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Modeling of asteroid spectra – M4AST⋆

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ABSTRACT

Context. The interpretation of asteroid spectra provides the basis for determining the chemical composition and physical process that modified the surface of the asteroids. The increasing number of asteroid spectral measurements has lead to well-developed methods for analyzing asteroid spectra. There is however no centralized database for all the published data and a set of standard routines is also required.

Aims. We present a public software tool that combines both data archives and analyses of asteroid spectra.

Methods. Our project M4AST (Modeling for asteroids) consists of an asteroid spectral database and a set of applications for analyzing asteroid spectra. These applications cover aspects related to taxonomy, curve matching with laboratory spectra, space weathering models, and mineralogical diagnosis.

Results. M4AST project is fully available via a web interface. The database contains around 2700 spectra that can be either processed in M4AST and/or downloaded. The paper presents the algorithms we developed for spectral analyses based on existing methods. The robustness of routines is proven by the solutions found for spectra of three different asteroids: (9147) Kourakuen, (99 942) Apophis, and (175 706) 1996 FG3. The available results confirm those in the literature. M4AST applications can also be used to characterize any new asteroid spectra.

Conclusions. M4AST is a robust and reliable tool dedicated to asteroid spectra.

Key words. minor planets, asteroids: general – methods: data analysis – techniques: spectroscopic

1. Introduction

Spectroscopic studies of celestial bodies connect astronomy with fundamental physics on both atomic and molecular levels. The interpretation of the visible and near-infrared reflectance spectra of asteroids provides a powerful remote method for characterizing their surface composition. The mineralogical and the chemical properties of these objects provide direct information about the conditions and processes that were present during the very early stages of the evolution of the solar system. Another important aspect related to asteroids is their relative accessibility to spacecraft investigations. This enables their scientific study and the detailed assessment of their future use as space resources. The choice of targets and the planning of space missions are based on the ensemble of physical and dynamical parameters of these objects, which are properties inferred from ground-based observations.

Asteroid spectra have been obtained since the late 1960s. McCord et al. (1970) published the first spectral measurements in the 0.3–1.1 μm wavelength region for the asteroid (4) Vesta, and found that its spectrum is similar to those of basaltic achondritic meteorites. The most important surveys in the 1980s for measuring the spectral characteristics of asteroids were the Eight-Color Asteroid Survey (ECAS, Zellner et al. 1985), and the 52-color survey (Bell et al. 1988). All these results showed the diversity of asteroid surface composition.

In the past two decades, the development of CCD spectrographs have made it possible to obtain spectra of significantly fainter asteroids with a much higher spectral resolution than achievable with filter photometry. Several spectroscopic surveys have been performed, including SMASS (Xu et al. 1995), SMASS2 (Bus & Binzel 2002b), and S^3OS^2 (Lazzaro et al. 2004). Other spectroscopic surveys have been dedicated only to near-Earth asteroids such as SINEO (Lazzarin et al. 2005) or the survey performed by de León et al. (2010). The total number of asteroid spectra resulting from these surveys is on the order of thousands and has led to a mature understanding of their population.

Currently, the spectral data of asteroids continues to grow. The most important spectral surveys for asteroid have made their data available online. There is no centralized database containing all the asteroid spectra[1]. Moreover, the exploitation of these data in terms of the construction of mineralogical models, comparison to laboratory spectra, and taxonomy is treated individually by each team working in this field. While the spectral databases for asteroids have become significant in size and the methods for modeling asteroid spectra are now well-defined and robust, there are no standard set of routines for handling these data.

We developed M4AST (Modeling for Asteroids), which is a tool dedicated to asteroid spectra (Popescu et al. 2011; Birlan & Popescu 2011). It consists of a database containing the results

⋆ M4AST is available via the web interface:
http://cardamine.imcce.fr/m4ast/

[1] Some of these data are archived within the Small Bodies Node of the Planetary Data System (http://pds.nasa.gov/).

of the observational measurements and a set of applications for spectral analysis and interpretation. M4AST covers several aspects related to the statistics of asteroids – taxonomy, curve matching with laboratory spectra, modeling of space weathering effects, and mineralogical diagnosis. M4AST was conceived to be available via a web interface and is free for access to the scientific community.

