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VNIR spectral modeling of Martian Dark sand dunes inside Kasei Vallis (data acquired by MEX-OMEGA): first results

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Abstract. Knowledge regarding the surface composition of Mars and other bodies of the inner solar system is fundamental to have an understanding of their origin, evolution, and internal structures. Approaches to qualitative and quantitative analysis of remotely-acquired spectra have been successfully used to infer the presence and abundance of minerals and to discover compositionally associated spectral trends. Both empirical and mathematical methods have been applied, typically with full compositional knowledge, for predicting the compositional information. In this work we analyze some OMEGA/MEX spectra to derive the surface composition. Preliminary results are reported, and the modeling limitations discussed.

Key words. Spectroscopy: Visible,NIR – Spectroscopy: mineral compositions – Solar System: Mars

1. Introduction

Gaussian curves are one of the models currently used to analyze the absorption bands in the reflectance spectrum of a mineral, provided various techniques for statistical fitting and best fit evaluation are used (Hawthorne & Waychunas 1988). Electronic absorption features have been usually considered to be Gaussian-like (Singer 1981), or modified Gaussians (Sunshine et al. 1990), when analyzed as log reflectance versus photon energy. The assumption is made that absorption bands have Gaussian shapes in energy, or in optical length, respectively, and thus the area of the absorption band is related to the probability of an electronic transition to take place, although vibrational interactions may modify band shapes and contribute to asymmetric profiles in crystal field spectra (Sunshine et al. 1990). To model reflectance spectra using a number of absorption components, two different approaches have been extensively used. One is the continuum removed approach which implies fitting the spectral components after removal of the background absorptions. The natural logarithm of the reflectance domain simplifies the continuum removal, because multiple component absorptions become additive, allowing the continuum to be subtracted from the natural logarithm of the reflectance spectrum. The continuum removal technique, al-

Send offprint requests to: L. Pompilio though useful in identifying the weakest spectral features, implies that the continuum parameters are subjectively estimated. A different approach is based on simultaneously fitting both the continuum and the absorption components. This approach requires inferring the continuum shape at least, while both the continuum and band parameters are concurrently computed. Continua can be represented as straight-line segments, polynomial curves, Gaussians, cubic splines, etc. Here we perform the spectral analysis of two Martian spectra acquired inside Kasei Vallis, using the high resolution Visible/Near-Infrared imaging spectrometer, OMEGA onboard the Mars-Express spacecraft. Spectral data have been extracted from cube number 3, orbit 100, at centre spatial coordinates 32.96 N, -53.78 E. The spectral range here investigated spans from 0.39 to 2.65 m, which is particularly well-suited for analysis of Fe-bearing mineral assemblages (Sunshine & Pieters 1993, 1998 and references in all). In this region OMEGA has sampled spectrally similar dark and bright materials, from the bottom of a channel and top of a nearby highland, respectively (fig. 1a). A quick overview of the MOC NA E13-00548 image (fig. 1b) shows that the low albedo material forms dune shaped bodies lying on wrinkle terrains. Both spectra show blue slopes toward long wavelengths, two broad absorptions near 1 and 2 m, likely to be due to Fe^{2+} in pyroxene, and a prominent charge transfer band toward the UV (fig. 2). The low-albedo spectrum shows bluer slope and red shift of the absorption bands with respect to the high albedo spectrum.

