyzed by Raman and FTIR.

Overall, our results suggest that dissolution of S into the melts at low fO<sub>2</sub> is accomplished through bonding with Si, and is accompanied by significant structural changes that lower melt viscosity (Mouser et al., 2021). Lower melt viscosities will affect many aspects of Mercury's evolution, from magma ocean dynamics, to melt migration in the mantle, to eruption dynamics and degassing.

Session III

# **Challenges of observing Mercury**

## Spectral Characterization of Solar System Airless Bodies Analogues

K. L. Donaldson Hanna<sup>1</sup>, A. C. Martin<sup>1</sup>, L. Rosello Del Valle<sup>1</sup>, A. N. Shackelford<sup>1</sup> and P. Tripathi<sup>1</sup>.

<sup>1</sup> *Department of Physics, University of Central Florida, Orlando, FL, USA.*

To best interpret spectral remote sensing observations of Mercury and other Solar System airless bodies (e.g., the Moon and asteroids), laboratory measurements of well-characterized analogue sample are needed. Research at the University of Central Florida (UCF) focuses on understanding how airless bodies like Mercury formed and evolved into what we observe today, specifically what surface processes have altered the crust and how have those surface processes modified the spectral signature of those crustal materials. Laboratory facilities include three spectrometers: (1) a Bruker Vertex 70V Fourier Transform Infrared (FTIR) spectrometer, (2) a Thermo Nicolet iS50 FTIR spectrometer, and (3) an ASD LabSpec4 High-Res spectrometer. Our Bruker FTIR spectrometer has the capability of measuring hemispherical and diffuse reflectance and emissivity across the 5 – 50  $\mu\text{m}$  (2000 – 200  $\text{cm}^{-1}$ ) with a wide range beamsplitter and DLaTGS detector, and using (a) a Bruker Integrating Sphere accessory placed in the FTIR sample compartment, (b) a SpecAc Diffuse Reflectance accessory placed in the FTIR sample compartment, and (c) a bespoke environment chamber capable of simulating the near surface conditions of Solar System airless bodies, which is attached to the emission port of the FTIR. Our Thermo Nicolet spectrometer has the capability of measuring diffuse reflectance across the  $\sim 0.4 - 25 \mu\text{m}$  (25,000 – 400  $\text{cm}^{-1}$ ) using a combination of beamsplitters and detectors, and a Pike EasiDiff Diffuse Reflectance accessory placed in the sample compartment of the FTIR. Our LabSpec4 High-Res spectrometer has the capability of measuring reflectance across the 0.35 – 2.5  $\mu\text{m}$  range using a contact probe, a muglight, or a small diameter reflectance probe (2 mm spot size). Our analogue sample catalog includes synthetic minerals with compositions relevant to Mercury, returned Apollo regolith samples from each of the Apollo landing sites, synthetic Apollo glass samples, carbonaceous chondrite meteorites, terrestrial minerals with compositions relevant to the Moon and asteroids, and physical mixtures of minerals with potassium bromide (KBR) to simulate high-porosity regolith samples. Using these lab facilities and analogue samples, our research has focused on characterizing changes to spectra due to: (1) the near surface thermal gradients, (2) particle size, porosity, and albedo, and (3) space weathering processes.



## Laboratory studies to validate an indirect method of sensing carbon enrichments in the LRM with MIXS

A.R.D. Fox<sup>1</sup>, A. Martindale<sup>1</sup>, T.L Barry<sup>1</sup>, S.T Lindsay<sup>1</sup>,  
J.C. Bridges<sup>1</sup>, E.J. Bunce<sup>1</sup>, B. Charlier<sup>2</sup>, G.P Hall<sup>1</sup>, O. Namur<sup>3</sup> and T. Tikkanen<sup>1</sup>

<sup>1</sup>University of Leicester (UK). <sup>2</sup>University of Liège (Belgium). <sup>3</sup>KU Leuven (Belgium)

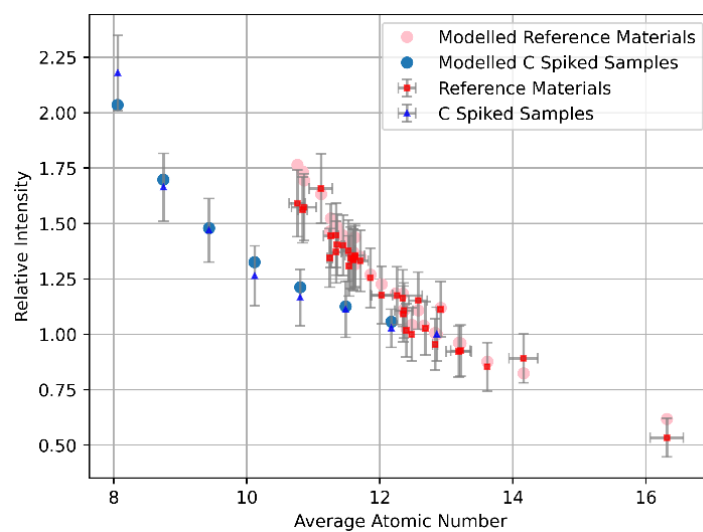
Making spatially resolved observations of carbon on Mercury's surface is of great scientific importance in the context of Mercury's Low Reflectance Material (LRM) [Rothery+ 2020, Space Sci Rev]. This measurement will be extremely difficult to perform with BepiColombo's science payload. We present and examine the plausibility of an indirect sensing method with the Mercury Imaging X-ray Spectrometer (MIXS). We consider the changes in spectral background which are seen when observing areas of enriched carbon abundance, potentially allowing us to identify further supporting evidence for graphite as the dominant darkening phase in the LRM.

Low atomic number material scatters X-rays very efficiently and, if correlated with LRM, observations of this scatter increase could be interpreted as supporting evidence of carbon's presence. In order to test the effectiveness of this method, we carried out lab-based testing with the MIXS Ground Reference Facility which uses the MIXS Qualification Model detector, an X-ray source and rotating, multi-sample stage, all housed in a high-vacuum chamber. Under standardised conditions, we made observations of the scattered X-ray intensity from a catalogue of terrestrial reference materials and samples of graphite-spiked dolerite. We use a physical model to make predictions of these scatter intensities as observed in the laboratory system. Agreement has been found between the trends predicted by the model and those observed experimentally (Figure 1).

With validation of the physical plausibility of this method and validation of the model, we predict observations with MIXS from Mercury. We forward model different solar conditions that were recorded by the MESSENGER spacecraft [Nittler+ 2020, Icarus] to estimate the sensitivity to carbon that this method provides after given integration times. We consider different compositional terranes as reported by Peplowski+ 2019 [JGR: Planets]. Most extensively, we consider observations of the Rachmaninoff basin, which has been interpreted to be among the most carbon rich deposits on Mercury's surface [Klima+ 2016, Geophys Res Lett] and thus the target of greatest interest for this method.

With our laboratory verified model, we predict that resolving carbon enrichments, at the levels anticipated from MESSENGER results [Peplowski+ 2016, Nat GeoSci Lett], requires integration times of order hundreds of seconds even under extremely energetic solar flares. We propose targeted 'stare' observations, as are planned BepiColombo's extended mission, of LRM rich deposits including Rachmaninoff. These observations will require serendipitous solar activity during the observations, as was successfully observed by MESSENGER [Weider+ 2016, Geophys Res Lett].

**Figure 1:**



*Scattered X-ray intensities from experimental observations of reference materials (red squares) and graphite-spiked samples (blue triangles). Plotted against average atomic number of the sample and used to verify modelled predictions (circles).*

## Mid-Infrared Studies of Hermean Analogues at IRIS Labs, Universität Münster

Andreas Morlok<sup>1</sup>, Christian Renggli<sup>2</sup>, Stephan Klemme<sup>3</sup>, Alexander Sehlke<sup>4</sup>, Alan Whittington<sup>5</sup>, Bernard Charlier<sup>6</sup>, Olivier Namur<sup>7</sup>, Aleksandra N. Stojic<sup>1</sup>, Maximilian P. Reitze<sup>1</sup>, Iris Weber<sup>1</sup>, Harald Hiesinger<sup>1</sup>, Joern Helbert<sup>8</sup>

<sup>1</sup>Institut für Planetologie, Wilhelm-Klemm-Strasse 10, 48149, Germany <sup>2</sup>Max-Planck-Institut für Sonnensystemforschung, Justus-von-Liebig-Weg 3, 37077 Göttingen, Germany <sup>3</sup>Institut für Mineralogie, Corrensstrasse 24, 48149 Münster <sup>4</sup>NASA Ames Research Center, Moffett Field, CA 94035, USA <sup>5</sup>The University of Texas at San Antonio <sup>6</sup>University of Liege, Department of Geology, 4000 Sart-Tilman, Belgium <sup>7</sup>Department of Earth and Environmental Sciences, KU Leuven, 3001 Leuven <sup>8</sup>Institute for Planetary Research, DLR, Rutherfordstrasse 2, 12489 Berlin, Germany

The MERTIS (MERcury Radiometer and Thermal Infrared Spectrometer) is the mid-infrared instrument (7  $\mu\text{m}$ -14  $\mu\text{m}$ ) onboard of BepiColombo. For the interpretation of the expected data, we compile a database of mid-infrared spectra (All spectra together with further information are accessible via our database <http://bc-mertis-pi.uni-muenster.de/>) of a wide range of end-member minerals but also of analogues:

