

MODELLING OF SPECTRA WITH AND WITHOUT DUST FROM MARTIAN SURFACE BASED ON INFRARED DATA

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Abstract

This article aims to show mineral composition of Mars surface based on TES spectra (Thermal Emission Spectrometer-Mars Global Surveyor), measured in infrared thermal range. It presents how, based on TES data, spectra from selected Martian regions were modelled and interpreted after prior removal of atmospheric influences from the spectra using the Radiative Transfer Algorithm and Deconvolution Algorithm. The spectra from dark area of Cimmeria Terra and light Isidis Planitia were elaborated in cited publications.

In the case of light areas ex. Arsia Mons, spectrum of dusty weathered surface of Mars was obtained (also after removal of atmospheric influences) from averaging spectra of dusty regions of Mars. Those aforementioned spectra were used in modelling Martian surface aiming to determine their mineral composition. Deconvolution Algorithm was chosen from the mentioned methods as a tool for the modelling.

The spectra described above were used for the Martian surface modelling, such as the Hellas Basin and Martian meteorites SNC (Shergottites, Nakhilites, Chassignites), in order to determine their mineral composition. As a modelling tool one of the following methods of deconvolution algorithm can be chosen. Spectra for the modelling were obtained from the PFS spectrometer (Planetary Fourier Spectrometer) - (Mars Express) and mineralogical composition of basalts from the southern part of Poland were used for this purpose.

The method of modelling which was used to determine the mineral composition of Mars and dust can be used in determining mineral composition of selected areas on the Earth from aerial and satellite levels, e.g., soil and vegetation with the use of spectral libraries and spectra of individual plant species.

Keywords: Mars, deconvolution algorithm, infrared spectrometry, Martian dust, spectra modelling.

1. INTRODUCTION

Mars infrared spectra indicate that the majority of regions of the planet is composed of basalt, volcanic rock [1]. It is confirmed by studies carried out primarily by Martian Viking landers missions 1, 2 and Mars Pathfinder lander and wheeled robotic Mars rover named Sojourner, which investigated the selected areas directly from the surface of Mars, using the XRFS apparatus (X-Ray Spectrometer Fluorescence) and APXS (Alpha Particle X-Ray Spectrometer), [2], [3], [5]. Later research mission

was studied by rovers Spirit and Opportunity with APXS apparatus and mini-TES (Thermal Emission Spectrometer). With this equipment it was possible to determine the elemental composition of selected areas of Mars (Chryse Planitia and Utopia Planitia, the area of Meridiani Planum and Gusev Crater), and then after conversion to oxides, determine the mineral composition [2], [4],[5], [6]. Slightly later hematite has been discovered at Terra Meridiani using the TES apparatus and sulfates on the Valles Marineris and clay minerals on the polar caps, with the OMEGA apparatus (Observatoire pour la Mineralogy, l'Eau, les Glaces et l'Activité). [7]. Last mission of Curiosity rover sent to Gale crater brought the most interesting discovery, where using the CheMin (Chemistry & Mineralogy X-Ray Diffraction), SAM (Sample Analysis at Mars) and APXS apparatus (Alpha Particle X-Ray Spectrometer) it confirmed the presence of minerals which indicate the turbulent past of Mars. However, for those studies, data from a small portion of Mars was used, which does not reflect the total global petrological construction of the planet.

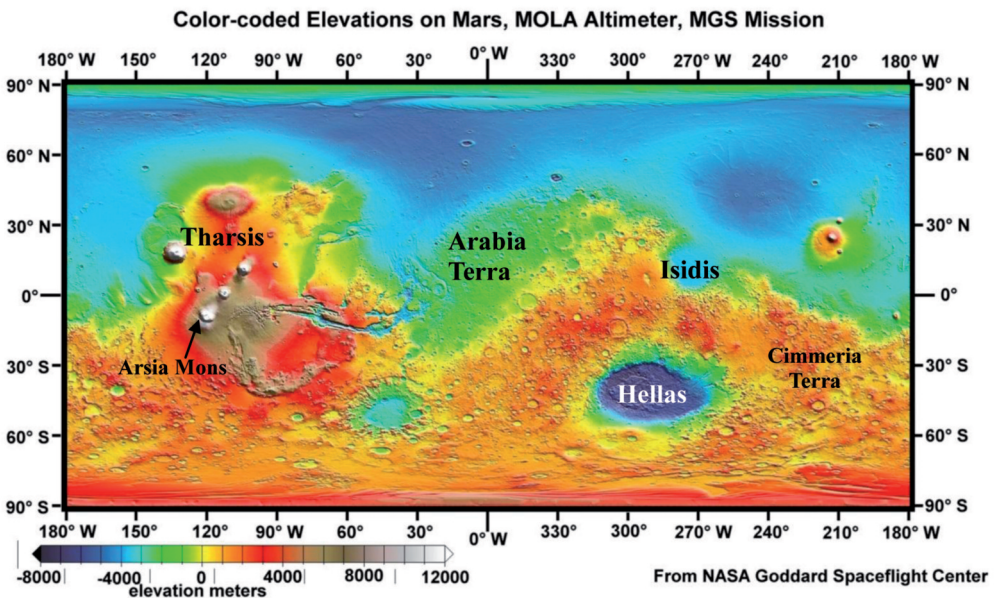


Fig. 1. Elevation map of Mars from MOLA apparatus (Mars Orbiter Laser Altimeter) (Mars Surveyor) with marked areas discussed in the article [NASA Goddard Spaceflight Center, data from MOLA, 1997-2006]. [<http://www.lpi.usra.edu/science/treiman/greatdesert/workshop/credits/mola.html>]

Infrared spectroscopy, among others, is used as a method of structural analysis for the study of minerals and rocks. Infrared absorption is caused by vibrations of functional groups and chemical bonds in the molecule of the test compound. Waves of the infrared range have length similar to the length of chemical bonds. Passing through the sample of the test substance, the radiation vibrates chemical bonds of length corresponding to the wavelength absorbed. It is possible to determine the bonds present in the sample due to the fact that each compound has its own characteristic vibration. The vibrations are quantized, that is, they can take only specific, discrete values. The relationship between the frequency of the absorbed radiation ω and initial – E1 and final – E2 internal energy of the molecule is essential. Transitions between the quantized energy states give rise to complex band and linear spectra. Most generally, transitions between energy states of the molecule consist in a simultaneous change of vibrational and rotational electron energy. Near infrared absorption corresponds to changes in energy due to vibrational crossings, resulting from mutual vibrations of individual atoms in the molecule. Rotational energy states associated with the rotation of the molecule

is located very close to each other and the transitions between them correspond to far infrared or microwave frequency range. Superposition of those two types of energy gives a certain level called rotation-oscillation level, because it is assumed that, approximately, the energy of each level is equal to the sum of rotational and vibrational energy. The wavelength of absorbed radiation determines the position of absorption band of the molecule in the infrared spectrum. The band corresponding to the longest wavelength band is called primary because it represents the smallest value of the vibrational energy in the molecule. Diatomic molecules have only one fundamental absorption band, however, multiple bands also occur corresponding to the baseband, known as overtones.

Group frequencies are vibrations associated with certain elements of structure of the molecule and are determined by movements of the nuclei of atoms during vibrations. The vibrations retain its character as they are related to the presence of the established groups in the molecule and are presented in a relatively fixed wavelengths. Some of the vibrations are only active in the Raman spectrum. In each group of the frequencies, we should be aware of factors which determine the number and position of the absorption bands. Those factors are: masses of atoms in a molecule, force constants of bonds between atoms of the molecule, symmetry of the molecule and the vibration noise. The following types of vibrations of molecules can be distinguished: symmetric and asymmetric stretching, scissoring (bending), rocking, wagging and twisting.

2. METHODOLOGY OF RESEARCH

Modelling the transfer of radiation emitted or reflected by the atmosphere with the specified component concentration characteristics of the atmosphere and surface, compared to the actual measurements, gives a very similar spectrum of the surface. An estimation of the size of grains of dust and ice crystals can be attempted [8]. Factor analysis was used for this purpose.

Factor analysis allows to conclude that even before a separation of the contributions of the atmosphere and surface, TES spectra obtained from Martian surface heated during the day exhibit high albedo (e.g. *Isidis Planitia*) (fig. 1) and can be modelled by only three emissivity components: crystals of ice, dust and black body, [9] as opposed to the surface with low albedo, where in addition to the components of the atmosphere, surface emissivity spectrum has to match. Such is the area of Cimmeria Terra where minerals were chosen to model its surface [1]. The impact of Martian dust was removed by using the aforementioned methods of radiation-transfer (Radiative Transfer Algorithm) and deconvolution (Deconvolution Algorithm) [1]. A good match was observed between the model-derived spectrum of Martian dust and the measured spectra with a high degree of haze and / or a high angle of radiation emission. There is also a good match between the derived spectrum of dust and TES spectra of the atmosphere only and between the surface spectra derived using the dust spectra of high atmospheric haze. Consistency is also observed between the measurements of atmospheric dust taken during the day and night [10].

