Composition of surface units on Mercury from surface reflectance measurements during the first and second MESSENGER flybys. Mario D'Amore (mario.damore@dlr.de)[1], Jörn Helbert[1], Alessandro Maturilli[1], Deborah L. Domingue[2], Noam R. Izenberg[3], Sean C. Solomon[4], [1]Institute for Planetary Research, DLR, Berlin, Germany; [2]Planetary Science Institute, Tucson, AZ 85719, USA; [3]Johns Hopkins University Applied Physics Laboratory, Columbia, MD 20723, USA; [4]Carnegie Institution of Washington, Washington, DC 20015, USA.

Introduction: During MESSENGER's first two flybys of Mercury, the Mercury Atmospheric and Surface Composition Spectrometer (MASCS) obtained reflectance spectra of large areas of the planet's surface [1,2]. The resulting dataset is composed of several hundred spectra that have not yet been corrected for effects of observing geometry or photometry. Under the hypothesis that surface compositional information can be efficiently separated from other contributions by the use of statistical techniques, we have employed principal component and cluster analyses to identify and characterize spectral units along the MASCS ground tracks. Under the same hypothesis, we applied a linear decomposition algorithm to the data, employing newly available visible–near-infrared (VNIR) biconical reflectance spectra of candidate materials from the DLR Planetary Emissivity Laboratory (PEL). We fixed the reflectance measurement conditions to match a portion of the flyby viewing area on the planet and used those measurements to estimate the mineralogical composition of Mercury surface material. We then used a second set of samples shocked to high temperature (> 500ºC) to investigate how thermally shocked material might modify the interpretation.

Spectral Unit Characterization: To retrieve and characterize the number and spectral shapes of the distinguishable components present in the dataset, we apply principal component analysis (PCA), a well-established technique in remote sensing [3-5]. PCA expresses the data in a new vectorial basis set, for which the data covariance is minimized. PCA essentially reduces the dimensionality of the dataset and allows modeling of the data as a linear combination of the principal components or eigenvectors. The dimensionality of the new set measures the number of components that influence the system. We evaluated the eigenvalue ratio [3] and the reconstruction error, and we inspected visually the goodness of fit of model spectra to observations. Applying the covariance matrix decomposition, spectra in the dataset are assembled in matrix form as $\mathbf{D} = \mathbf{R} \cdot \mathbf{C}$, where **D** is the matrix of the data, **R** the matrix of reconstruction vectors, and **C** the matrix of relative concentration coefficients. The goal of PCA is to decompose **D** into two matrices. **R** will consist of the principal eigenvectors calculated from the covariance matrix of **D**. Application to the full MASCS dataset shows that in general seven eigenvectors are sufficient to reconstruct the data within the error. The first eigenvector always displays a strong positive or "red" slope with increasing wavelength, probably strongly linked to effects associated with viewing geometry variations, and all eigenvectors show distinctive spectral signatures. The concentration coefficients in the **C** matrix indicate that spectral units display geographical variation. Because we do not photometrically correct the data, we can clearly see the dependence of the coefficients on geometrical parameters. We apply the Mahalanobis transformation [6], a decorrelation technique, to partially remove dependence on observation angle in the retrieved concentration coefficients. Thanks to this analysis we resolved isolated spectral units within the two flyby viewing areas that also show a strong correlation with surface units mapped with the MESSENGER imaging system.