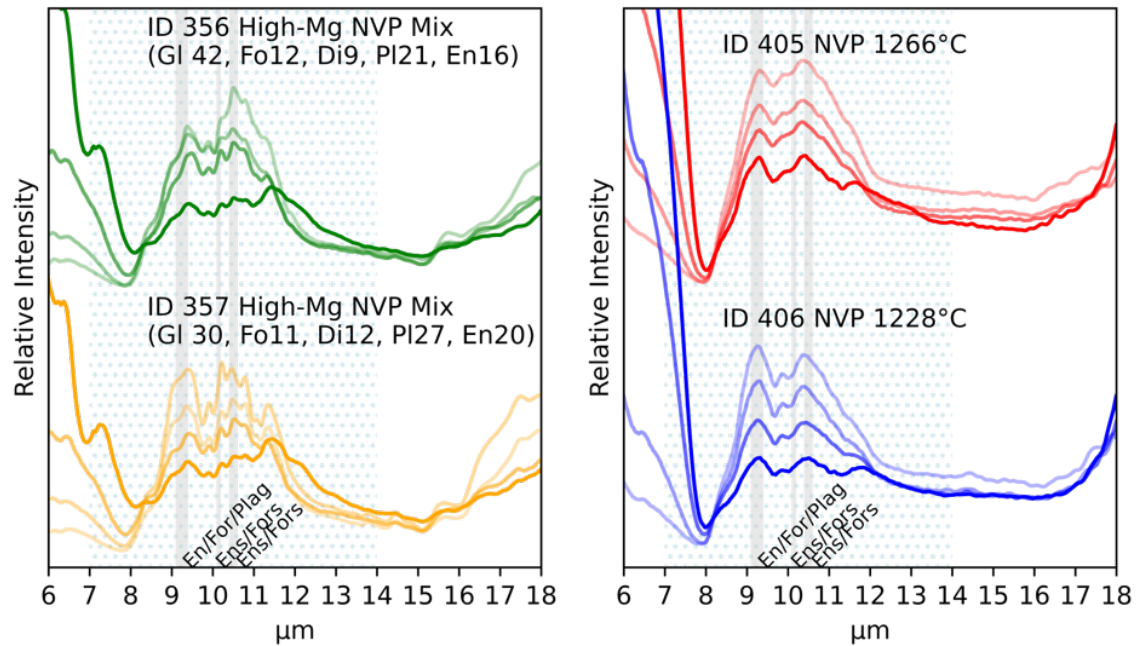
-Synthetic phases as basis for further mixtures of hermean analogues (e.g. Morlok et al. (2021) Icarus 361, 114363 and Morlok et al. (2023) Icarus 396, 115498), and study of run products from petrological experiments of the hermean surface (e.g. Sehlke and Whittington (2015) JGR Planets 120, 11; Namur and Charlier (2017) Nature Geoscience 10, 9-13; Morlok et al. (2023) Icarus 396, 115498; Morlok et al. (2024) Icarus 415, 116078) (Fig.1).

-Sample Processing: Space Weathering and impacts change the original material by the formation of glass and nanophase iron (e.g. Weber et al. (2023) Icarus 404, 115683; Stojic et al. (2023) Icarus 391, 115344), mineral/gas interaction will produce surface reaction layers (e.g. Renggli et al. (2023) JGR Planets 128, 12).

All these samples are first characterized in detail (SEM, EMPA, Raman) and then studied in the mid-infrared either as sieved bulk materials (0-25  $\mu\text{m}$ , 25-63  $\mu\text{m}$ , 63-125  $\mu\text{m}$ , and 125-250  $\mu\text{m}$ ) with a Bruker Vertex70v, or in-situ using a Hyperion 3000 FTIR Microscope.

Variations in spectra from samples with similar composition but formed under varying parameters and experimental settings (Fig.1) demonstrate the need for a systematic study of analogues. Samples exhibit varying abundances of glass, forsterite, pyroxene and feldspar.

We will present an overview and comparison of our work on hermean analogs in Münster in the last 12 years with several collaborators.



**Figure 1:** (NVP: Northern Volcanic Plains region on Mercury) Representative reflectance spectra of **(left)** a study of mineral/glass mixtures (Namur and Charlier (2017) *Nature Geoscience* 10, 9-13; Morlok et al. (2023) *Icarus* 396, 115498) and **(right)** hermean lava analogues of the NVP region (Sehlke and Whittington (2015) *JGR Planets* 120, 11; Morlok et al. (2024) *Icarus* 415, 116078) quenched at different temperatures. The spectral features show the range of pyroxene, forsterite and glass to be expected depending on formation history. Dotted region: spectral range of the MERTIS instrument. Saturated color: finest grain size fraction (0-25μm), bright color: coarsest fraction (125-250 μm). Grey shades areas: characteristic bands for enstatite (Ens), forsterite (For) and plagioclase (Plag).

## A database of emissivity spectra for Mercury analog materials measured in the TIR spectral range under Mercury conditions

Alessandro Maturilli<sup>1</sup>, Jörn Helbert<sup>1</sup>, Giulia Alemanno<sup>1</sup>, Aurelie Van der Neucker<sup>1</sup> and Oceane Barraud<sup>1</sup>.

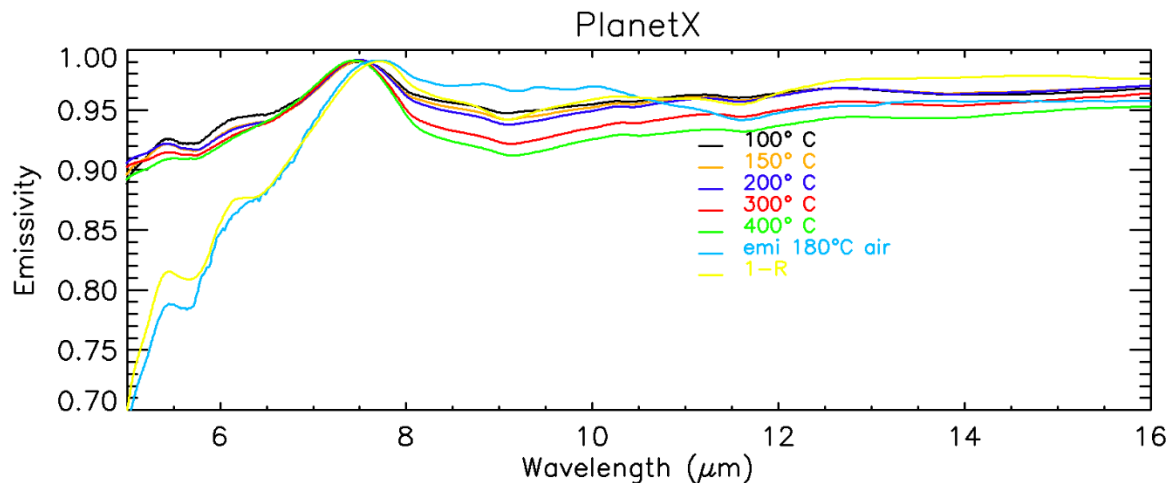
<sup>1</sup> Institute for Planetary Research, DLR, Rutherfordstrasse 2, 12489 Berlin, Germany.

The ESA-JAXA mission BepiColombo to the planet Mercury started its long road in 2018 and it's almost arrived at the innermost planet of our solar system: end of 2024 - beginning of 2025 the last 3 Swingbys (MSB#4-6) at Mercury will occur, then the spacecraft will be placed in orbit around Mercury and the nominal mission will start, at end of 2025.

One element of the MPO (Mercury Planetary Orbiter) is the MERTIS imaging spectrometer, that will record TIR spectra of the surface allowing to map its mineralogical composition and the identification of rock-forming minerals. Thanks to its deepspace view (routinely used for calibration at Mercury) MERTIS is able to observe the planet Mercury during the MSB#5, providing the first ever high spectral resolution spectra of the planet in the TIR spectral range (7-14  $\mu\text{m}$ ).

At the Planetary Spectroscopy Laboratory (PSL) in the Institute for Planetary Research of the German Aerospace Center (DLR) a facility allows to measure the emissivity of solid or powdered samples in vacuum and at high temperatures, typical of the daytime on the Mercury surface.

To prepare for the analysis of the MERTIS measured spectra, in the last 10 years we measured the emissivity spectra for a long list of analogs, all of them acquired in vacuum and for temperatures spanning the one on the surface of Mercury (typically, from 100/150°C to 400/450°C, step 100°C). The database contains many entries for plagioclases, olivines, orthopyroxenes, feldspathoids, sulfides, basalts, glasses, komatiites, lunar simulants, chondrites, grafite, and mixtures of some of those minerals/rocks.



**Figure 1:** Emissivity spectra of the PlanetX Mercury simulant (vacuum,  $T$  100-400°C) vs emissivity under purged air (at 180°C) vs bidirectional reflectance in the same spectral range.

Measuring Mercury analogs exactly under the same conditions of pressure and temperature as present on the surface of Mercury is crucial for the interpretation of MERTIS measured spectra. To illustrate this concept, Figure 1 shows the spectra of PlanetX, a mercury simulation mixture created at DLR. Typical effects shown in the picture are: a)  $1-R \approx E_a \neq E_v$  (where  $R$  is bidirectional reflectance,  $E_a$  is emissivity in air, and  $E_v$  is emissivity in vacuum), b) The maximum in emissivity (Christiansen

feature, CF) peaks at different wavelengths for  $E_v$  respect to 1-R and  $E_a$ , c) The CF position and shape in  $E_v$  are influenced from the sample surface temperature, a linear shift with T is usually observed.

## **The effect of bulk sample porosity on MIR spectra**

M.P. Reitze<sup>1</sup>, I. Weber<sup>1</sup>, A. Morlok<sup>1</sup>, H. Hiesinger<sup>1</sup>, K.E. Bauch<sup>1</sup>, J.-H. Paskert<sup>1</sup>, and N. Schmedemann<sup>1</sup>, J. Helbert<sup>2</sup>

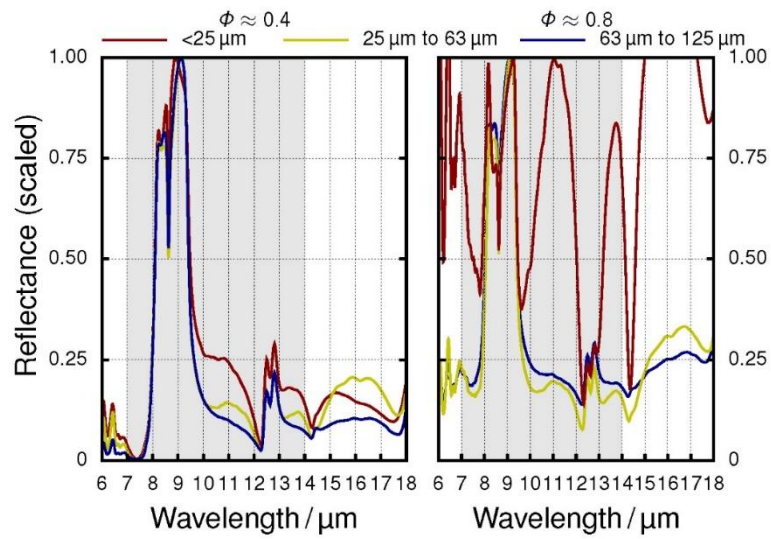
<sup>1</sup>*Institut für Planetologie, Wilhelm-Klemm-Str. 10, Universität Münster, 48149 Münster, Germany.*

<sup>2</sup>*Institute for Planetary Research, DLR, Rutherfordstr. 2, 12489 Berlin, Germany*

In the last years several studies investigated the effects of particle size and porosity on MIR spectra [e.g., Shirley & Glotch, 2018, JGR Planets, Izawa et al. 2021, Icarus, Martin et al. 2022, 2023, Icarus]. These questions are essential because the surface of planetary bodies without atmosphere is covered by regolith which properties affect remote sensing MIR spectra. However, even the porosity of the lunar regolith is unknown and could not be determined with the data gathered yet [e.g., Hapke 2016, Icarus]. On the other hand, some remote sensing data suggest very high porosities of the lunar or asteroidic regoliths, known as fairy castle structure [e.g., Ohtake et al., 2010, Space Science Reviews; Vernazza et al. 2012, Icarus; Hapke 2016, Icarus]. Therefore, the effect of the porosity on the MIR spectra is important for the upcoming MERTIS observations of Mercury.