This paper presents M4AST as follows: in Sect. 2, we briefly review the general methods used to analyze asteroid spectra. In Sect. 3, we describe the structure of the database, and in Sect. 4 we give details about the M4AST interfaces and their use. Section 5 presents the algorithms behind the different models implemented in M4AST. Section 6 shows some examples of spectral analysis and discusses the applicability of the models. We end up with the conclusions and further perspectives.

2. Methods for asteroid spectra analysis

"Asteroids" actually means "star-like" and viewed through a telescope, as these planetesimals are merely a point source of light. A panoply of new observational techniques (e.g. spectroscopy, photometry, polarimetry, adaptive optics, radar, etc.) has transformed these star-like objects into individual little worlds.

One of the techniques used to characterize the surface of asteroids is reflectance spectroscopy in the visible and near-infrared wavelength regions. Diagnostic features in spectra related to electronic and vibrational transitions within minerals or molecules are detectable in the 0.35–2.50 μm spectral range. The overlapping of the absorption bands from different mineral species provides a distinctive signature of the asteroid surface. Olivine, pyroxene (clino- and ortho-pyroxene), iron-nickel (Fe-Ni) metal, spinel, and feldspar are some of the most important minerals that can be identified by carefully analyzing the reflection spectra of the asteroid (McSween 1999).

The analysis of reflectance spectra can be done using several methods, such as taxonomic classification, comparison with laboratory spectra, band parameter determination, and modeling of the space weathering effects. We briefly discuss below the methods implemented via M4AST.

2.1. Taxonomy

Taxonomy is the classification of asteroids into categories (classes, taxons) using some parameters and no a priori rules. The main goal is to identify groups of asteroids that have similar surface compositions. The classification into taxons is the first step for further studies of comparative planetology. In the case of asteroids, a precise taxonomic system gives an approach to a specific mineralogy for each of the defined classes.

Taxonomic systems of asteroids were initially based on asteroid broadband colors (Chapman et al. 1971), which allowed us to distinguish between two separate types of objects, denoted "S" (stony) and "C" (carbonaceous). Based on the increasing amount of information from different types of observations, new taxonomic classes were defined. Historically, the most widely used taxonomies are the following: Tholen (1984) and Barucci et al. (1987), which used data from the Eight-Color Asteroid Survey (Zellner et al. 1985); Bus & Binzel (2002a), which used data from the SMASS2 survey; and DeMeo et al. (2009), which is an extension of a previous taxonomy scheme into the near-infrared.

Statistical methods are used for defining taxonomic systems of asteroids. We point out two of them, namely principal component analysis (PCA) and the G-mode clustering method.

Principal component analysis (PCA) is a method for reducing the dimensionality of a data set of M variables, involving linear coordinate transformations to minimize the variance. The first transformation rotates the data to maximize the variance along the first axis, known as the principal component 1 (PC1), then along the second axis – the second principal component, and so on. Overall, the new coordinates are ordered decreasingly in terms of the dispersion in the principal components.

The G-mode is a multivariate statistical clustering method that allows us to classify a statistical sample consisting of N elements with M variables. The parameter G is the analog of the distance in a NxM space. This statistical distance between an object and a taxonomic class shows the similarities of the characteristics of this object to those of its class (Birlan et al. 1996). One of the advantages of this method is that even if only a subset of variables are available for an object (only part of the spectrum), a preliminary classification can still be achieved.

2.2. Spectral comparison

Spectroscopy of different samples performed in the laboratory provides the basis upon which compositional information about unexplored planetary surfaces can be understood from remotely obtained reflectance spectra. Thus, confronting the spectral data derived from telescopic observations with laboratory measurements is an important step in study of asteroid physical properties (Britt et al. 1992; Vernazza et al. 2007; Popescu et al. 2011).