2.1 Deconvolution algorithm

The algorithm is based on the factor analysis and it involves matching a linear combination of the spectra of atmospheric components and the surface to measured spectra. Next, a set of matching shapes of spectral components of the atmosphere are removed from the measured spectra to obtain a clean surface spectrum. It can occur that while using this method, during matching the spectra of individual minerals, the main mineral component does not match the observed shape. Those minerals are then removed. That is until only components whose shapes are suitable for the measured spectra are left in the model. The same adjusting procedure is repeated for all the minerals that have chemical composition similar to those still left from separation using the factor analysis method.

Deconvolution algorithm takes two assumptions:

- 1) measured emission spectrum can be modelled using linear combination of spectra of the surface and the atmosphere. It is assumed that the spectrum of the surface can be described using linear combination of the spectra of individual minerals and the spectral contribution of the atmosphere can also be derived by linear combination of spectra of its components;
- 2) during matching the spectral shape of the measured spectrum, all constituents of the atmosphere and surfaces are taken into account.

The infrared spectrum of the surface is normalized against a portion of the probed surface area. The linear mixing of components in emission spectrum is a sum of surface concentration products of each component and its emission factor. In addition to the emission factor of surface components, atmosphere transmission also contributes to the shape of the measured spectrum. It is assumed that the transmission of atmospheric constituents does not depend on the size of the ice crystals and dust. Hence the expression, describing the shape and intensity of the spectrum can be approximated by the product of two summations: the summation of each component of the surface multiplied by the emission factor and the transmission ratio of each component of the atmosphere multiplied by its concentration: [1], [2], [3], [4]

$$\left(\sum_{i=1}^n c_i \cdot e_i \right) \cdot \left(\sum_{j=1}^m a_j \cdot t_j \right) = d \quad (1)$$

d – shape of the mixed spectrum;

c_i – concentration of the i -th component of the surface;

e_i – emission factor for the i -th component of the surface;

a_j – concentration of the j -th component of the atmosphere;

t_j – the transmission coefficient for the j -th component of the atmosphere.

Equation (1) is not linear because of the starting components..

In order to perform a linear deconvolution an approximation is used, which linearizes the relationship of the three components of the spectrum (2).

$$x \cdot y = \alpha \cdot x + \beta \cdot y + \gamma \cdot i \quad (2)$$

where:

x - spectrum of the emission factor;

y - spectrum of the transmission ratio;

i – spectrum of the black body;

$\alpha \beta \gamma$ – constants.

Using this approximation to the expression [9] system of linear equations is obtained describing the mixture of emission and transmission spectra by ever changing concentrations of the atmosphere and surface components: (3)

$$\alpha \left(\sum_{i=1}^n c_i e_i \right) + \beta \left(\sum_{j=1}^m a_j t_j \right) + \gamma i = d \quad (3)$$

Concentrations of minerals derived with this method should be scaled because the initial components of the sum are multiplied by additional constants: α and β . For this purpose, the actual concentration of the surface components can be derived from the formula: (4) [10].

$$c_i' = \frac{\alpha c_i}{\sum_{i=1}^n \alpha c_i} \quad (4)$$

In a deconvolution process, a mineralogical part is based on the choice of the minerals whose spectral shape fits the measured spectrum originating from Mars. The infrared spectrum of the surface is modelled by applying the linear combination of spectra of selected minerals, which then are normalized against the measured surface area with the previously separated atmosphere. Note that the selection of minerals in Martian rocks are obtained only as relevant percentage values [1]. Minerals are selected on the grounds of the expected composition of Martian rocks such as basalt and its derivatives, that is, from silicate minerals: pyroxenes, amphiboles, alkali and plagioclase, feldspars and carbonates optionally present apart from other oxides and hydroxides and olivine. The additional use of weathered basalts allows for modelling the Martian surface spectra showing a high content of dust on the surface and in the atmosphere.

PFSLook software has been developed for this purpose (fig. 2, 3). The program is written in C++ based on adding the spectra of minerals in the relevant percentage - the final spectrum containing 100% of the minerals.

This modelling method used to determine the mineral composition of the Martian surface and dust can, in turn, be used to determine the mineral composition of selected areas of Earth with the use of aerial and satellite imagery, e.g. soil and vegetation with the use of spectral libraries of minerals and various spectra of selected plant species.

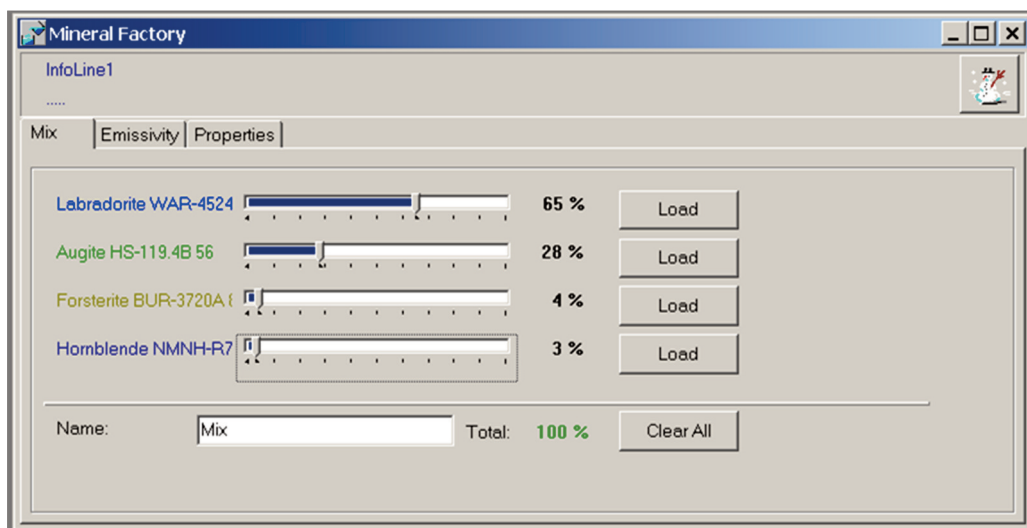


Fig. 2. PFSLook software, linear addition of infrared spectra of minerals [Software made by M. Morawski to own calculations (modification 2010)].

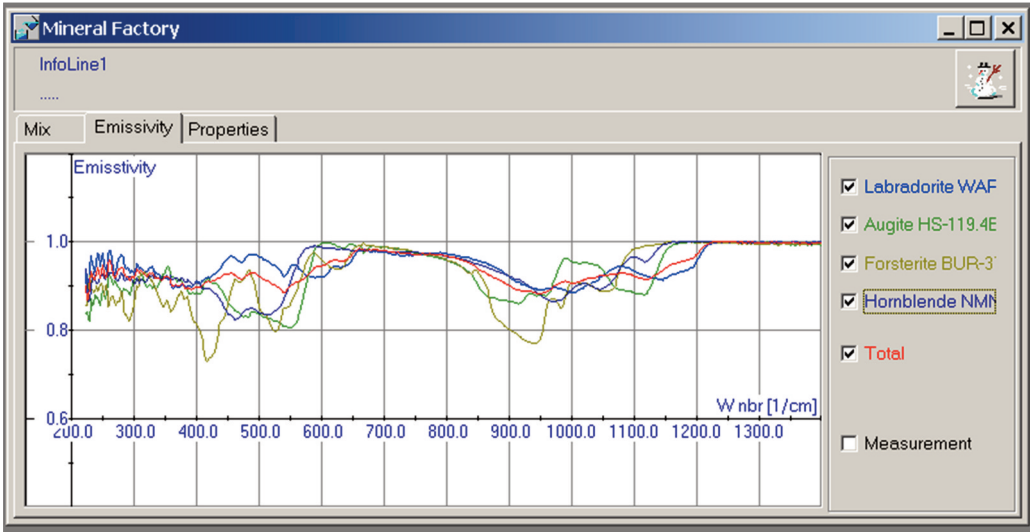


Fig. 3. Result of linear addition of minerals spectra - red spectrum [Software made by M. Morawski to own calculations (modification 2010)].

3. MODELLING OF MARTIAN SURFACE

Mars surface modelling involves the use of infrared spectra of minerals ($200\text{--}1800\text{ cm}^{-1}$) from the ASU library available at speclib.asu.edu (2009) using the deconvolution method. The spectra were used in a suitable percentage according to a predetermined desired mineralogical composition of the rock. The resulting spectra were later compared to the above mentioned spectra of Mars with separated atmosphere.