It is well-known that a decreased grain size lead to stronger volume scattering, whereas an increased grain size lead to stronger surface scattering. We were able to show that the porosity and our standard grain size fractions listed in the IRIS MERTIS Infrared database are correlated, if our standard preparation routine is applied. Higher porosities are simulated using a mix of IR-transparent KBr powder and mineral powder. First results indicate that the grain size plays only a subdued role but the main effect is related to the porosity (Fig. 1). The most important change takes place in the wavelength region of the CF. Its form changes from U-shaped to strongly V-shaped and shifts to longer wavelengths and it is not the global minimum in the reflectance spectra anymore. However, part of this behavior is related to the measurement setup as the sample cups are composed of alumina, which highly reflects infrared radiation. To avoid this, we covered the alumina cups with an emission standard material with very low reflectance and assumed than a linear spectral mixture of the mineral and the blackbody-like material. With this procedure, we were able to produce “corrected” spectra. Nevertheless, effects of the porosity remain in the spectra which show the need for further investigations.

This shows the need for future analog-samples that we need in addition to chemical, mineralogical and physical properties also a handle on the porosity. In addition, the measurements setups have to be evaluated in terms of a correct simulation of the regolith surface.



**Figure 1: Quartz (ID 13) spectra (scaled to 1 at  $9 \mu\text{m}$ ) for 3 different grain sizes and 2 different porosities. Volume scattering is strongly enhanced in the small-grained, high porosity spectrum. Higher densities show only subdued changes in the region of the TFs. One of the most important changes is the form and position of the CF in the high porosity-spectrum.**



# DigiGREF: A Digital Analogue of the Mercury Imaging X-ray Spectrometer Ground-Reference Facility

Graeme P. Hall<sup>1</sup>, Adrian Martindale<sup>1</sup>, Alberto Paganini<sup>2</sup>, John. C. Bridges<sup>1</sup>, Simon T. Lindsay<sup>1</sup>,

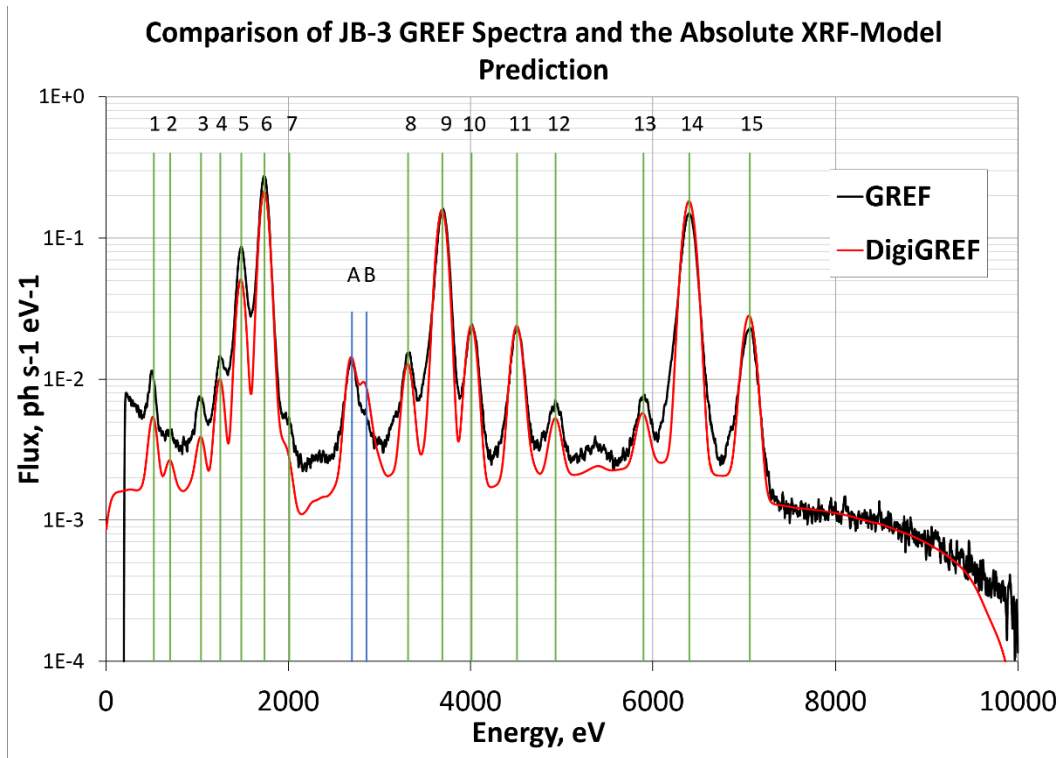
Tuomo V. Tikkanen<sup>1</sup>, Julia A. Cartwright<sup>1</sup>, Adam R. D. Fox<sup>1</sup>, and Emma J. Bunce<sup>1</sup>

<sup>1</sup>*School of Physics and Astronomy, University of Leicester, Space Park Leicester, 92 Corporation Rd, Leicester LE4 5SP, UK*

<sup>2</sup>*School of Computing and Mathematical Sciences, University of Leicester, University Road, Leicester, LE1 7RH, UK*

This work presents a new X-ray fluorescence simulation (DigiGREF), designed as a digital analogue to the Mercury Imaging X-ray Spectrometer (MIXS) ground-reference facility (GREF). MIXS is a novel instrument onboard the BepiColombo mission to Mercury, and requires characterisation with reference targets, which can be achieved in a laboratory setting with the flight qualification model (FQM). A new ground-reference facility (GREF) has been built to facilitate this task. The FQM focal-plane assembly (FPA) was installed in a vacuum chamber, partially simulating the Mercurian environment, which can be used for ground-testing whilst BepiColombo is in flight. DigiGREF is the first step towards a computer simulation of the emission and detection of X-ray fluorescence, which will eventually allow the elemental abundances of Mercury's surface to be accurately determined. DigiGREF solves the standard fluorescence integral, defined in a 3D geometry, using a Monte-Carlo integration technique. X-ray emission processes simulated include photoemission, and both Compton and Rayleigh scattering. To account for the geometry at Mercury, the new model incorporates planar sources, and volumetric targets. The model works by dividing the source, target and detector surface into a number of elements and then tracing the photons from every element of the source to every element of the target. The interactions at each target element are then calculated and the resulting photon emissions mapped to every element in the detector surface. An electron random-walk simulation is also presented, used to simulate an X-ray tube (XRT) input spectrum, as currently used in the GREF. The detection process is simulated using known response functions for the FQM detector. The simulated spectrum is tested against a well characterised geological standard, Japanese Basalt 3.

DigiGREF successfully modelled the fluorescence peaks for all major constituents, plus source Rh-L $\alpha$  and Rh-L $\beta$  scatter-peaks, along with a background spectrum derived from scattered photons. DigiGREF produces a spectrum with an  $R^2$  value of 0.9513 (Figure 1), which we consider a good approximation for a first-order simulation. Although quantification of low-Z elements is uncertain due to fundamental parameters, other work aims to improve this using the scattered background spectrum. The XRT spectrum is also tested and generates a spectrum with an  $R^2$  value of 0.9900, when compared to the experimental spectrum. Thus, we consider DigiGREF a good first-order approximation of X-ray fluorescence and it forms a suitable basis for future development, eventually leading to analysis of data returned by MIXS during the BepiColombo orbital mission in 2026-2028



**Figure 1:** A plot showing the DigiGREF spectrum for JB-3 plotted over the GREF data. The DigiGREF spectrum shows that all of the expected elemental fluorescence peaks are present (identifier in brackets): O-K $\alpha$  (1), Fe-La (2), Na-K $\alpha$  (3), Mg-K $\alpha$  (4), Al-K $\alpha$  (5), Si-K $\alpha$  (6), P-K $\alpha$  (7), K-K $\alpha$  (8), Ca-K $\alpha$  (9), Ca-K $\beta$  (10), Ti-K $\alpha$  (11), Ti-K $\beta$  (12), Mn-K $\alpha$  (13), Fe-K $\alpha$  (14), Fe-K $\beta$  (15), and the scattered Rh-La (A) and Rh-L $\beta$  (B) peaks

Session VI

# **Mercury's iron paradox**

## **Experimental preparation of analogue samples for Mercury – possibilities and limitation**

Olivier Namur<sup>1</sup>, Bernard Charlier<sup>2</sup>, Manon Lecaille<sup>2</sup>

<sup>1</sup> *Department of Earth and Environmental Sciences, KU Leuven, Belgium* 1. <sup>2</sup>*Department of Geology, University of Liege*

Experimental petrology is a discipline focused on reproducing magmatic conditions from shallow to deep planetary environments. This involves using various experimental facilities to recreate the melt and mineral compositions found in low-pressure lava flows, as well as in deeper crustal and mantle sections of planets or planetesimals.

Mercury is a unique planetary body characterized by extremely reducing conditions and a volatile-rich (particularly sulfur-rich) silicate mantle, which upon melting produces volatile-rich lavas (Weider et al., 2015, EPSL; Namur et al., 2016, EPSL). Additionally, it has been suggested that Mercury's crust may contain moderate to large quantities of graphite (Peplowski et al., 2016, Nature Geoscience).