2. Spectral modeling

The Modified Gaussian Model (MGM (Sunshine et al. 1990)) had a great emphasis, particularly in the last decade, for its implications for interpretation of remote sensing measurements. To model complex absorptions the MGM exploits modified Gaussians (Gaussians in wavelength) superimposed onto a continuum linear in energy. The original purpose of the MGM was to describe a single electronic absorption band with only one distribution, thus to make the spectral decomposition more stable and physically realistic. The MGM has been successfully applied to model crystal field transitions due to transition elements in various crystal sites (Sunshine & Pieters 1993, 1998), as well as both oxygen-metal and intervalence charge transfer bands (e.g., McFadden & Cline 2005). Therefore, the MGM has been used to decompose superimposed and overlapping absorptions in mafic minerals and mixtures (e.g. Sunshine & Pieters 1993), solid solution series (olivines and pyroxenes (Sunshine & Pieters 1998)), natural rock samples and meteorites (McFadden & Cline 2005), and unknown remote spectra of the Moon and asteroids (Hiroi et al. 1995). All these efforts were addressed to establish a direct correspondence between the individual Gaussians and physical processes responsible for the occurrence of absorption bands in reflectance spectra, and thus resolve absorption bands accounting for each component of a multimineralic material. A different technique of spectral analysis grounds on the comparison between the "unknown" spectra and suitable spectral libraries including huge amounts of measurements of natural materials. The comparison is usually achieved via automated techniques, such as multivariate statistics applied to numerical or geometrical parameters. In the present investigation, the algorithm used for spectral comparison is the Spectral Angle Mapper (SAM), which is implemented within the Envi package (Research Systems, Inc). The result is the objective evaluation of the best likelihood through a numerical score indicating the goodness of the spectral match. The materials used as Martian analogues have been selected for their implications for planetary geology, thus including basaltic rocks, mafic mineral separates and mixtures of them measured in the laboratory, and SNC meteorites from the RELAB Public Database. The mafic rocks here included, mostly cumulates and basalts, have different textural characteristics, compositions and in turn geologic implications. Compositions of all the reference materials have been measured using techniques other than reflectance spectroscopy (electron micro-