It is shown in the paper [1] that the spectrum of Mars from Cimmeria Terra is qualitatively similar to the terrestrial spectrum basalt from the Deccan Indian subcontinent (fig. 5). Deccan Basalt gives a very similar shape of the spectrum to that developed in the publication from Cimmeria Terra, independently by two methods - radiative transfer (Radiative Transfer Algorithm) and deconvolution (Deconvolution Algorithm). Cimmeria Terra area has relatively low dust influence as indicated by low albedo (Lambertian albedo <0.18) [11], therefore, not weathered rocks can be used for comparisons with larger particle sizes of $700\text{--}1\,000$ microns which – theoretically - do not contain minerals that have been subjected to weathering.

Results from the quantitative analysis of mineralogical composition show that Deccan basalt consists mainly of plagioclase (65%), contains calcium pyroxene (28%), opaque minerals (4%) and 3% residues [1], (Fig. 4). This paper also presents a laboratory model of the spectrum which is an approximation of the Martian rock spectrum, created by the superposition of spectra of suitable minerals. It contains 66% plagioclase, 17% calcium pyroxene, 7% iron smectites and 10% rest. The comparison of the two is made, Deccan and laboratory, after averaging of TES spectral resolution (fig.5), (tab.1), [1]. As for the rest, hornblende was used for a comparison, which is an amphibole and often accompanies basalts. The base plagioclase consists of labradorite, bytownite, anorthite. Labradorite is often used in the modelling of spectra as plagioclase containing Na and Ca and often forming part of basalt [12]. TES measurements have not detected weathered minerals, in this case, phyllosilicates, which include clay minerals, but it is assumed that they may be present in the spectrum below 15% [1]. Therefore, smectite has been used as a product of weathering of volcanic rocks.

The above-mentioned spectra from the dark and dusty, light area of Cimmeria Terra, were averaged and subjected to own modelling using PFSLook software by deconvolution method using mineral spectra library in the thermal emissivity band (ASU Thermal Emission Spectral Library) [13].

For comparison the same operation of spectrum modelling for basalt of Deccan basalt composition was performed [1], using online library (ASU Thermal Emission Spectral Library). All of the following descriptions of the modelling are attempts to match better components of known weathered and not weathered basalts to the Martian surface spectra with separated atmosphere, taken from the papers [1], [10], [12].

Immediately, it can be noticed that the shape of the spectrum is given by primarily dominant components: mineral plagioclase group - labradorite and calcium pyroxene - augite. The other of those minerals was chosen because of its shape fitting the spectrum of Mars. Diopside mineral from the library has sharper spectral characteristics that would be able to interfere with the spectrum and therefore, is not suitable for the modelling of Martian surface. Minerals that have been detected in dark Deccan basalt indicate the content of magnetite so that mineral was also used for modelling. As it can be seen (fig.12) modelled spectrum basalt gives perfect shape with respect to the spectrum of Deccan basalt measured directly. In the range of about 950- 1110 cm^{-1} slight maximum can be observed, because of pyroxenes - in this case - from augite. Selected percentage composition, (tab.1, column 2), [1] established by Christensen gives a better approximation of the shape of the spectrum of Mars, namely smoothes the 950 - 1110 cm^{-1} area of the band. This is achieved by using a lower content of pyroxene mineral and for smoothing the spectrum - smectite is used (fig.4, fig.12). This is a small peak, but it is characteristic of the Martian meteorites that have similar mineralogical composition to basalt. For example, Nakhla meteorite has olivines, clinopyroxenes (augite), plagioclase (anorthite) and Fe-Ti oxides and even carbonates such as siderite.

Pyroxene often included in the meteorites is bronzite. It is a Mg and Fe pyroxene (orthopyroxene). If you change augite for bronzite you get smoother part of 950 – 1110 cm^{-1} band with no maximum. The spectrum takes the form most similar to the spectrum of Mars from the Cimmeria Terra (fig.4), (fig.5), (fig.12). It turns out that bronzite is a pyroxene that is most useful for modelling, to get the best match with the Martian spectra.

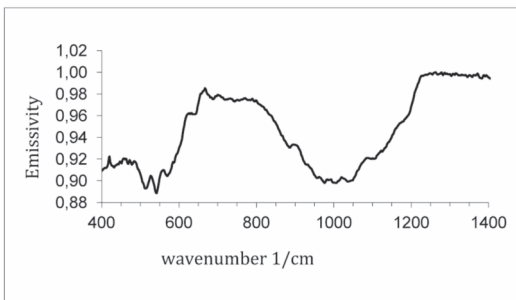


Fig. 4. The spectrum model based on Deccan basalt spectrum using the Deconvolution Algorithm [13].

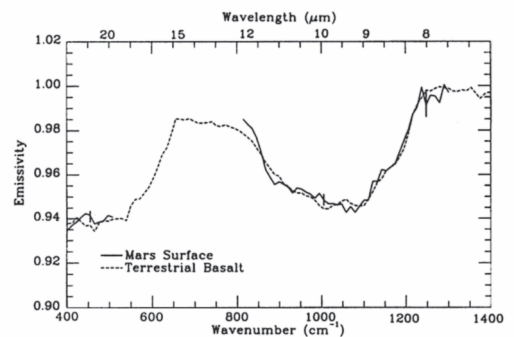


Fig. 5. Comparison of the Cimmeria Terra spectra and Deccan basalt with atmosphere separated by the Radiative Transfer Algorithm [1], (Tab.1).

Turning to modelling of the Martian surface spectra using radiative transfer and deconvolution methods [1],[9] already selected percentage composition of minerals was used. The first method uses 2% quartz, 53% plagioclase, 19% clinopyroxene, 12% olivine, 11% layered silicate and 2% gypsum. However, in the second - 3% quartz, 45% plagioclase, 26% clinopyroxene, 12% olivine, 15%

phyllosilicate (tab. 2a), [1]. One of the phyllosilicates found in rock on larger scale is biotite and therefore it was used for spectrum. After modeling of the spectrum, it was found that the first percentage composition is so much better, it smoothes 400-540 cm^{-1} range. This is done by reducing the percentage content of clinopyroxene (augite) and phyllosilicate (biotite) than in the second case. Pyroxene and biotite in the band have very deep minimum. In both cases, a small peak is observed around 1000 cm^{-1} , which is derived from augite, and is not observed in the spectrum of Mars.

When we limit the number of minerals and apply only basic minerals in both methods, plagioclase and clinopyroxene, we notice that the shape of the spectrum becomes similar to the shape of the percentage composition of Deccan basalt where plagioclase and pyroxene are most abundant (tab. 2b), [1]. In contrast, when we use 100% fixed percentage composition: 56% labradorite and 44% augite as a blend of 70% and the remaining 30% will be hematite, we receive an interesting spectrum with a smooth part 900 – 1,100 cm^{-1} of the spectrum (tab. 2b), [1]. It can be seen (after self-modeling as well), that the part of the peak at around 600-700 cm^{-1} takes the exact shape of the measured spectrum of Deccan basalt.

For comparison, the spectra of some basalts and mafic rocks occurring in Poland with known percentages of minerals can be shown. Basalts from the Mountain of St. Anne's (Sankt Annaberg), (50° 27' 22" N, 18° 10' 3" E), (tab.3) consist of 58% augite, 14% nepheline, 12% olivine and 10% magnetite and the rest are apatite, zeolite and calcite [14]. The modeling nepheline was replaced with microcline, because spectral library does not contain the nepheline spectrum. Looking at the shape of the spectrum of basalt from the Mountain of St. Anne's (fig.6) (fig.13), we can see that its shape resembles that of the spectrum of famous Martian meteorite ALH84001 (fig.7), where augite pyroxene is the dominant component which is visible around 940- 1060 cm^{-1} band, where the maximum originating from the mineral and the minimum in the range of ~ 510 cm^{-1} can be observed. Carbonate mineralization has been identified in the ALH84001 meteorite and bacteria may be responsible (fig.13). In contrast, the entire spectrum of basalt from Mountain of St. Anne's is similar in shape to the spectrum of Mars, which confirms that the surface of Mars in Cimmeria Terra area is made of basalt.

Gabbro is the deep-sea basalt equivalent which is the rock that emerges within the earth's crust. It has the same mineral composition as basalt, having developed only macroscopic mineral crystals. An olivine gabbro of Nowa Ruda, (50° 34' 45.17" N, 16° 30' 5.25" E), (tab.3) in the Sudety could be an example, which contains 57% bytownite or labradorite, 15% augite, 10% enstatite and 15% olivine (forsterite). The rest are ilmenite, magnetite and apatite. The shape of the gabbro spectrum resembles the spectrum of the ALH77005 meteorite, (fig. 6) (fig. 7), which is composed mainly of lherzolite - alkaline igneous rock of peridotite class, consisting mainly of pyroxene (rhombic and monoclinic or ortho and clinopyroxene). Especially around 450 cm^{-1} band, with a maximum derived from forsterite, the similarity is clear (fig. 13).