In this contribution, we illustrate how various experimental techniques can advance our understanding of Mercury and assist in calibrating BepiColombo's geochemical and spectroscopic instruments.

Low-pressure experiments using gas mixing or muffle furnaces can produce large quantities (up to several grams) of glassy or glass-and-crystal analogue material under oxygen fugacity conditions relevant to Mercury. A limitation of this method is the vaporization of highly volatile elements such as carbon and sulfur during the experiments, which prevents their physical dissolution in the silicate melt. This issue limits the extent to which these samples can be used for calibration purpose of spectroscopic instruments (MERTIS). However, for purely chemical calibration (MIXS), elemental sulfur and carbon can be mixed with the experimental powders before laboratory measurements.

To dissolve volatiles into the glass phase, methods at low pressure (evacuated silica tubes, i.e., 1 atm) or high pressure (piston cylinder, multi-anvil press) can be used. These methods, however, produce only small quantities of material (milligrams). While these amounts may suffice for in situ mid-infrared measurements (e.g., Morlok et al., 2023, Icarus), they are insufficient for high-temperature emissivity measurements or MIXS detector calibration.

A significant challenge remains the production of large quantities of pure Fe-free silicate minerals (forsterite and enstatite). Tests are currently underway to synthesize these minerals from pure oxides or by reducing Fe-bearing terrestrial minerals. Another challenge is that some phases produced in experiments (e.g. MgS) are unstable in air meaning that the lifetime of experimental products is fairly limited.

## Measurements of X-ray fluorescence of iron minerals

Martin Hilchenbach<sup>1</sup>, Oliver Stenzel <sup>1</sup> and Azar Arghavanian <sup>1</sup>.

<sup>1</sup> *Max Planck Institute for Solar System Research, Justus-von-Liebig-Weg 3, 37077 Göttingen*

Iron minerals have been analysed at the XAFS beamline of the Elettra Sincrotrone Trieste in the excitation energy range of 5 to 9 keV and the fluorescence and scattered light was detected with a radiation detector analog to the MIXS detector of the BepiColombo ESA mission to Mercury. The response of the detector had been calibrated at the BESSY synchrotron in Berlin in a previous campaign. The detector unit could be rotated by 90° around to the incoming polarised synchrotron excitation beam while keeping the sample at the same position. We will report on the results of these measurements for a series of iron minerals (e.g. olivine, limonite, hematite, pyrite, magnetite, pyrrhotite) and discuss the influence of polarisation as well as slight absorption differences on the interpretation of the Fe signal analysis.

## How poor of transitional elements are Mercury surface rocks?

Carli C.<sup>1</sup>, Landi A.I.<sup>2</sup>, Pratesi G.<sup>2</sup>, De Angelis S. Anna G. and Capaccioni F.<sup>1</sup>.

<sup>1</sup> IAPS-INAF (via del fosso del Cavaliere 100, Rome). <sup>2</sup>Earth Science Department, University of Florence

Abundance of iron on the surface of Mercury is up to date considered very low and none reflectance spectra suggest clear evidence of iron in silicates (e.g. Klima et al. 2014, 6<sup>th</sup> WHISPERS). This could be a consequence of low iron abundance in hermean lavas combined to the effects of space weathering. Nevertheless, even a small amount of iron (e.g. 1%) in pyroxenes shows important absorptions (e.g. Klima et al. 2007, M&PS) and no laboratory experiments on pyroxene and olivine (e.g. Brunetto et al. 2006, ICARUS) show a complete suppression of the 1  $\mu$ m absorptions due to Iron.

Conversely, if iron is very low, could other transitional elements, present in olivine or pyroxene even in low amounts, be detected from the surface of Mercury? For instance, the absorption related to the Hollows observed on Mercury around circa 650-700 nm (Vilas et al. 2016, GRL) are in the same spectral range where absorptions due to Cr<sup>3+</sup>, Ti<sup>3+</sup>, Ni<sup>2+</sup> in the crystal field of olivine or pyroxene occur (Lucchetti et al. 2018, JGR).

In the future, we would like to explore from a petrological point of view, using both modeling and experiments, if small amounts (e.g. up to 1% at least) of these elements could enter in mafic minerals at hermean conditions. The subsequent step will be to explore which spectral properties could have those minerals, or mineral assemblages, in the visible to near infrared and in the mid-infrared, in vacuum and at different temperature, to identify potential parameters helpful to VIHI (Cremonese et al., 2020, SPACE SCI.REV.) and MERTIS (Hiesinger et al. 2020, SPACE SCI.REV.).

A further interest will be to understand how the space weathering, simulating it in the laboratory, affects silicates where iron is negligible, but other transitional elements are present in the crystal lattice.

## High-pressure melting experiments of Fe-Si metal alloys, as proxy for Mercury's core

Amber den Hartog<sup>1</sup>, Jurrien Sebastiaan Knibbe<sup>1</sup> and Wim van Westrenen<sup>1</sup>.

<sup>1</sup> Faculty of Science, Vrije Universiteit Amsterdam, Boelelaan 1105, 1081 HV Amsterdam

The reducing conditions of Mercury, indicated by a low surface abundance of Fe and high surface abundance of S (Nittler et al., 2011), suggest that Si is likely the dominant light element in Mercury's core (Chabot et al., 2014). Geodetic observations indicate that the outer core is in liquid state (Margot et al., 2007) and imply that the pressure of Mercury's core-mantle boundary is between 5 and 6 GPa (Knibbe et al., 2021). Constraining models of the interior structure and the evolution of Mercury's core by these observational constraints requires knowledge of the Fe-Si phase diagram at high pressure and high temperature. Additionally, the dynamics of Mercury's core that generate the observed magnetic field may depend on the fluxes of light elements through the core. These fluxes depend on the solid/liquid fractionation of light elements including Si and on the variation of the liquidus with pressure.

We are performing high-pressure and high-temperature experiments on Fe-Si metallic alloys to study the liquidus, solidus and eutectic of the Fe-Si phase diagram. We use a multi-anvil press for experiments at 7.2 GPa to simulate conditions in the upper part of Mercury's core. We additionally use a piston-cylinder press at 1 GPa to study the variation of the phase diagram with pressure. Experiments at higher pressure are available in literature (Edmund et al., 2022). SEM-analysis shows that a completed series of experiments on metallic Fe - 10wt% Si samples have produced fully solid, fully liquid and partially molten samples. Compositions of all phases are being quantified by EMPA to determine the compositional boundaries of the solid+liquid field. Series of experiments on Fe - 6wt% Si and Fe - 14wt% Si are in preparation.

In this workshop, we will present our experimental results and compare them with available literature data at ambient pressure and at higher pressure (Edmund et al., 2022). These results contribute to improving models of Mercury's interior, which aim at constraining the composition of Mercury's core using observational data by MESSENGER and BepiColombo.

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## Spectral properties of synthetic plagioclases as planetary analog materials

Clarisse Peignaux<sup>1</sup>, Jessica Flahaut<sup>1</sup> and François Faure<sup>1</sup>.

<sup>1</sup> Centre de Recherches Pétrographiques et Géochimiques (CRPG), UMR7358, CNRS/Université de Lorraine, 15 rue Notre-Dame des Pauvres, 54500 Vandœuvre-lès-Nancy, France.

Plagioclases signatures have been identified on various planetary surfaces. Being the main rock-forming mineral within the Moon's primary crust, anorthite is ubiquitous in the lunar highlands, as evidenced by meteorites, returned samples and remote sensing instruments (e.g., Donaldson-Hanna et al. (2014), *JGR: Planets*). On Mars, increasing detections of feldspar-bearing rocks with the visible near-infrared (VNIR) spectrometer CRISM are raising questions about the nature of the Martian crust (e.g., Payré et al. (2024), *Minerals*). As for Mercury, gamma ray spectroscopy excludes an anorthite-rich flotation crust, rather suggesting that albite is a major mineral on the surface (e.g., Evans et al. (2012), *JGR: Planets*).

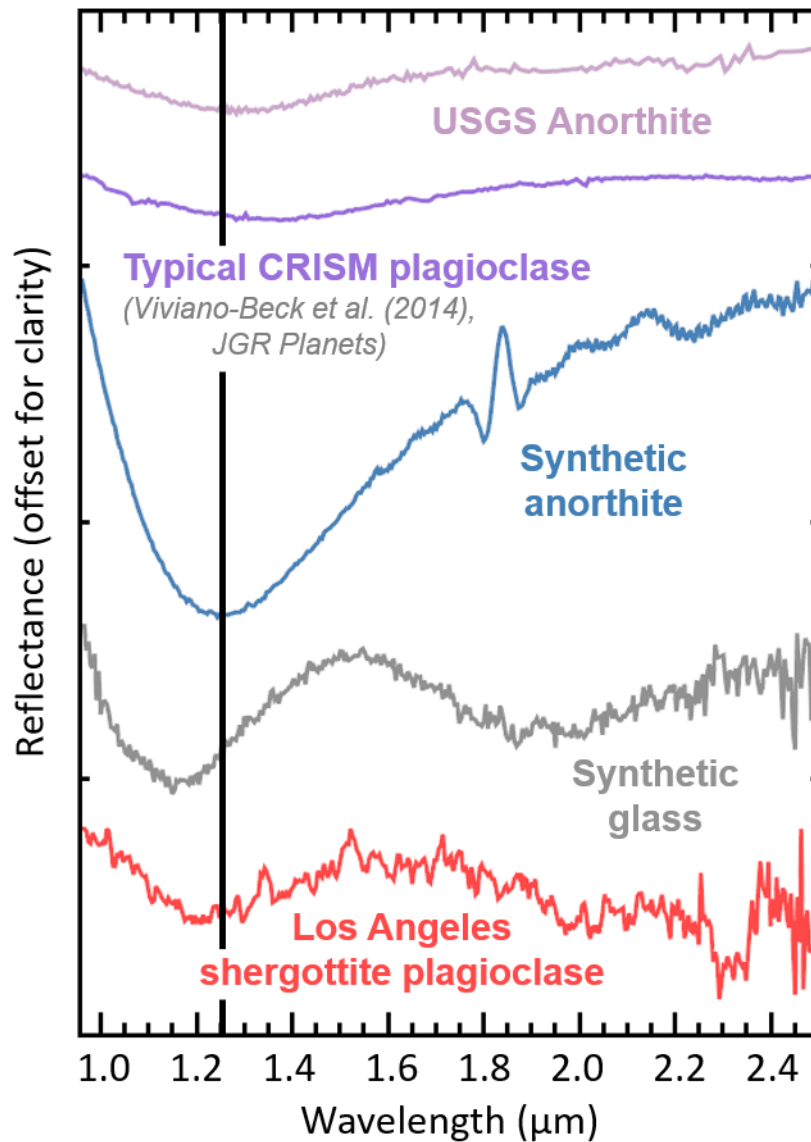
To further understand the composition and nature of planetary crusts, we investigate the VNIR spectral properties of synthetic plagioclases as a function of their composition (An#, iron content) and magma redox state. Our measurements aim to better constrain past and future spectroscopic detections of plagioclases on planetary surfaces.