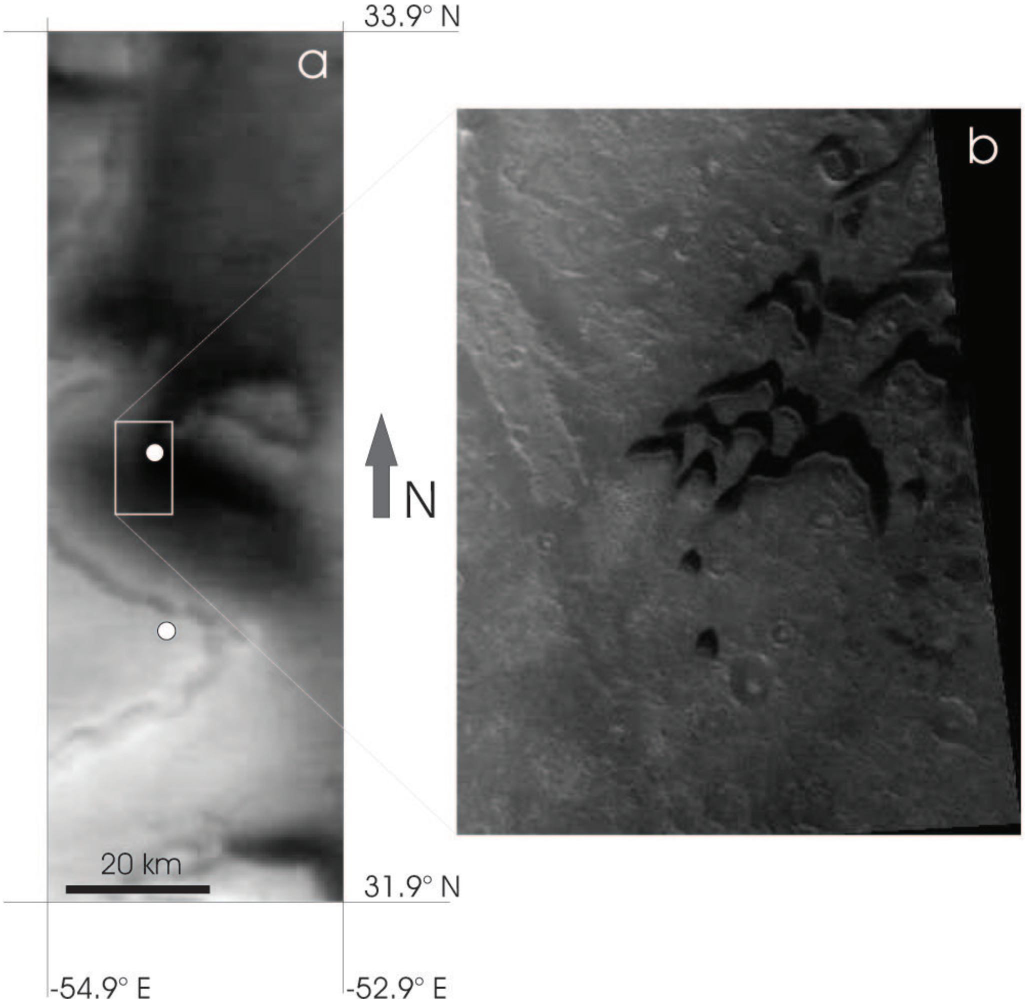

Fig. 1. a) OMEGA albedo map of the area selected for this study. The total albedo has been extracted at 1 μm. The white dots indicate pixels from which the spectra have been acquired. b) MOC NA E13-00548 image showing the peculiar morphology of low albedo materials within the channel.

probe analyses, optical microscopy, and X-ray fluorescence).

3. Results

The unconstrained MGM decomposition of both spectra results in a number of Gaussians ranging from 7 to 10, superimposed onto a three parameter continuum. Results of the MGM modeling were evaluated via statistical criteria for the best fit evaluation. Comparison with spectral libraries of Martian surface analogues has been also achieved and the results used for the interpretation. So far, the criterion used to evaluate the best fit to the measured spectrum constrains the RMS error to be of the same order of magnitude as the observational error associated with each measurement (Sunshine et al. 1990). In the present study, we use a noise level directly derived from remote measurements. It is calculated as the maximum difference between the reflectances measured at two close channels of the spectrometer. It re-