Gabbro from Sobótka (50° 53' 55" N, 16° 44' 40" E), (Tab.3) area in the Sudety consists of 52% labradorite, 35% augite and 10% enstatite. Augite substituted with bronzite in the spectrum of gabbro from Sobótka we will get a smooth part of the spectrum in the range of 950- 1110 cm^{-1} , which starts to resemble the Cimmeria Terra spectrum (fig. 14), as well as some characteristics of the ALH84001 meteorite spectrum (fig. 7) due to a minimum at ~ 510 cm^{-1} band and a small peak at around 900 and 1000 cm^{-1} bands which is due to pyroxene. The transformed spectra also show similarity to the modelled spectra of the surface of Mars by using two methods: radiative transfer (Radiative Transfer Algorithm) and deconvolution (deconvolution algorithm), where only basic minerals, labradorite and augite were used.

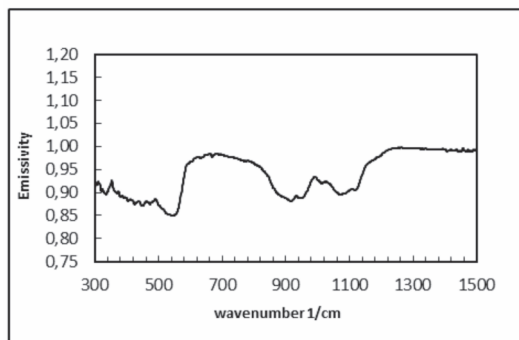


Fig. 6. The modelled spectrum of basalt based on the mineral composition of basalt from Mountain of St. Anne's (Sudety) using a deconvolution algorithm [13], (Tab.3).

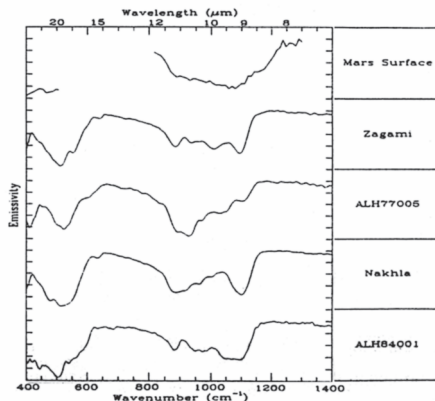


Fig. 7. Martian meteorites spectra [1].

To summarize, we can note that:

- Compliance of Deccan basalt rock spectrum with the spectrum from Cimmeria Terra is qualitative.
- Mineralogical analysis of Deccan basalt is quantitative and based on the available ingredients acquired from ASU online library. speclib.asu.edu (2009).
- In order to form the laboratory mineral superposition in the spectrum matching the spectrum from Cimmeria Terra, deconvolution method was used (fig. 12-16).
- Finally, the comparison was made of the quantitative analysis and mineral spectral superposition with chosen mineral components composition (using deconvolution), of such percentage as table 1 indicates [1], (ASU library speclib.asu.edu (2009)).

The areas of Mars with higher albedo (> 0.18) are considered to be dusty. Dust can be both on the surface and suspended in the atmosphere. The particle size is estimated at < 40 microns. Apart of Hellas, other areas with high dust coating can be found in Arabia Terra and Tharsis [11], [12]. Although high albedo spectrum can sometimes be modelled with only three ingredients: dust, ice crystals and black body, after the separation of the atmosphere as in the paper [12] the surface shows a complex spectral shape that can be modelled by a deconvolution and a selection of appropriate ingredients. Looking at the spectrum of the atmosphere separated from the dusty surface of Mars (fig. 9), deep minima can be observed in the vicinity of $820\text{-}830\text{ cm}^{-1}$ band, 1380 cm^{-1} and $1,580\text{ cm}^{-1}$ band. The spectrum of weathered basalt with a particle size of $0\text{-}10$ microns almost exactly fits the spectrum of the surface of Mars, with the exception of the $1380\text{-}1580\text{ cm}^{-1}$ band, where $1,380\text{ cm}^{-1}$ minimum is not present in the spectrum of weathered basalt. A minimum at $1,580\text{ cm}^{-1}$ and sharp peak at 1630 cm^{-1} is from the water bound in the minerals, and $820\text{-}830\text{ cm}^{-1}$ minimum is interpreted as originating from carbonates (fig. 9), [12]. Indeed, carbonates have minima in those areas (calcite, magnesite) but also clay minerals. Carbonates as well as clay minerals are formed in the presence of water, but clay minerals are usually products of chemical weathering of plagioclase and pyroxene, basalt minerals and inorganically form on a large scale. Carbonates are minerals not commonly found in igneous rocks, however, their existence can also be considered as probable. They may be, but not directly, weathering products of olivine contained in the basalt.

For dusty surface modeling, fine grained clay minerals spectrum was used as available in ASU library speclib.asu.edu (2009), because shapes of their spectra are similar to the shape of the spectrum of dusty surface of Mars, but also to the shape of weathered basalt which in terrestrial conditions began to erode into clay minerals. Products of such basalt weathering are primarily smectites such as montmorillonite, its variant - hectorite and palygorskite, kaolinite and dickite. When a spectrum from the dusty area is modelled adding the appropriate percentage of major components of basalt (augite 20% and andesine 20%) 30% dickite and 30% palygorskite, then the shape of such spectrum starts to resemble the spectrum of the surface of Mars. Palygorskite plays a major role here because it has a double peak shape similar to the dusty surface of Mars, only shifted from 1380 cm^{-1} to 1430 cm^{-1} band. The water absorption peak is also shifted from 1630 cm^{-1} to 1700 cm^{-1} band. Deep, wide dickite minimum reaching the areas of $1,640\text{ cm}^{-1}$ band deepens the shape of the spectrum at this point, resembling the shape of the spectrum of weathered basalt, compared with the spectrum of dusty surface of Mars (fig. 8).

Mineral composition of the basalt from Mountain of St. Anne's [14], (tab. 3) indicates typical earth basalt. The same as modelled mineral composition of the Deccan basalt with augite replaced by bronzite, may in fact reflect the potential rock on which weathering of minerals occurred. Thus, dusty Martian spectrum modeling can also rely on superposition of clay minerals spectrum mixed with the spectrum of not weathered basalts. 40% of the spectrum of basalt from Mountain of St. Anne's mixed with 40% palygorskite, 10% dickite and 10% calcite does not give the perfect match to the spectrum of dusty surface of Mars, but is much closer to its shape, it may in fact suggest the occurrence of clay minerals and a little of carbonates on the surface of Mars. The use of the Deccan basalt as the base gives a better smoothing of the spectrum around $880 - 1,120\text{ cm}^{-1}$ band. A minimum at 830 cm^{-1} is shifted to 880 cm^{-1} , which is because of the influence of calcite (fig.8). When hectorite is added to this mixture in a percentage of 70% to 30% (hectorite), it gives the minimum at around 830 cm^{-1} band and the deepened minimum and maximum of water absorption peak at $\sim 1540\text{ cm}^{-1}$ (min) and 1630 cm^{-1} (peak), which resembles the shape of the spectrum of dusty Martian surface, as hectorite has minima in these exact places (fig. 15).

Basalt on Earth can erode to the depth of a few to dozens of meters. Weathered basalt lavas in the Polish Sudety mountains are a good example. Weathered are can be divided into different zones like: smectite- kaolinite zone and kaolinite – halloysite zone – iron minerals weathering zone, e.g. pyrite. The waste of Krzeniów [14] contains 90-100% smectite, 5-10% kaolinite, magnetite and goethite. For the purpose of modeling 90% of smectite, 7% of kaolinite and 3% magnetite proportion was established (fig. 8). Conversely, another waste of Dunin at the Sudety mountains [14] contains halloysite, kaolinite and magnetite, where 90% halloysite, 7% kaolinite and 3% magnetite proportion was established. Immediately you will notice that the spectrum of Krzeniów weathering is similar in shape to the dusty surface of Mars. It has the minimum of about $1,070\text{ cm}^{-1}$ band, which is not present in the spectrum from Mars and the minimum of $1,550\text{ cm}^{-1}$ and the water absorption peak of $1,630\text{ cm}^{-1}$ band, also visible in the spectrum of Mars. Waste of Dunin gives a very smooth spectrum with virtually no visible water absorption peak that is caused by the presence of halloysite, which does not have such a peak, as it is dehydrated form of hydrohalloysite. If one adds to those spectra 10% calcite, there will be a minimum at 880 cm^{-1} and the deepened minimum at $1,550\text{ cm}^{-1}$ band caused by calcite. However, the occurrence of calcite mineral on Mars is very controversial because of the presumably not sufficiently abundant aquatic environment where it could form in such quantities. Despite all this, calcite mineral fits well to the shape of the spectra of dusty Martian surface.