Previous studies demonstrated the limitations of working with terrestrial analog rocks, since mineral mixtures and alteration are known to alter plagioclases' spectra (e.g., Barthez et al. (2023), *JGR: Planets*). In the present study, we use experimental petrology to synthesize pure, unaltered plagioclases, before analyzing their VNIR spectra at the CRPG hyperspectral remote sensing laboratory (Flahaut et al., this meeting).

Starting glass materials were obtained after melting reagent grade oxides in a muffle furnace to ensure homogeneous mixing. Desired compositions comprise both plagioclase endmembers (anorthite and albite) with different iron-enrichments, as Fe<sup>2+</sup> is known to cause the diagnostic VNIR absorption feature of plagioclases around 1.25  $\mu\text{m}$  (Adams and Goullaud (1978), *LPSC Proceedings*). Dynamic crystallization experiments were conducted in a 1-atm vertical furnace using platinum wire loops-supported small pellets of the starting mixture to grow large grains of plagioclase (targeted size: > 32 microns). Redox state was controlled with CO-CO<sub>2</sub> gas mixtures, allowing for varying iron partitioning. Quenched samples were initially mounted in epoxy resin for characterization (optical microscope, SEM). Reflectance spectra were then measured on epoxy-free samples using Hyspex VNIR3000N and SWIR640 hyperspectral cameras.

Millimetric anorthite (An<sub>93.80-98.45</sub>) were successfully synthesized and unprecedented VNIR signatures of synthetic plagioclases were measured (Figure 1). Contrary to natural plagioclase spectra, hydration features are absent, allowing for accurate analysis of the feldspar-related absorption parameters. Future steps include unmixing the residual glass and plagioclase spectral signals, as plagioclase transparency leads to contamination by the underlying glass, as well as analyzing pure albites, and plagioclases of intermediate compositions.





**Figure 1:** Reflectance spectra (continuum-removed) of one of our synthetic anorthite sample (grey and blue curves) are compared to a spectrum acquired on a plagioclase crystal of the Los Angeles shergottite (red curve). All spectra were acquired in similar laboratory conditions using the Hypslex SWIR640 camera. A CRISM type spectrum of Mars plagioclase (dark purple curve) and the USGS HS201.3B anorthite spectrum (light purple curve) are also shown for comparison. The vertical black line highlights the VNIR absorption band of plagioclase, usually centered around 1,25  $\mu\text{m}$ .

Session V

# **Surface-environment interactions**

## **X-Ray Photoelectron Spectroscopy: a Critical Tool for Understanding the Compositional and Chemical Effects of Space Weathering**

Noah Jäggi<sup>1</sup>, Adam K. Woodson<sup>1</sup> and Catherine M. Dukes<sup>1</sup>.

<sup>1</sup>Laboratory for Astrophysics and Surface Physics, University of Virginia, 395 McCormick Road, Charlottesville, 22904 VA, USA

Mercury's exosphere is produced by the ejection of surface atoms that reflect the mineralogy of the planet's regolith. Relevant ejection processes include desorption (thermal, photon and electron stimulated), ion sputtering (or ion stimulated desorption) and micrometeorite impact vaporization. Laboratory studies generally focus on analyzing the ejecta from these processes by mass-spectroscopy, particle counting and optical methods, while neglecting complementary changes to the substrate. To fully understand the underlying physics of exospheric production, a holistic approach is necessary – one that includes quantifying compositional, chemical, and physical changes to the substrate after processing, in addition to the characteristics of the ejecta.

For conditions relevant to Mercury and other airless extraterrestrial objects, sputtered and desorbed atoms are ejected from the outermost few nanometers of the surface. However, methods such as energy-dispersive X-ray (EDX) spectroscopy, Raman spectroscopy, and Fourier-transform infrared (FTIR) spectroscopy necessarily gather information over a much greater depth, on the order of a micron. These methods are therefore unable to resolve near-surface chemical and structural changes that occur with sputtering and desorption; X-ray photoelectron spectroscopy (XPS), on the other hand, is ideally suited for this purpose.

We will present past and ongoing work, performed in the Laboratory for Astrophysics and Surface Physics at the University of Virginia, employing XPS to characterize compositional and chemical changes at the surfaces of mineralogical samples resulting from ion irradiation and controlled heating. Such studies include the sputter-removal of moderately volatile metals from smooth and granular mineral surfaces, surface alteration of ion-irradiated Ca and Mg sulfides though to be relevant to Mercury, and thermal diffusion of adsorbates along the surfaces of mineral samples.

## **Oxygen ion irradiation experiments on planetary analogue materials: A Mercury perspective**

Haruhisa Tabata<sup>1</sup>, Koki Yumoto<sup>1</sup>, Oya Kawashima<sup>1</sup>, Yudai Suzuki<sup>1</sup> and Tomohiro Usui<sup>1</sup>

<sup>1</sup> Institute of Space and Astronautical Science (ISAS), Japan Aerospace Exploration Agency (JAXA).

Mercury has a tenuous atmosphere supported by ions from the surface material (Killen et al., 2019; McClintock et al., 2019). Of ion species detected to date, hydrogen and oxygen are of interest in view of understanding the redox condition of surface materials. In this study, we developed a laboratory instrument capable of irradiating oxygen ions and neutral oxygen atoms to solid samples. Although the instrument was originally developed to simulate the oxygen ion irradiation environment on Phobos, a moon of Mars, we seek a possibility to apply the apparatus to investigate the surface environmental condition of Mercury.

The oxygen irradiation experimental apparatus consists of a plasma source induced by a 2450 MHz microwave source coupled with a quartz-glass reaction tube of ~30 cm. Oxygen supplied from the gas cylinder to the reaction tube was maintained at a pressure of 10–100 Pa by continuous pumping. A current probe is installed at downstream of the reaction tube to measure oxygen ion flux by applying a negative voltage. As an initial experiment, we irradiated oxygen for 30 hours to olivine (Pakistan, ~Fo90), Alkaline olivine basalt (Hawaii), and a Phobos simulant (Miyamoto et al., 2021). We measured visible (0.4–0.9 nm) and infrared (1.3–20 μm) reflectance spectroscopy on the samples before and after irradiation to examine changes in the reflectance.

After the irradiation for 30 hours, an increase in reflectance (i.e., brightening) and a decrease in spectral slope (i.e., bluing) over the 400–900 nm range was observed for the olivine and olivine basalt. Phobos simulant changed from the original dark black color to gray, consistent with the reflectance increase from the initial value (~3%) to >15%. In infrared region, while the overall reflectance remained nearly unchanged, the weakening of sharp peaks was observed. The observed bluing trend in olivine and olivine basalt is similar to that of the spectral changes reported in previous studies that examined the spectra of olivine and iron oxide mixture (Bou-Orm et al., 2022), indicating the potential formation of iron oxides. These results suggest that the irradiation of oxygen could modify surface materials on planetary bodies, and the investigation of such an effect is important for interpreting remote sensing spectral observations.

## **Laboratory simulation of ion impact and back-scattering signal investigation on Mercury surface**

E. De Angelis<sup>1</sup>, R. Rispoli<sup>1</sup>, Richards G.<sup>1</sup>, M. Moroni<sup>1</sup>

and ELENA Lab-Sci team: A. Milillo<sup>1</sup>, A. Mura<sup>1</sup>, S. Orsini<sup>1</sup>, C. Plainaki<sup>2</sup>, A. Aronica<sup>1</sup>, L. Colasanti<sup>1</sup>, N. Vertolli<sup>1</sup>, F. Nuccilli<sup>1</sup>, R. Sordini<sup>1</sup>

<sup>1</sup> IAPS-INAF Rome Italy, <sup>2</sup>ASI Agenzia Spaziale Italiana, Rome, Italy

The study of ion precipitation on Mercury's surface has several interesting aspects from a science and experimental point of view.

The solar wind interacting with planetary surfaces allows for the opportunity to study surface chemistry, exosphere and particle circulation. Moreover, planetary ions impacting on the night side have an effect that has to be considered to better understand precipitation and particle circulation.

At the INAF/IAPS laboratory there is the facility of an Ion and ENA (ENA-Energetic Neutral Atom) beam that provides the opportunity to investigate the interaction of selectable ion/neutral beams with several samples and detectors.

The possibility to replicate the impact of the solar wind on surfaces and the subsequent detection of escaping and back scattered particles can improve understanding of the phenomena within Mercury's environment. It also supports the foreseen BepiColombo mission, in particular the SERENA experiment (Search for Exospheric Refilling and Emitted Neutral Abundances), which is dedicated to studying the solar wind precipitation and release effect in terms of the generated charged and neutral particles.

The set-up provided by the ion beam, together with angular motor step and detector with high angular resolution, can allow reconstruction of the angular distribution of escaping/back-scattering particles.