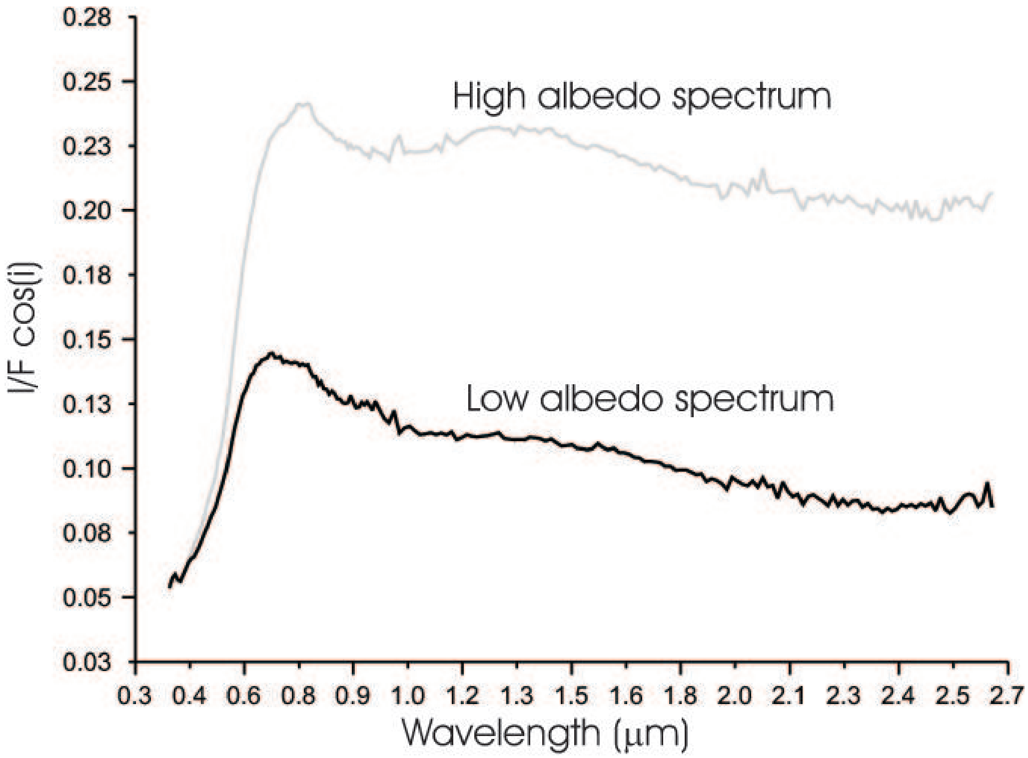

Fig. 2. OMEGA high- and low-albedo spectra used for this investigation.

sults higher than the RMS computed for each model, thus preventing the RMS to be used for detailed statistical evaluations. Based on the RMS values, we are unable to reject any of the models. In addition, the RMS effectively condenses the error at each wavelength into a single number; effectively ignoring the wavelength distribution of the errors. Thus, a poor fit at a few wavelengths are counter-balanced by a good fit at other wavelengths. Hence, we introduce a further parameter for statistical evaluations of MGM models. It is called the adjusted coefficient of determination (R2adj) and is interpreted as the fraction of the variance explained by the regression plane, weighted for the degrees of freedom allowed for each model. According to this criterion, the best regression model can be established by maximizing the R2adj. At least eight models give R2adj estimates higher than 0.999, thus allowing us to accept all these models without concern. It is obvious that we need to evaluate further parameters in order to establish if the statistically best fit to the data yields also a good description of the spectral properties of the test samples. The resulting models show that double-linear continua with negative coefficients provide acceptable models of the overall shape of the Martian spectra. However, the physical meaning of the continuum is not completely understood and as a result, its mathematical representation is the subject of active research. Therefore, there is no convincing evidence to reject any model on the basis of the continua characteristics. Band strengths are strongly dependent on the rock composition and can thus be used for quantitative estimates of relative abundances of minerals (e.g Sunshine & Pieters 1993). However, we suggest band strengths can be used as a criterion for rejecting certain model results. A statistically based criterion uses both the sensitiv-

Table 1. **LAS** MGM truth table. Criterion of 0 is reject and 1 is accept 1 preferred

Model	#G	RMS	R2adj	Cont.	S	FWHM	C	RD	Sum
1	7	1	1	1	1	0	1	0	5
2	7	1	1	1	1	0	1	0	5
3	8	1	1	1	1	1	1	1	7
4	8	1	0	1	0	1	1	0	4
5	8	1	0	1	1	0	1	0	4
6	9	1	0	1	0	1	1	0	4
7	9	1	0	1	1	1	1	1	6
8	9	1	0	1	0	1	1	0	4
9	10	1	0	1	1	1	1	1	6
10	10	1	0	1	1	1	1	1	6

Table 2. **HAS** MGM truth table. Criterion of 0 is reject and 1 is accept 1 preferred

Model	#G	RMS	R2adj	Cont.	S	FWHM	C	RD	Sum
1	7	1	1	1	1	1	1	1	7
2	7	1	0	1	1	1	1	1	6
3	8	1	1	1	1	0	1	1	6
4	8	1	1	1	1	0	1	1	6
5	8	1	1	1	1	0	1	1	6
6	8	1	1	1	1	0	1	1	6
7	9	1	0	1	1	0	1	1	5
8	9	1	0	1	1	0	1	1	5