It is also possible to model the basalt surface without dust by mixing its spectrum with the spectrum of the dusty surface at an appropriate percentage. Mixing the spectrum from dusty surface always causes smoothing of the shape of the spectrum from dust-free surface, it is dependent on the ratio in which they were mixed. It is even possible to get the spectrum of the surface mixed with

some additional peaks, and so is the case of mixing 70% of weathered basalt from Krzeniów with calcite and 30% basalt from Mountain of St. Anne's (tab. 3). In contrast, the mixture of 70% Deccan basalt with bronzite and 30% waste of Dunin smoothes and reduces the minima of the spectrum of basalt preserving the overall shape of the spectrum (fig. 16). It follows that even if we consider a given area as dust-free, it may be coated with a little amount of dust which will not be particularly visible in the spectrum.

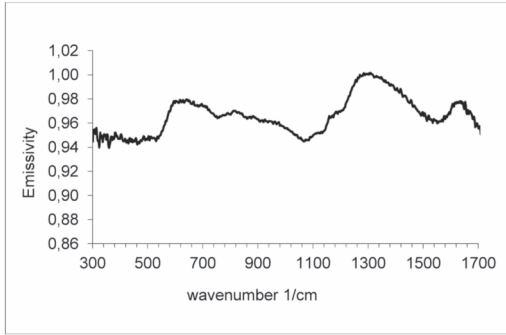


Fig. 8. Weathered basalt spectrum modeled based on the weathered basalt from Krzeniów (the Sudety) using the Deconvolution Algorithm [13].

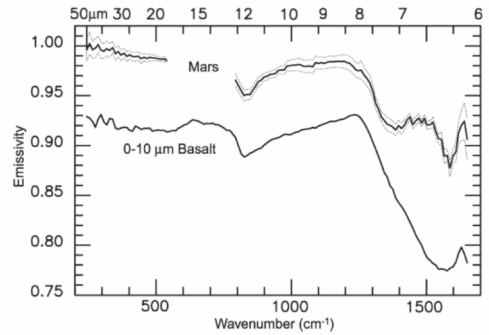


Fig. 9. Comparison of the spectra of Martian dusty surface and fine grain basalt with separated atmospheric influence by the Radiative Transfer Algorithm [12].

Sometimes, the problem of matching the spectra in the range of about 800 cm^{-1} to about 1,400 cm^{-1} is due to the different wavelengths in the Christiansen frequency range in compounds (fig. 10). That frequency identifies oxygen compounds such as molecules belonging to the crystal matrix of minerals and is defined by SCFM. ($\text{SCFM} = \text{SiO}_2 / \text{SiO}_2 + \text{CaO} + \text{MgO} + \text{FeO}$). SCFM is an association of Christiansen frequency with the transparent area of the part of the spectrum responsible for the oscillation of SiO_2 molecule. For example, the Christiansen frequency of quartz (fig. 11) fits around 7.6 microns (1,315 cm^{-1}). Between 8.2 and 9.2 microns (1,219 and 1,086 cm^{-1}) is the residual radiation (reststrahlen) and the broad transparency peak is around 11.5 microns (869 cm^{-1}) [16], [17].

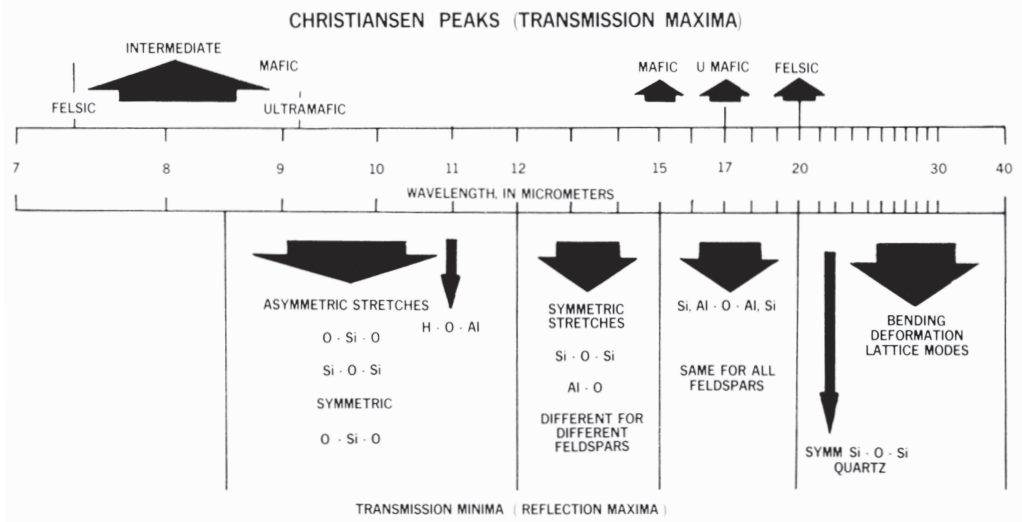


Fig.10. The example showing the Christiansen frequency in mafic rocks in transmittance [15].

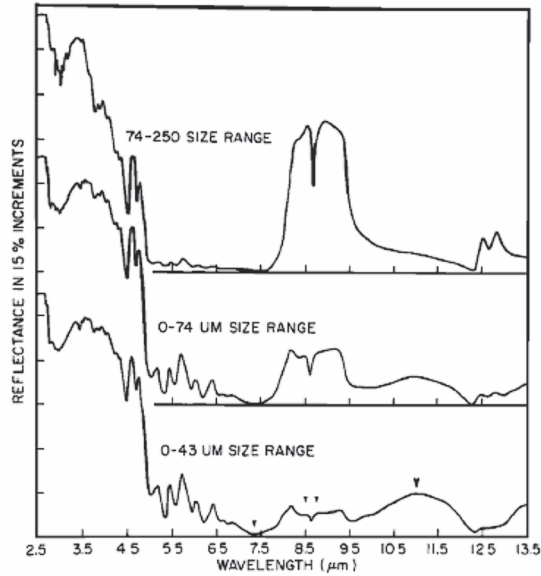


Fig. 11. The example of reflectance quartz spectra in three size range. The Christiansen frequency is pointed by single small arrow, double arrow points band derived from residual radiation (reststrahlen) and thicker arrow indicates the transparency peak [16].

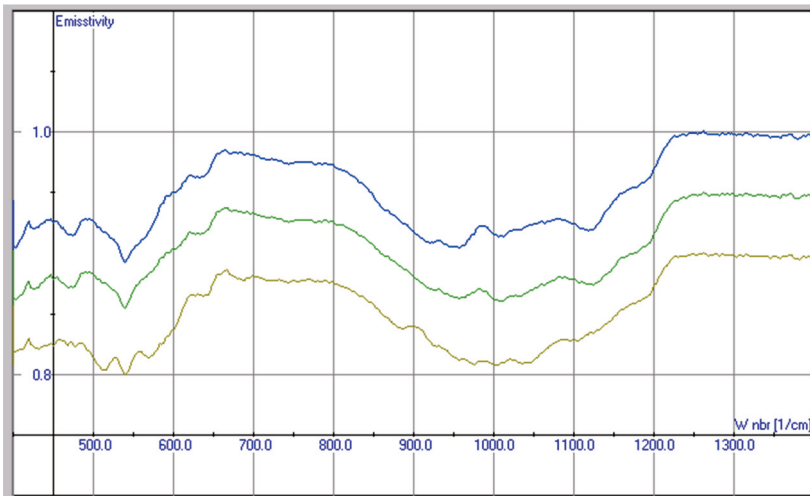


Fig. 12.

- 1-(first from the top) spectrum of Deccan basalt, 65% labradorite, 28% augite, 4% forsterite, 3% ormlende, according to [1] (tab. 1).
 - 2-(second from the top) The modeled spectrum of Deccan basalt, 66% labradorite, 17% augite, 7% smectite, 10% hornblende, according to [1] (tab. 1).
 - 3-(third from the top) Deccan basalt spectrum with bronzite instead of augite, 65% labradorite, 28% bronzite, 4% forsterite, 3% hornblende.
- Mineral spectra for modeling come from the ASU library speclib.asu.edu (2009).