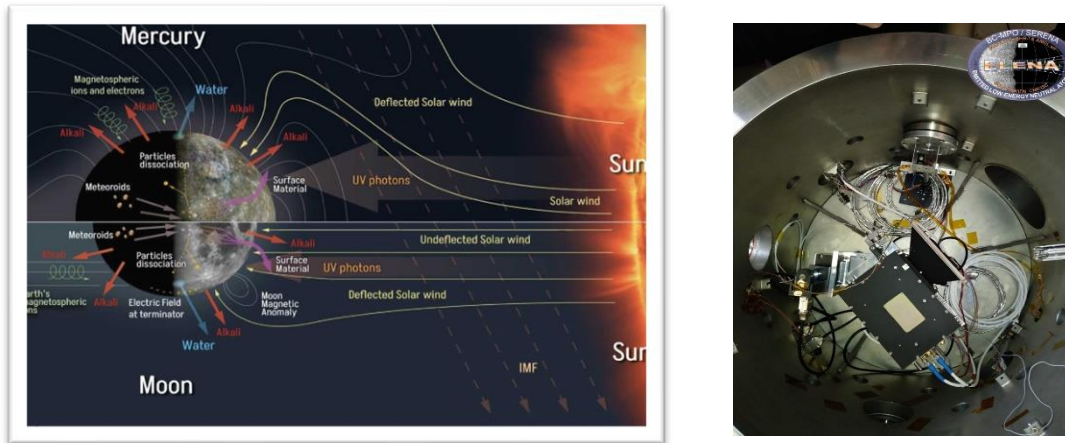
In order to fully simulate Mercury's environment, the charged particle beam can be made into a beam of accelerated neutral atoms, with a neutralisation cell applying a charge exchange effect, to simulate the generated neutral abundances.

Moreover, it is recently proposed to extend the current facility to a higher energy range (10-30 keV) that will enable simulation of the accelerated ions precipitating onto the surface.

The overall set-up provided by ion sources, surface analogues and the angular sensitive detector (as for the ELENA Flight Spare sensor) can simulate the entire phenomena of ion impact on Mercury's surface and the reconstruction of angular distribution.

A specific description of the facility and experiment baseline will be presented.

Open points and topics for discussion will also be provided in terms of necessary collaboration between laboratories and expertise to best carry out a global and complete experiment.



**Figure 1:** **Left** Processes affecting two solar system bodies (Mercury and the Moon) with ion impact on surface and following effects depicted. **Right** SERENA/ELENA Flight Spare inside the vacuum chamber @IAPS/INAF

## The effects of ion bombardment on the surface of Mercury

R. G. Urso<sup>1</sup>, G. A. Baratta<sup>1</sup>, D. Fulvio, M. E. Palumbo<sup>1</sup>, C. Scirè<sup>1</sup>

<sup>1</sup> *INAF-Osservatorio Astrofisico di Catania, via Santa Sofia 78, 95123 Catania, Italy*

Solar particles and cosmic rays continuously bombard the surface of atmosphere-less surfaces in the solar system, causing strong alterations in both the surfaces' physical properties and chemical composition. In turn, these alterations induce modifications in the spectral properties of the surface materials. Despite the presence of a magnetic field, the surface of Mercury is exposed to a high flux of solar particles. These particles are responsible for the sputtering of neutral particles and ions from the planet's surface, with evidence of this process obtained by MESSENGER'S observations (e.g., Sun et al. 2022).

Laboratory experiments allow us to study the effects induced on planetary surfaces by energetic charged particles (e.g., Rothard et al. 2017, Martinez et al. 2022). The Laboratory for Experimental Astrophysics at INAF-Osservatorio Astrofisico di Catania (Italy) is equipped with facilities to simulate and characterize the alteration induced by energetic charged particles on a variety of samples, including minerals, organics, and meteorites. The facility is equipped with a ultra-high vacuum ( $P < 10^{-6}$  mbar) chamber where samples are exposed to a 200 keV ion beam (400 keV for double ionization). After the exposure, samples can be characterized by means of UV, Visible, and infrared spectroscopy as well as Raman spectroscopy (Brunetto & Strazzulla 2005, Palumbo et al. 2004). Furthermore, an ongoing implementation will allow us to perform the in-situ reflectance spectroscopy during ion bombardment and the ex-situ reflectance spectroscopy up to 900 °C.

We here present our facility and our studies on the effects of ion bombardment on laboratory analogues of the surface of Mercury. In particular, we produced analogues as pellets of mineral mixtures (including jadeite and nepheline) and samples collected on the mount Etna (Italy) that were then exposed to 200 keV ions ( $H^+$ ,  $He^+$ , and  $Ar^+$ ). Our study aims to produce data in support of the interpretation of remote sensing observations of Mercury, to shed light on the changes induced by energetic charged particles on the spectra of analogues (e.g., the variation of spectral slopes, darkening, or brightening) and to relate the spectral changes to the timescale of exposure to ion bombardment.

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## **The Electron Impact Facility at the University of Leicester: Opportunities for Mercury Science**

S.T. Lindsay<sup>1</sup>, A. Martindale<sup>1</sup>, E.J. Bunce<sup>1,2</sup>, N.A. Carr<sup>1</sup>, J.A. Cartwright<sup>1,2</sup> and M.C. Sharman<sup>1</sup>.

<sup>1</sup> *School of Physics & Astronomy, University of Leicester, Leicester, UK*

<sup>2</sup> *Institute for Space, University of Leicester, Leicester, UK*

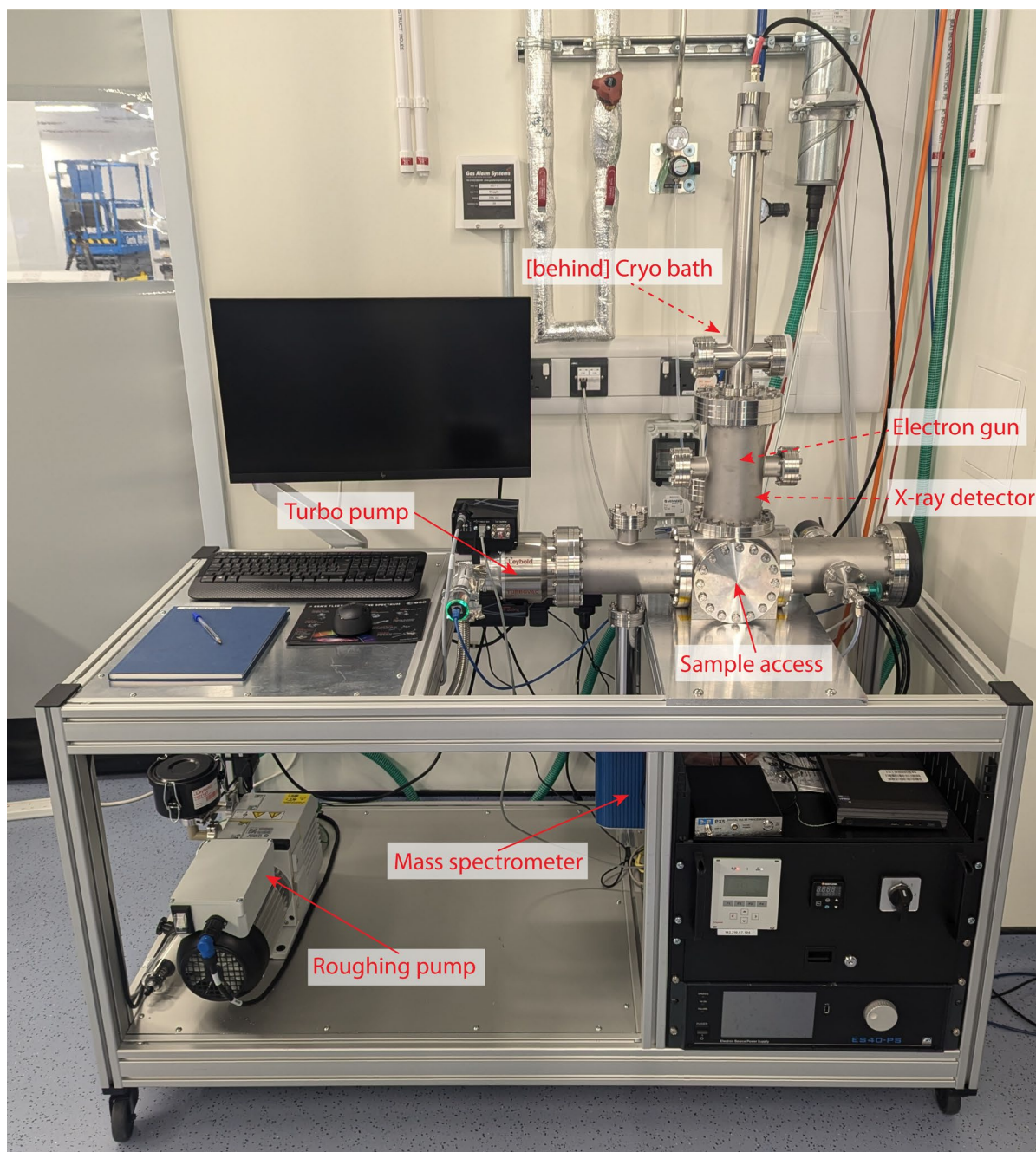
Mercury is subject to bombardment by energetic particles, including electrons that precipitate in “aurora-like” features organized by the planet’s magnetic field. Precipitating electrons with sufficient energy cause the emission of X-rays, which have been observed by MESSENGER XRS [Starr+ (2012), *JGR*; Lindsay+ (2016), *PSS*]. Related electron populations have been observed in situ above the Mercury surface by MESSENGER [Dewey+ (2017), *JGR*] and BepiColombo [Aizawa+ (2023), *Nature Communications*]. Further characterization of such X-ray emission can provide insights about surface composition and magnetospheric activity and structure, and is a primary science objective of BepiColombo MIXS [Bunce et al. (2020), *SSR*]. If precipitation occurs within permanently shadowed regions, this may present a unique opportunity to measure the surface composition within these areas, which likely host water ice.

In order to better characterize electron-induced X-ray emission, and make the best use of data returned by BepiColombo MIXS, we require ground truth measurements taken under controlled lab conditions. The Electron Impact Facility (EIF), under commissioning at Space Park Leicester, will be a key part of this preparation.

EIF consists of an ultra-high vacuum chamber with a 155x155x155 mm test compartment (interior manifold ~100mm diameter sphere). A sample stage placed at the centre of this compartment is connected via a copper cold finger to a liquid nitrogen cryo bath, providing sample cooling. A Henniker Scientific ES40C1 electron gun, producing a 0 - 5 keV electron beam with current on sample of up to 100  $\mu$ A, is mounted vertically above the test compartment. An ultra-high vacuum (UHV)-adapted Amptek FastSDD X-ray detector is mounted alongside the electron gun, providing high energy resolution (122 eV @ 5.9 keV) measurements of X-rays emitted from the sample. A Lesker Element 200 RGA mass spectrometer mounted to the chamber measures species desorbed or sputtered from the sample, and allows leak analyses.