ity of the model to detect absorption bands and the precision of the available data to fix a minimum threshold for the Gaussian intensities to be rejected. We use the same threshold as used for RMS evaluations. Hence, we could reasonably reject band intensities lower than this value. The distribution of the FWHM (full width at half maximum) as a function of band centers is compared with the existing database of MGM-derived band parameters. In particular, we use computations from decomposition of pure pyroxene separates and Martian meteorites (McFadden & Cline 2005). Based on published FWHM data, a number of models must be rejected. However, FWHM is influenced by a number of variables, such as saturated bands, amorphous and/or opaques materials, continuous chemical variations within crystals. In addition, the test spectra are likely to be the result of a number of overlapping electronic absorption processes due to different mineral species. Although the spectral interference of absorption bands has not been documented in detail in the case of solid rocks, it has been observed that it strongly affects both the band shape (broadening) and position (shifting) (Pompilio et al. 2006). Finally, the analysis of residuals can help our discussion through the identification of large discrepancies between the measured data and the models used to describe them. The residuals which exceed the amplitude of the noise threshold at certain wavelengths reasonably could be rejected. A further criterion to reject unacceptable models based on the residuals distribution accounts for the relative positions of band centers and residual peaks (Sunshine & Pieters 1993). The systematic positive offset between maximum residual errors and derived absorption band centers points out poor fit models. Besides, the symmetric distribution of residual peaks with respect to modeled band centers has been attributed to a band saturation phenomenon, which does not require additional Gaussians. In the present investigation, the fundamental criteria introduced by (Sunshine & Pieters 1993) for the evaluation of residual errors distributions do allow rejection of a number of models. After these statistical criteria are applied, we obtain a unique result for each test spectrum analysis, as shown in the truth tables 1 and 2. The best fit model of the high albedo spectrum shows absorption bands diagnostic of low- and high-Ca pyroxene, probably mixed together. Even though band widths are quite broad, we are unable to resolve further hidden components. The low albedo spectrum shows a further absorption which could be contributed by plagioclase. Unfortunately, without further knowledge about composition, we are forced to use a different method of spectral analysis. In particular, we use the mathematical comparison of the spectral morphologies via the Spectral Angle Mapper algorithm (SAM). The reference spectral libraries include particulate SNC meteorites, and mafic minerals (pyroxene, olivine and plagioclase), mafic rocks (basalts and gabbros), both solid and particulate. According to this method, we establish the best likeness with basaltic materials and plagioclase among the minerals. Partially this result is in agreement with some evidence of MGM decomposition. However, our concerns about the results of the MGM decomposition applied to unknown spectra analysis still subsist.

4. Concluding remarks

The spectral analyses reveal the MGM decomposition of solid rock samples can be used to obtain qualitative estimates of the main mineral components, at least. Statistically objective evaluation of the spectral models is complicated by the increased observational error of remote with respect to laboratory measurements. This suggests additional efforts are required to provide a better understanding regarding the spectral modeling of both laboratory and in-situ measurements of bulk rocks and particulate mixtures. The very preliminary results of the spectral analysis of Martian spectra allow us to establish the best match with basalt spectra. Basalts are very common rocks throughout the inner Solar System and at the surface of Mars, as has been inferred by numerous studies of spectral data even before OMEGA measurements. In addition, the occurrence of Tharsis lava flows and Early Hesperian ridged plain materials on the highlands surrounding Kasei Vallis has been inferred by a number of authors (Tanaka 1986,Robinson & Tanaka 1990). Nevertheless, further work is still required to improve the identification of different kind materials that OMEGA spectrometer is able to sample with very high spectroscopic detail on the Martian surface. Merging together different kind of remote data will indeed help our ability of achieving qualitative and quantitative information. In our opinion, the key for a clear understanding of Martian surface composition is to improve our geological knowledge, thus having an understanding of:

1. Hydraulics and depositional settings within mega outflow channel systems;
2. Material provenance;
3. Distribution of similar materials within the same area or different geologic context.

By collecting all the information required to provide a geologic description of phenomena as complete as possible, we could certainly have a look at Mars with an unbiased ”vision”.

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