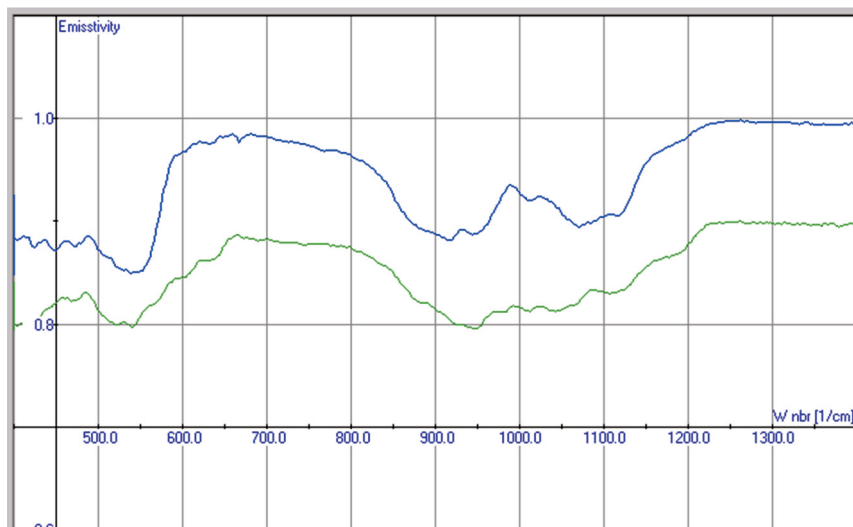


Fig. 13.

1 (first from the top) The spectrum of basalt from the Mountain of St. Anne: 58% augite, 20% microcline, 12% forsterite, 10% magnetite.

2 (second from the top) The spectrum of gabbro from Nowa Ruda, 57% labradorite, 15% augite, 10% enstatite, 15% forsterite + apatite, magnetite, ilmenite 3% (tab. 3).

Mineral spectra for modeling come from the ASU library speclib.asu.edu (2009)

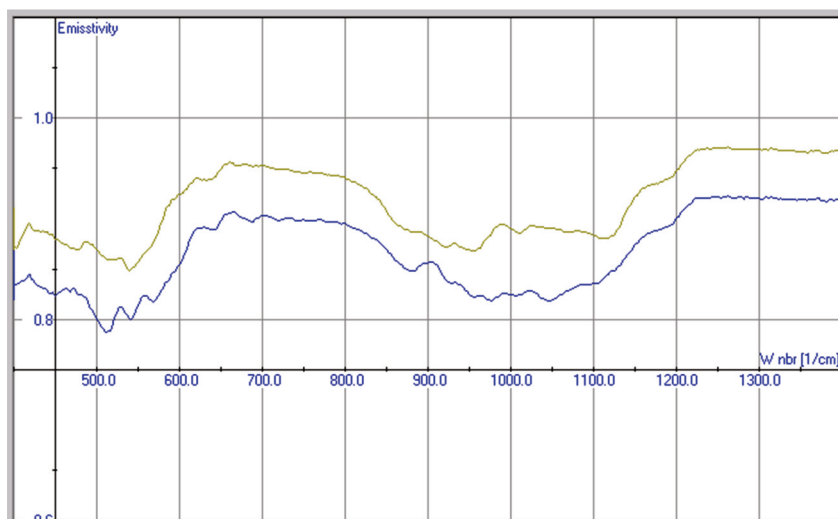


Fig. 14.

1 (first from the top) The spectrum of gabbro from Sobótka: 52% labradorite, 35% augite, 10% enstatite.

2 (second from the top) The spectrum of gabbro from Sobótka with bronzite instead of augite: 52% labradorite, 35% bronzite, 10% enstatite (tab. 3).

Mineral spectra for modeling come from the ASU library speclib.asu.edu (2009).

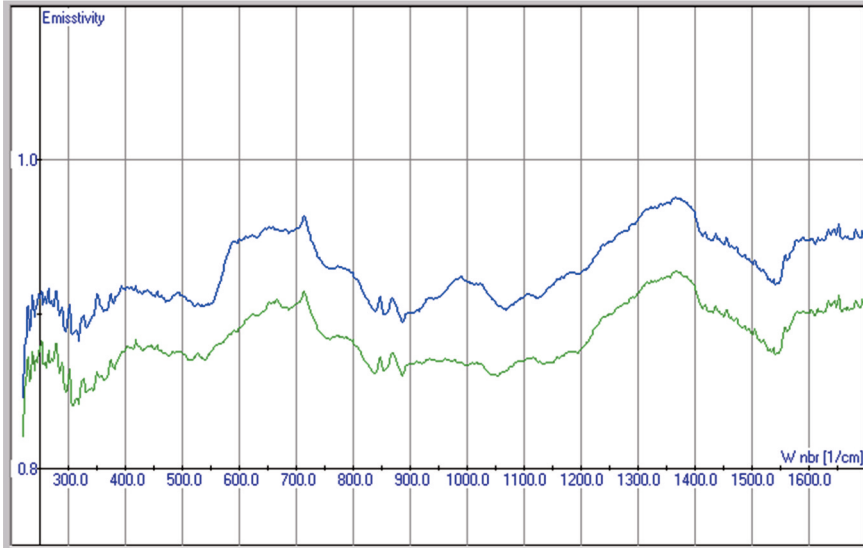


Fig. 15.

1 (first from the top) spectrum of the mixed 70% (40% basalt from the Mountain of St. Anne (Tab.3) + 40% palygorskite, 10% of calcite and 10% dickite) + 30% hectorite.
 2 (second from the top) spectrum of the mixed 70% (40% (labradorite 65% bronzite 28% magnetite 4% ferrohornblende 3%) + 40% palygorskite, 10% of calcite and 10% dickite) + 30% hectorite.

Mineral spectra for modeling come from the ASU library speclib.asu.edu (2009).

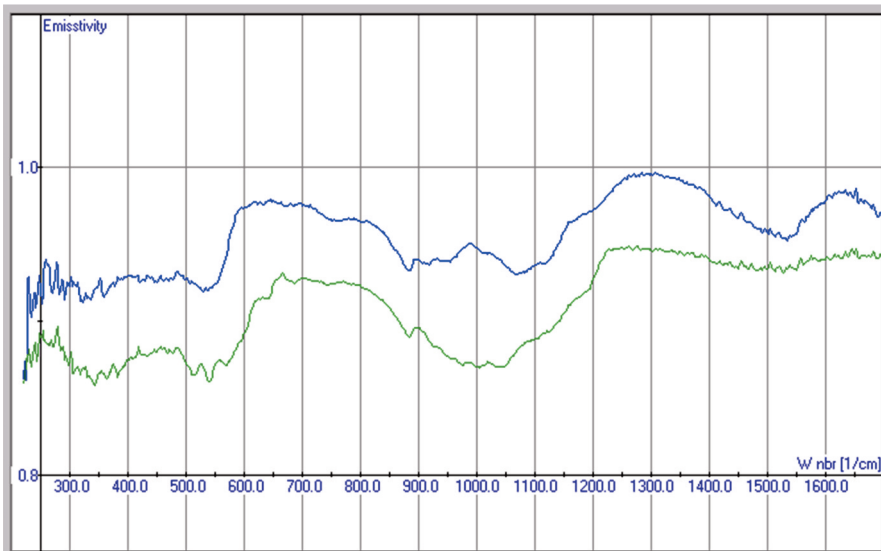


Fig. 16.

1 (first from the top) Mixed spectrum 70% of Krzeniów weathering of calcite + 30% basalt from the Mountain of St. Anne (Tab.3).
 2 (second from the top) Mixed spectrum 70% (labradorite 65% bronzite 28% magnetite 4% ferrohornblende 3%) + 30% waste of Dunin.

Mineral spectra for modelling come from the ASU library speclib.asu.edu (2009).

The percentage of minerals in the rock, used in modelling

Tab. 1. The percentage of minerals in the sample of Deccan basalt and model sample [1].

minerals	Mineral content measured in%	Modelled content in %
plagioclase	65	66
Ca pyroxene	28	17
Minerals dark	4	0
Fe- smectite	0	7
other	3	10
the sum	97	100

Tab. 2a. Percentage of minerals selected by deconvolution algorithm and by radiative transfer algorithm in the spectrum of Cimmeria Terra after atmosphere separation [1].

minerals	Radiative transfer method, the composition in%	Deconvolution method, the composition in%
quartz	2	3
plagioclase	53	45
clinopyroxene	19	26
olivine	12	12
phyllosilicates	11	15
gypsum	2	0
the sum	99	101

Tab. 2b. Percentage of minerals selected by deconvolution algorithm and by radiative transfer algorithm in the spectrum of Cimmeria Terra after atmosphere separation [1].

minerals	Radiative transfer method, the composition in%	Deconvolution method, the composition in%
plagioclase	65	56
clinopyroxene	35	44
sum	100	100

3.1. Description of clay minerals used for modelling

Polygorskite $(\text{Mg, Al})_2\text{Si}_4\text{O}_{10}(\text{OH}) \cdot 4\text{H}_2\text{O}$ Frequently of hydrothermal origin can be found in igneous rocks, where it forms a gap filling. It occurs in melaphyrs and porphyre crevices. In sedimentary rocks it is genetically related to the processes occurring during sediment accumulation (lake and lagoon forms). It often occurs in paragenesis with montmorillonite. Very fine-grained variety is present in sedimentary rocks, sometimes as the main ingredient.