We anticipate a wide range of applications simulating environments across the solar system, including Mercury. Illuminating Mercury analogues with electrons will allow us to characterize their response to a known spectrum in a repeatable and controllable manner, establishing ground truth to support MIXS observations. In support of potential observations of particle-induced X-ray emission from permanently shadowed regions, EIF’s cryo capability will allow us to maintain water-ice and ice/rock mixtures under UHV while characterizing their response to illumination by electrons. We also intend to characterize the response of MIXS’ optics to in situ electron populations, using silicate glasses of the same composition.





**Figure 1:** The Electron Impact Facility.

# **Poster session**

## Experimental investigation of silicate sulfidation kinetics

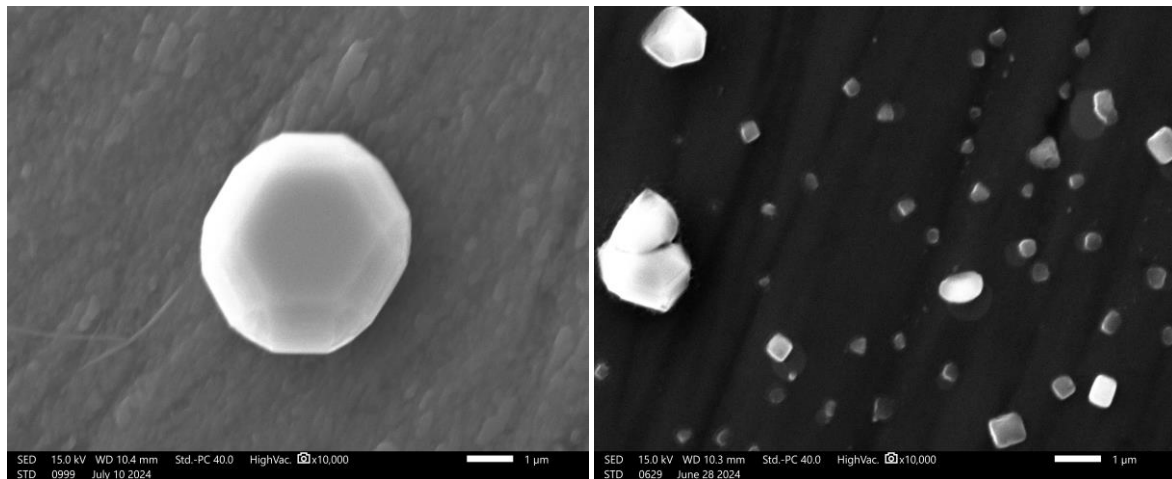
R.C. Erftemeijer<sup>1</sup>, C.J. Renggli<sup>1</sup>, T. Müller,<sup>2</sup> and T. Kleine<sup>1</sup>.

<sup>1</sup> Max Planck Institute for Solar System Research, Justus-von-Liebig-Weg 3, 37077 Göttingen, Germany.

<sup>2</sup> Department of Mineralogy, Georg-August Universität Göttingen, 37073 Göttingen, Germany.

Since the detection of a relatively high (up to 4 wt.%) sulfur abundance on Mercury's surface by NASA's MESSENGER mission, much debate arose about the nature of this enrichment. Volcanic degassing might have played a major role, releasing sulfur from the interior of the planet and triggering chemical reactions between the volcanogenic sulfur and the surface rocks, forming sulfides such as niningerite (MgS) and oldhamite (CaS). Formation and decomposition of these sulfides might play an important role in the formation of hollows – rimless, flat-floored depressions encircled by bright haloes – on Mercury's surface. Still, the processes controlling the behavior of sulfur at reducing conditions remain poorly constrained. We are performing a systematic analysis of the reactions between gaseous sulfur and silicate minerals using high-temperature experiments to improve our understanding about the kinetics of these crucial processes.

For each experiment, a silicate mineral with a polished surface – olivine, diopside, or albite – and sulfur powder are mounted into separate graphite buckets, and placed in an evacuated silica glass tube. Experiments were performed at temperatures ranging between 600 and 1200 °C. Furthermore, for each mineral and temperature, the run time was varied from an hour to a week. Preliminary results show a dependence of the degree of sulfidation on all these factors (Figure 1). More sulfidation decreases the ability of infrared light to penetrate through the sulfide coating, affecting the spectral properties of the mineral. In this poster presentation, the first results of this study and their implications are shared with the community.



**Figure 1:** Secondary electron images of sulfides on an olivine (left) and a diopside (right), after an experiment at 800 °C for 24 hours.

## Experimental REE-partitioning between (Ca,Mg)S and silicates

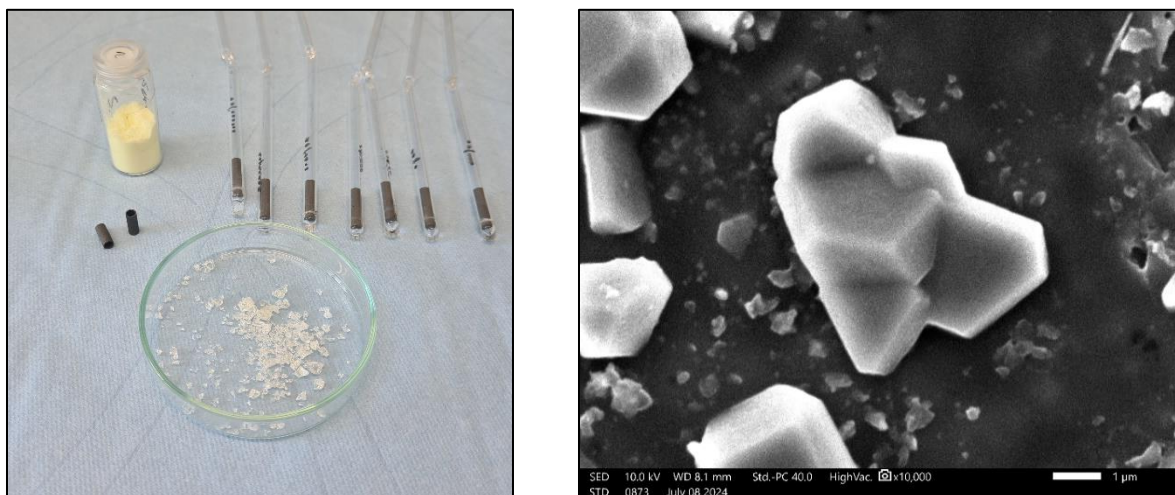
M. Nieuwenhuis<sup>1</sup>, C. J. Renggli<sup>1</sup>, M. Piralla<sup>1</sup>, T. Kleine<sup>1</sup>

<sup>1</sup> Max Planck Institute for Solar System Research, Justus-von-Liebig-Weg 3, 37077 Göttingen, Germany

Alkaline earth sulfides such as oldhamite (CaS) and niningerite (MgS) occur only under very reducing conditions as predicted for Mercury and are observed in reduced meteorites such as enstatite chondrites (EC). These sulfides form by a number of processes, as magmatic phases [1,2], via silicate sulfidation reactions [3-5], or as early condensates of the solar nebula [6] in the formation of ECs. Oldhamite in particular is a major carrier of rare earth elements (REE) in ECs [6], and possibly also in the crust and mantle of Mercury. The different formation processes likely result in different degrees of REE partitioning, due to different formation conditions and mechanisms. Here, we conduct experiments on the partitioning of REE between the sulfides and glass in gas-solid reactions.

We perform partitioning experiments in evacuated silica glass ampoules containing graphite crucibles with a REE-doped glass of anorthite-diopside eutectic composition and S powder (Fig. 1). Heated to 600 – 1200 °C for 24 – 168 h, the S forms a reduced gas phase and reacts with the sample material forming CaS and MgS crystals on the polished glass surface (Fig. 1). The run products are analyzed by electron microscopy (Fig. 1) and for their REE contents by femtosecond-LA-ICP-MS. Here, we present our preliminary results.

[1] Malavergne et al. (2014) EPSL. [2] Namur et al. (2016) EPSL. [3] Piani et al. (2016) GCA. [4] Lehner et al. (2013) GCA. [5] Renggli et al. (2022) EPSL. [6] Crozaz & Lundberg (1995) GCA.



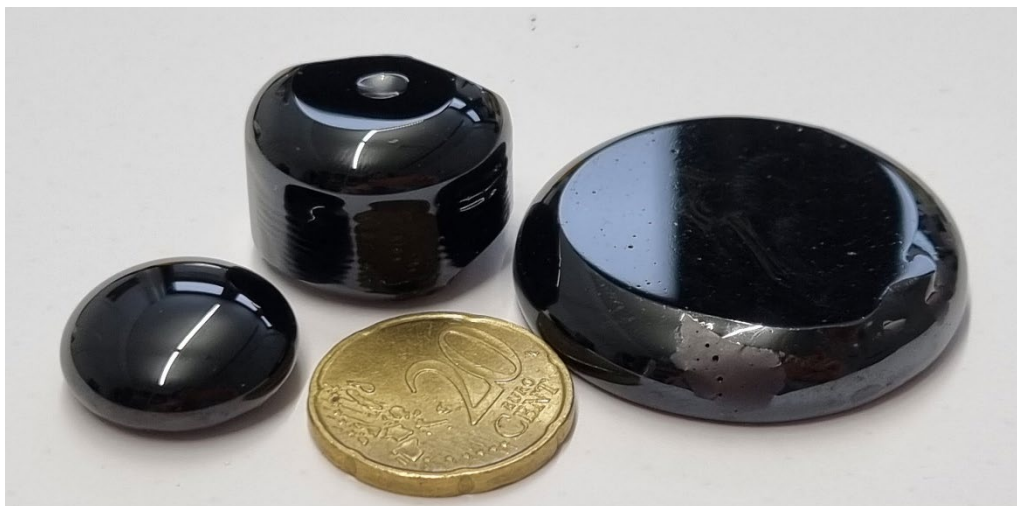
**Figure 1:** Left: Ready-to-go silica glass ampoules with C-crucibles. Right: Secondary electron image of a CaS crystal on a polished glass surface at 10'000x magnification.

## Synthesis of natural basaltic glass discs to be used as terrestrial planet analogues.

Lauren Jennings<sup>1</sup>, Solmaz Adeli<sup>2</sup>, Ana-Catalina Plesa<sup>2</sup>, Stephan Klemme<sup>1</sup>, Andreas Morlok<sup>3</sup>, Maximilian P. Reitze<sup>3</sup>, and Iris Weber<sup>3</sup>.