Spectral Analysis: The newly available VNIR biconical reflectance spectra data from the PEL laboratory are then used to constrain the composition of the surface areas observed. To sidestep the photometrical correction problem, we analyze only a small portion of the surface, thus limiting the range in emission and phase angles observed by MASCS. The instrument operated in our laboratory, a Bruker IFS 88v, acquires biconical diffuse reflection spectra over the wavelength interval 0.5-25 µm. We acquired a dataset for characteristic mineral samples, fixing the emission and incidence angle at the target to 45º. This design gave us a set of observations directly applicable to surface regions viewed at a similar geometry, including areas between 130° and 150°E during the first flyby (M1) and 20° and 40°E during the second (M2). Each of these areas included a mix of terrains. During M1, MASCS viewed fresh crater ejecta and spectrally intermediate terrain and small areas of high-reflectance red plains, intermediate plains, and possibly low-reflectance blue plains, whereas the viewing area during M2 included fresh crater ejecta, intermediate terrain, small areas of high-reflectance red plains and intermediate plains, and regional low-reflectance material [7]. The choice of the laboratory samples was based on a subset of the candidate Mercury minerals selected in support of BepiColombo Mercury Thermal Imaging Spectrometer (MERTIS) data analysis [8]. Measured samples included calcium-rich plagioclase feldspar, magnesium-rich olivine and pyroxene, a representative glassy phase, and titanium-rich oxide. For the samples analyzed we used the smaller grain size (0-25 μm) routinely produced by PEL, because the low spectral contrast observed in thermal infrared spectra of Mercury may indicate a grain size on the order of tens of microns [9]. Moreover, all the materials were thermally shocked after the reflectance observations and measurements were reacquired. Our purpose was to simulate the sort of thermal cycle that "cooks" surface material on Mercury every solar day, because our previous work indicated that thermally induced structural change can occur in common rock-forming minerals, such as plagioclase [9][10]. We co-analyzed the laboratory and MASCS datasets by combining a local PCA to retrieve the concentration of end-member minerals with an iterative linear decomposition algorithm, based on least-square minimization and iterative elimination of negative concentrations. Each run produces a vector of areal fractional concentration (mass fraction divided by density and particle size) for each input end-member. The residual error is expressed as a single value of the root mean square (RMS) misfit.

Results: The fit of model to observations appreciably improve when thermally shocked materials are used as reference end-members instead of only their unshocked equivalents. The spectra modeled with the mixed library show a good match, even if some zones of high residual signal are present, particularly near 900 nm wavelength. Such misfit indicates the absence of representatives of Mercury's surface spectral behavior in this region. Whether the missing end-members are extremely shocked materials or other minerals will be explored in future work.

In general, the results from the application of simple linear decomposition are quite similar for the two flybys. The surface appears to be composed mainly of thermally shocked minerals, with the exception of feldspars that are also present as unshocked minerals. The best fit is obtained with a surface that is dominantly plagioclase feldspar, up to 70%, one-third unshocked and two-thirds shocked. The remaining areal fraction, according to fit results, consists of a thermally shocked glassy phase, up to 30%, and an accessory shocked olivine (between a few percent and 10%). During the first flyby the most unusual composition seen was at a small crater near 136°E viewed almost vertically by MASCS; this exotic composition was also seen in previous cluster analyses of the entire dataset. The cluster analysis separated clearly the western regional low-reflectance terrains, centered approximately at 0.5°N, 130˚E, from the intermediate terrain to the east [7], where no distinct compositional units could be inferred from the derived mineral compositions. The western terrains are nevertheless compositionally heterogeneous, possibly consisting of two different units, as also indicated by the cluster analysis. The second flyby presents a more constant profile, one for which the fitting procedure indicates a high areal fraction of plagioclase feldspar (between 65% and 70%), shocked glassy phase (between 20% and 30%), plus minor magnesium-rich olivine (a few percent). An exception is a single spot at 320˚E, where the indicated olivine fraction is ~10%. This spot is located on a transition from high-reflectance red plains or intermediate plains to low-reflectance blue plains and adjacent to a crater chain [7]. The cluster analysis clearly separates the high-reflectance red plains, the low-reflectance blue plains, and some larger craters as distinct spectral units.

Conclusions: Combined PCA and cluster analysis have demonstrated an ability to successfully separate several surface spectral units in a manner that matches observations with MESSENGER's camera system. The analysis appears to be robust to effects induced by not correcting the spectral data for variations in lighting and viewing geometry. As a further step, we applied to a subset of the MASCS flyby data a combination of PCA and linear decomposition into spectra of mineral samples measured at equivalent lighting and viewing geometry both before and after thermal shocking [8]. The inferred mineralogical concentrations vary with the terrain viewed, but the separation of true local features and "noise" features remains challenging. Broadly, the surface composition is compatible with basaltic material, consistent with a volcanic origin for much of the viewed terrain [7]. Clearly, non-linear effects on the spectra of mineral mixes have not been considered here, but our experience with PEL data tell us that linear decomposition should at least indicate the major constituents of a target mixture. An extensive laboratory test with reflectance data obtained at high temperature on synthetic mixtures is planned for the near future.

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