Montmorillonite $\text{Al}_2\text{O}_3 \cdot \text{SiO}_2 \cdot n\text{H}_2\text{O}$ belongs to the group of smectites. This group is widespread in sedimentary rocks and low temperature hydrothermal formations. It fills the crevices in igneous rocks. And creates very fine-grained, scaly crystals with a diameter not exceeding 1 mm. It occurs in dense, wax-like or earthy, powder-like structures. It sometimes creates fine-grained aggregates, taking „worm-like” or spherulitic forms. Montmorillonites are formed as a product of

weathering of igneous enamel - tuffs and tuffites in alkaline and strongly salinated environment. They are sometimes found in marine and lacustrine sediments usually accompanied by illite, kaolinite, halloysite, quartz and calcite. They are built of packets of type 2:1, which allows saturation with water, and in consequence causes swelling of the mineral.

Kaolinite $Al_4 [Si_4O_{10}] (OH)_8$: It is a weathering product of feldspars and other aluminosilicates. Kaolinite form in hydrothermal settings. It formed in acidic environment, by the action of juvenile waters rich in CO_2 , where it grows as small tablet or plate-shaped crystals. Kaolinite usually occurs in dense earthy and semi-crystalline clusters. Monomineralic accumulation are kaolin rocks. Subgroup includes minerals of two-layered dioctoedric packets of type 1:1, which allows water saturation.

Dickite $Al_4 [(OH)_8 Si_4O_{10}]$ Variety of kaolinite. Formed in hydrothermal and sedimentary environments. It occurs in porphyres, rhyolites and sedimentary rocks. Coincides with kaolinite. It occurs in clusters of fine, squamous, compacted conglomerates, forms coatings and sediments. It is soft, bendable and translucent. It is similar to kaolinite.

Hectorite $Na_{0.4}Mg_{2.7}Li_{0.3}Si_4O_{10}(OH)_2$ Variety of montmorillonite. Hydrothermal and sedimentary product. Occurs near volcanic rocks and tuffs.

Halloysite $Al_4 (OH)_8 / Si_4O_{10} \cdot 10H_2O$ Variety of kaolinite. Is formed in acidic environments, particularly in the presence of sulfuric acid as a result of weathering of pyrite and marcasite. The product of weathering of pyroclastic and igneous rocks and hydrothermal activity. It is a dehydrated variety of hydrohalloysite. It usually forms very small, very fine-grained tubular crystals visible under very high magnification and occurs in dense, massive clusters (resembling porcelain), earthy and powder-like ones. It is similar to montmorillonite and kaolinite, coincides with Gibbsite, montmorillonite, kaolinite, allophane and marcasite. [18]

Tab. 3. Examples of mineralogical composition of basalt and gabbro (extracted from [14])

gabbro composition of Lower Silesia - around Sobótka
52% labradorite (plagioclase)
35% augite (pyroxene Ca)
10% enstatite (pyroxene Mg-Fe)
the rest - ilmenite, magnetite, apatite
gabbro composition around Nowa Ruda
57% bytownite and labradorite (plagioclase)
25% augite (pyroxene)
15% olivine
the rest, ilmenite, magnetite, apatite
There are variations with 75% anorthite (plagioclase)
basalts from Mountain of St. Anne
58% augite (pyroxene)
14% nepheline (silicate from feldspathoid group)
12% olivine
10% magnetite
the rest - apatite, zeolite and calcite

4. MARTIAN DUST MODELLING FROM OVER THE HELLAS CRATER

There is a meteorite crater roughly 2,300 km in diameter on the southern hemisphere of Mars. Its deepest point is 7km located on the north-western side of the crater. Due to the prevailing atmospheric pressure of about 11 mb at the bottom of Hellas crater, which is higher compared to the average pressure on Mars (6 mb) that the possibility of the occurrence of liquid water exists, since it has exceeded triple point of H₂O. Therefore, there is a high probability of water existence associated with minerals such as sulfates, carbonates, clays and oxides.

In order to model Hellas area, the simulated Mars surface composition was used made from powdered minerals in a suitable percentage [19]. In contrast, measurement samples of the simulated surface of fine-grained and silt form was obtained by the authors [19]. The percentage composition of minerals is chosen so that it reflects two dusty types of Martian surface: the silicate minerals type - P-MRS (Phyllosilicatic Mars Regolith Simulant) and a type with a high content of sulfates - S-MRS (Sulfatic Mars Regolith Simulant). The mineral composition of those two surfaces is presented in Table (Tab.4), [19].

Spectrometric Research shows that Hellas region is mainly built of non-weathered and weathered basalt, where clay minerals are predominant. Therefore, surface modeling is based primarily on modeling the mineral composition of different types of basalts.

The mineral composition of dust tells us a lot about the surface of Mars. Spectral minimum of dust from PFS in emissivity of the surroundings of Hellas has two characteristic bands: 1,075 cm⁻¹ and 1,160 cm⁻¹.

Modeling of this spectrum by linear addition of spectra (Deconvolution Algorithm) using aforementioned PFSLook software allows to conclude that with 80% of dust consisting of basalts (pyroxenes and amphiboles) other 20% are sulfates and clay minerals. In some spectra, from above the deepest areas of Hellas, sulfates constitute as high as about 50% of all the components (fig. 18).

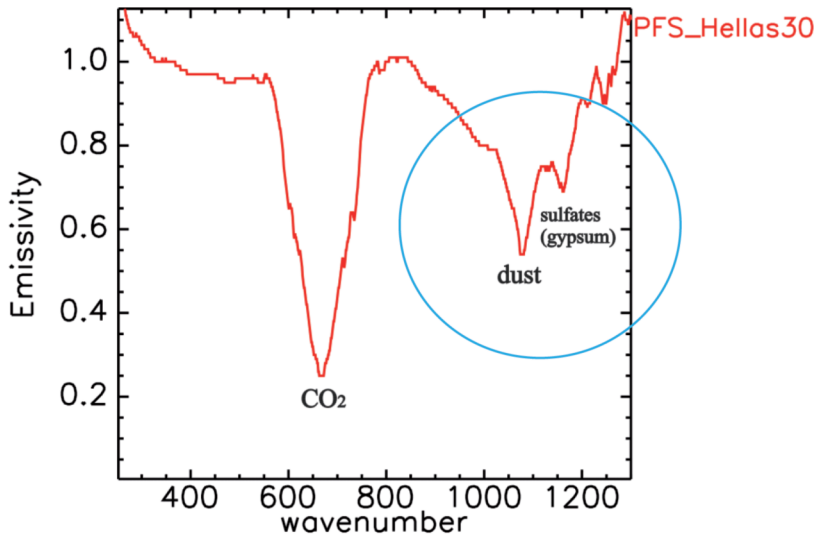


Fig. 17. PFS spectrum (red) of Hellas Planitia with 1160 cm⁻¹ band which is interpreted as sulfates (check the circle).

A minimum of 1160 cm⁻¹ of gypsum fit the spectrum of Hellas orbit no. 30. Gypsum comes from ASU Digital Spectral Library.

Other minima: CO₂ 667 cm⁻¹, dust 1075 cm⁻¹, CO₂ 1,250 cm⁻¹ [20].

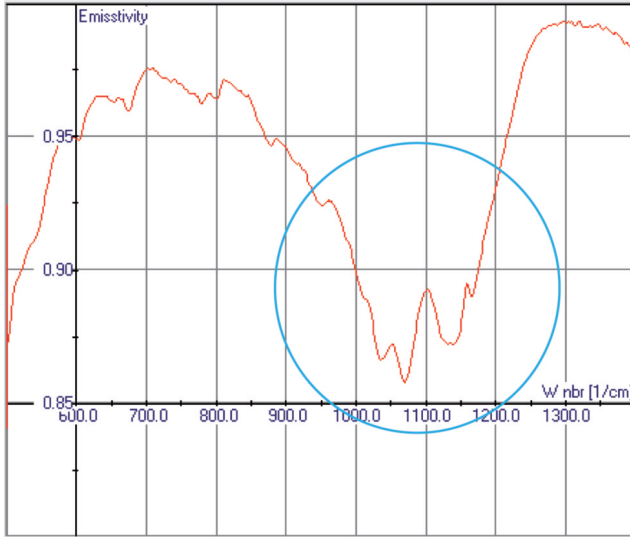


Fig. 18. Modelled dust spectrum with the use of linear addition method. It was used to model the mineralogical composition of the simulated soil of Mars labeled P-MRS and MRS-S [19] and gypsum mineral in relevant percentage (P-MRS 50% + gypsum 50%) 88% + S-MRS 12%. It represents a 47.6% of gypsum used for modeling. Two characteristic bands $1,075\text{ cm}^{-1}$ and $1,160\text{ cm}^{-1}$ (check the circle).