<sup>1</sup>Institut für Mineralogie, Universität Münster, Münster, Germany. <sup>2</sup>German Aerospace Center (DLR), Institute of Planetary Research, Germany. <sup>3</sup>Institut für Planetologie, Universität Münster, Münster, Germany.

Synthetic and natural glass samples are commonly used in experimental studies as analogues for crystallising lava. These glass samples are analysed as fragments or pulverised such that they can fit the physical constraints of the analytical instrument. However, orbital spectroscopic instruments (such as MERTIS on BepiColombo or the VenSpec suite on EnVision) analyse a much greater field of view. As such, the aim of this work was to generate large basaltic glass discs with a surface area that meets the size requirement of the Planetary Spectroscopy Laboratory (PSL, Berlin) emissivity chamber (4 to 5 cm). The method developed involved the use of dual box furnaces and a steel ring mould. A natural tholeiitic basalt from the Weilheim region in Bavaria, Germany, was crushed into mm and smaller-sized fragments. These fragments were then heated in one box furnace to a temperature of 1400°C to form a viscous melt. The melt was then poured into the steel ring mould that had been placed inside the second box furnace at a temperature below the glass transition temperature (600°C) to quench and then anneal for an hour. The resulting glasses were intact with little to no crystals and a homogenous chemical composition. Various sizes and quenching temperatures were also tested to determine the dimensions that could be achieved using this method. The widest glass has a diameter 36.64mm and the tallest glass has a height of 16.67 mm (see Figure 1). The lowest quenching temperature tested was 460°C. The successful synthesis of these glasses presents an opportunity to study the surface of terrestrial planets. For example, surface alteration and devitrification studies can be completed over a greater surface area and analysed with little risk of interference from the sample housing. Additionally, the level of control over the shape and size of natural glasses means this method could be utilised in other glass alteration studies or to investigate internal glass thermodynamics.



**Figure 1: Tholeiite basaltic glasses made at Universität Münster. Dimensions are as follows: left (D: 18.43 mm, H: 8.13 mm, W: 5.10 g), centre (D: 23.84 mm, H: 16.67 mm, W: 18.8 g), right (D: 36.64 mm, H: 7.77 mm, W: 25.2144 g).**

## **Hermean surface analysis using MLA and spectral characteristics focusing on mineral mapping**

Azar Arghavanian<sup>1</sup>, Oliver Stenzel<sup>1</sup> and Martin Hilchenbach<sup>1</sup>.

<sup>1</sup> *Max Planck Institute for Solar System Research, Justus-von-Liebig-Weg 3, 37077 Göttingen, Germany.*

The surface of Mercury provides a unique opportunity for mineralogical and geological studies due to its distinct physical, spectral and morphological characteristics. This research explores the use of MESSENGER Laser Altimetry (MLA) data in combination with spectral data from the Mercury Atmospheric and Surface Composition Spectrometer (MASCS) onboard MESSENGER, which provides over 230 spectral channels from the near ultraviolet to the near infrared, for detailed mapping of Mercury's surface. Using the high-resolution data from the MESSENGER spacecraft, we aim to develop robust models capable of accurately identifying surface features and their likely different compositions.

Our methodology involves pre-processing the data to remove noise and improve signal clarity, followed by the application of artificial intelligence (AI) methods to topographic and lithological modelling of Mercury's surface. These algorithms are trained and validated using previously obtained spectral signatures of Mercury's common minerals. This study focuses on identifying the key spectral properties associated with the geochemical components of several northern mid-latitude features on Mercury, including craters, depressions and faculae, which are crucial for understanding the planet's geological history and surface processes.



## **Radiative transfer and travel time to characterize the surface**

Jean Barron<sup>1</sup>, Frédéric Schmidt<sup>1,2</sup> and François Andrieu<sup>1</sup>.

<sup>1</sup> *Université Paris-Saclay, CNRS, GEOPS, 91405, Orsay, France.*

<sup>2</sup> *Institut Universitaire de France, IUF, Paris, France.*

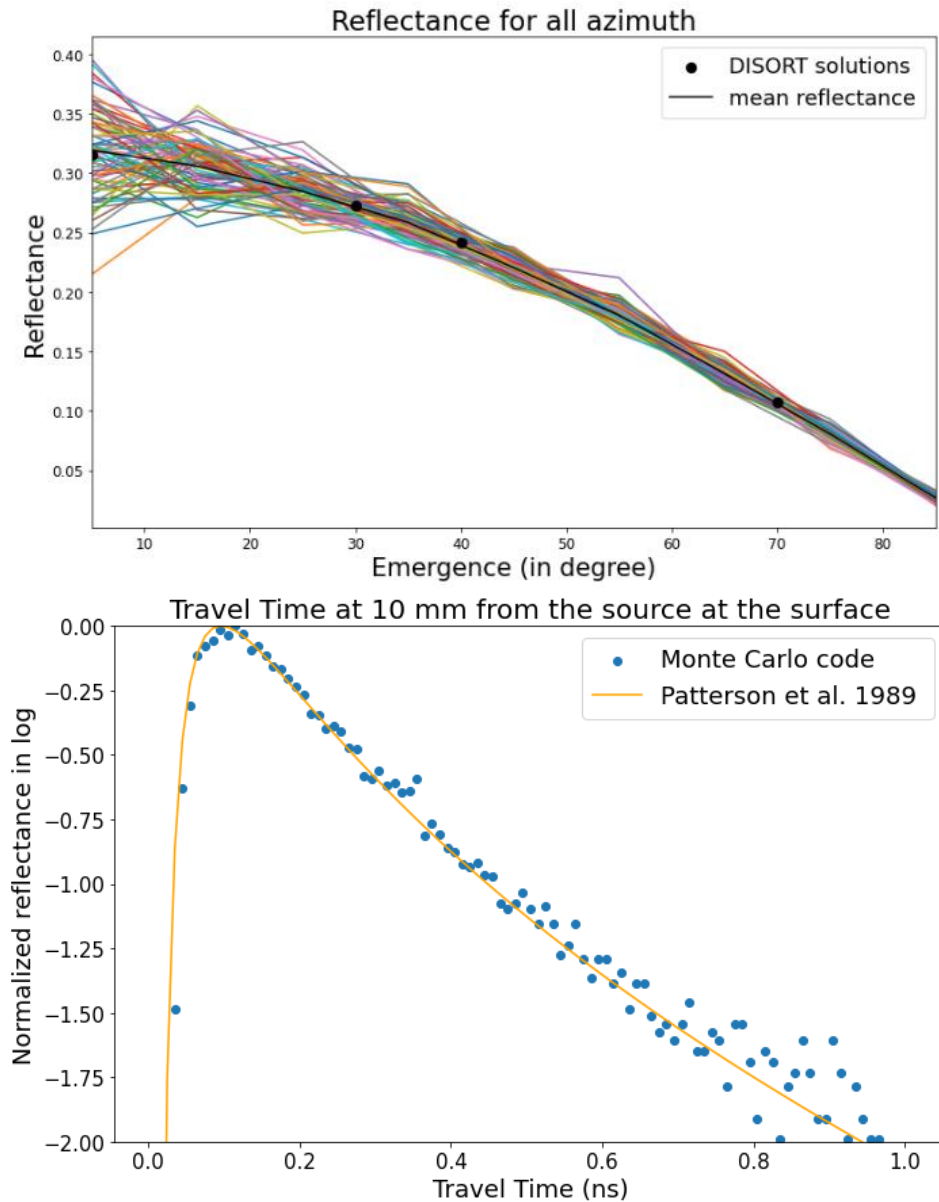
The next generation of lidar instruments will encompass the travel time measurement for each photon packet that would be available to characterize the planetary surface medium. For instance, the BepiColombo laser altimeter (BELA) (Thomas et al., 2021) includes this capability to explore the herman surface. We propose here a tool to simulate in-silico the time transfer inside the planetary medium.

We propose a Monte Carlo approach based on the work from Farrell et al., 1992 and Boas et al., 2002. Our model computes the position of the ray during its travel through the medium. The main parameters are incidence angle, optical thickness, single scattering albedo, Henyey-Greenstein or isotropic phase function.

The validation of the model is mandatory in order to compute a coherent and physically correct simulation of light time transfer within a planetary surface medium. In the model, planetary surface mediums can be either described as a semi-infinite granular layer or a homogeneous slab above a bedrock with a certain albedo. The purpose here is to be able to replicate the simulations in the same conditions from previous works such as Gao et al., 2013, Gautheron et al., 2024 and Patterson et al., 1989. We first computed the reflectance in the same conditions as seen in Gao et al., 2013 in the case of a semi-infinite granular layer (Figure 1) which are an incidence angle of 50 degree, an optical thickness of 1000 and an isotropic phase function. The DISORT algorithm (Stamnes et al., 1998) gives a numerical solution for this case that is also computed and displayed. By comparing both DISORT and Gao et al., 2013, our simulation shows a very good agreement, confirming the validity of our model for angular distribution.

We propose then a method to compute the trajectory and the time travel of the rays in the medium, that would be simulating the response of a full waveform lidar. Knowing the speed of light in the medium and assuming its constancy according to optical properties, we evaluate the time travel in comparison with the analytical solution from Patterson et al., 1989. Results in Figure 1 shows a very good agreement that validates our algorithm.

We propose a new approach to efficiently simulate the travel time of photons inside a planetary surface. We conducted several tests to validate the approach. In the future, we will adapt this tool to planetary science cases, such as the mercury regolith for BELA, or the icy surface for GALA.



**Figure 1: (up)** Reflectance for all azimuth computed in the conditions of semi-infinite granular layer for an incidence of 50 degrees, single scattering albedo  $\omega = 1$ . Scattered rays follow isotropic diffusion law as expected ; black dots represents the DISORT solution ; black line represents the mean reflectance value for all azimuth ; color lines represents reflectance following the emergence for different azimuth. **(down)** Histogram of time travel for an instance of semi-infinite granular layer compared with the analytical solution from Patterson et al., 1989. Here the source of the rays is isotropic at a depth  $z_0$  and observed at a distance 10 mm. The absorption coefficient is  $0.005 \text{ mm}^{-1}$ , the scattering coefficient is  $1 \text{ mm}^{-1}$  and the speed of light is  $299792458 \text{ m/s}$ .