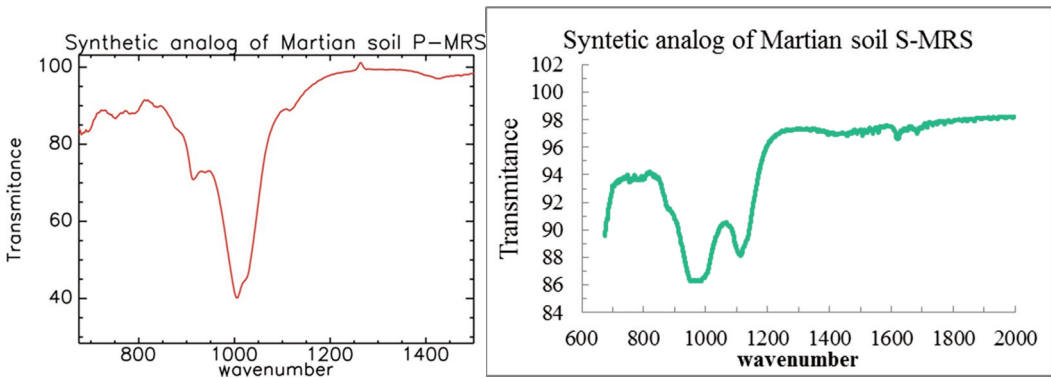


Fig. 19. P-MRS and MRS-S spectra [19] directly measured in the laboratory from samples. P-MRS (19a) and S-MRS (19b) spectral composition was used for modeling Mars dust by the linear addition method. Measurements made in the Oil and Gas Institute in Warsaw.

Figure 17 presents an example of the spectrum measured above the area surrounding Hellas, with visible minima at 1075 cm^{-1} and $1,160\text{ cm}^{-1}$, from the PFS spectrometer (Planetary Fourier Spectrometer), installed on the Mars Express probe. $1,160\text{ cm}^{-1}$ band probably comes from sulfates, which can be located both on the surface and in the dusty atmosphere ($1,075\text{ cm}^{-1}$ band). Another spectrum (fig. 18) is a modelled spectrum of dust from above the surface of Hellas in order to determine its mineral composition. The similarity of the modelled and measured spectra is significant but they are not identical. Small shifts of characteristic minima and the emergence of additional secondary characteristics is within the boundary of error, despite the fact that the spectra especially from the vicinity of Hellas are very noisy. Obtaining accurate characteristic minima at $1,075$ and

1,160 cm^{-1} is a result of the assembly of simulated spectra P-ISC and S-MRS, where the 1075 cm^{-1} band is derived from the input of the P-MRS spectrum and 1,160 cm^{-1} band of S-MRS in suitable proportions which is explained by the drawings (fig. 19b).

Two spectra presented below (fig. 19 a, b) show laboratory measurements of samples P-MRS and S-MRS [19] in transmittance, which can be comparable to emissivity. Spectra show the primary spectra characteristics of the samples. Emissivity is substituted by transmittance due to no possibility to make a direct emissivity measurements.

Tab. 4. The percentage of minerals constituting P-MRS and MRS-S samples [19].

Mineralogical composition of Phyllosilicatic Mars Regolith Simulant (P-MRS) and Sulfatic Mars Regolith Simulant (S-MRS) in weight percent (wt%).

Component	P-MRS (wt%)	S-MRS (wt%)
Pyroxene, Plagioclase, Amphibole, Ilmenite (Gabbro)	3	32
Olivine	2	15
Quartz	10	3
Hematite	5	13
Montmorillonite	45	-
Chamosite	20	-
Kaolinite	5	-
Siderite	5	-
Hydromagnesite	5	-
Goethite	-	7
Gypsum	-	30

The occurrence of aforementioned minerals in Hellas crater is likely due to the possibility of weathering of volcanic rocks that are common there and presence of sulfur rich environment and high concentration of feldspars as a basic component of basalt, weathering of which is the cause of clay minerals formation. Due to higher atmospheric pressure on Hellas and fluvio-glacial processes, the presence of water as necessary for the formation of clay minerals is very likely. Hydrothermal processes could also contribute to the formation of this type of minerals [21].

SUMMARY AND CONCLUSIONS

This article presents a method by means of which the mineralogical composition of surface and dust in the atmosphere can be accurately analyzed. The method can also be used for other spectral ranges including infrared and visible radiation.

Final conclusions for the above analyses presented in this article can be formulated as follows:

Replacement of augite by bronzite in the Dekkan spectrum of percentage composition acquired using deconvolution method, consistent with measured directly from Dekkan basalt, gives the best results (tab. 1) (fig. 4), (Fig. 12) The spectrum of gabbro from Nowa Ruda [14], (fig. 13), (tab. 3) has the approximate shape of the Martian ALH77005 meteorite spectrum, (fig. 7), while the spectrum of gabbros from Sobótka (tab. 3) with bronzite (fig. 16) has features in common with the spectrum of ALH84001 the famous Martian meteorite (fig. 7).

Spectrum most similar in shape to dusty Martian surface are the mix of spectra of Mountain of St. Anne's basalt [14], (fig. 6), (tab. 3) and Deccan basalt with bronzite, clay minerals – palygorskite and dickite as well as calcite and 30% hectorite (fig. 15). However, during modeling one faces

a number of problems associated with modeling of dust influenced spectra in the range of about $800 - 1,400 \text{ cm}^{-1}$, which is explained by Christiansen frequency responsible for stretching and bending vibrations of molecules identifying compounds.

From among natural weathering of basalt, weathering of Krzeniów [14] deserves attention, because of the similarity to the spectrum of Mars (Fig. 8). The spectrum of Krzeniów weathering is similar in shape to the dusty surface of Mars. It has minima in the vicinity of $1,070 \text{ cm}^{-1}$ band which is not present in the spectrum of Mars and a minimum of $1,550 \text{ cm}^{-1}$ and the water absorption peak of $1,630 \text{ cm}^{-1}$, also visible in the spectrum of Mars.

Even the supposedly dust-free surfaces may have a certain amount of dust which is not distinguished clearly in the spectrum. This can be noticed using MOC camera (Mars Global Surveyor) and especially with high-resolution HiRISE camera (Mars Reconnaissance Orbiter) Supposed dust-free area after scanning with infrared spectrometer shows little signs of dust. Established composition of Martian dust above Hellas impact crater is (P-MRS 50% + 50% gypsum) 88% + S-MRS 12%. This represents a 47.6% gypsum used for modeling. This amount of gypsum shown in the spectra indicates an acidic environment associated with the presence of liquid water.

Linear method of adding the spectra allows for in-depth analysis of individual spectral components involved in the spectrum.

Acknowledgments

I would like to acknowledge contributions of Space Research Centre of Polish Academy of Sciences in data research, Maja Mroczkowska-Szerszeń of Oil and Gas Institute in Cracow for infrared measurements, Jörg Fritz of Museum für Naturkunde in Berlin for providing regolith Martian analogues and Krzysztof Zalewski for English translation corrections.

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MODELOWANIE WIDM ZAPYLONYCH I NIEZAPYLONYCH ZNAJĄCYCH MARSJAŃSKICH POWIERZCHNI NA PODSTAWIE POZYSKANYCH WIDM W PODCZERWIENI

Streszczenie

Artykuł opisuje próbę przybliżenia składu mineralogicznego powierzchni Marsa na podstawie gotowych widm z TES (Thermal Emission Spectrometer-Mars Global Surveyor), zmierzonych w podczerwieni, w zakresie termalnym. Przedstawione tu będzie, jak na podstawie danych z TES

zostały modelowane i zinterpretowane widma z wybranych terenów Marsa po uprzednim oddzieleniu wkładu atmosfery od całości widma, algorytmami: transferu promieniowania (Radiative Transfer Algorithm) i dekonwolucji (Deconvolution Algorithm). W cytowanych publikacjach opracowano widma z ciemnego obszaru Cimmeria Terra i obszaru jasnego – Isidis Planitia . W przypadku obszarów jasnych, przykładowo obszar Arsia Mons, widmo zapyłonej i zwietrzałej powierzchni Marsa zostało uzyskane (również po oddzieleniu wpływu atmosfery) z uśrednienia widm pochodzących z terenów o wysokim zapyleniu. Te opisane powyżej widma zostały wykorzystane do modelowania powierzchni marsjańskich, takich jak basen Hellas oraz meteoryty marsjańskie SNC, w celu ustalenia ich składu mineralnego. Jako narzędzie modelowania wybrano jedną z wymienionych metod Deconvolution Algorithm. Widma do własnego modelowania były pozyskane ze spektrometru PFS (Planetary Fourier Spectrometer)-(Mars Express) oraz wykorzystano w tym celu skład mineralogiczny bazaltów z południowej części Polski.

Słowa kluczowe: Mars, algorytm dekonwolucji, spektrometria w podczerwieni, pył marsjański, modelowanie widm.