Several spectral libraries are available for accomplishing this task, such as Relab[2], USGS Spectroscopy Laboratory[3], the Johns Hopkins University (JHU) Spectral Library, the Jet Propulsion Laboratory (JPL) Spectral Library[4], etc. We use the Relab spectral library in M4AST, which is one of the largest libraries and contains more than 15 000 spectra for different types of materials from meteorites to terrestrial rocks, man-made mixtures, and both terrestrial and lunar soils.

2.3. Space weathering effects

It is now widely accepted that the space environment alters the optical properties of airless body surfaces. Space weathering is the term that describes the observed phenomena caused by these processes operating at or near the surface of an atmosphere-less solar system body, that modify the remotely sensed properties of this body surface away from those of the unmodified, intrinsic, subsurface bulk of the body (Chapman 1996, 2004).

The objects that are most affected by the space weathering are silicate-rich objects for which a progressive darkening and reddening of the solar reflectance spectra appear in the 0.2–2.7 μm spectral region (Hapke 2001). Lunar-type space weathering is well-understood, but two well-studied asteroids (433 Eros and 243 Ida) exhibit different space weathering types. The mechanism of space weathering for asteroids is still currently far from being completely understood.

The latest approaches to the study of space weathering are based on laboratory experiments. Simulations of micrometeorites and cosmic ray impacts have been achieved using nanopulse lasers on olivine and pyroxene samples. These have

[2] http://www.planetary.brown.edu/relab/
[3] http://speclab.cr.usgs.gov/
[4] http://speclib.jpl.nasa.gov/

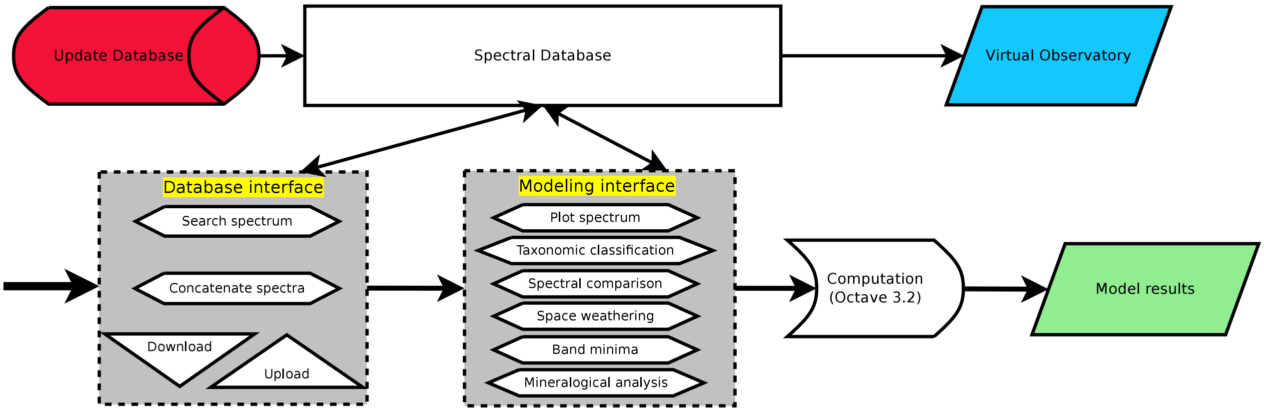


Fig. 1. Block diagram and work flow of M4AST.

shown that laser ablation lowers the albedo, dampens the absorption bands, and reddens the spectrum. These effects could explain the transition from "fresh" ordinary chondrite material to the observed asteroid spectra (Yamada et al. 1999; Sasaki et al. 2001). The spectral effects generated by the solar wind irradiation to silicate materials were investigated by Brunetto et al. (2006). On the basis of ion irradiation experiments, they found "a weathering function" that could be used to fit the ratio of the spectra of irradiated to unirradiated samples, which was implemented in M4AST.

2.4. Band parameters

The "traditional" method used for mineralogical analysis is based on different parameters that can be computed from the reflectance spectra of the object. These parameters give information about the minerals that are present on the surface of the asteroid, their modal abundances, and the size of the grains.

Cloutis et al. (1986) outlined an analytical approach that permits the interpretation of visible and near-infrared spectral reflectance to determine the mineralogic and petrologic parameters of olivine-orthopyroxene mixtures, including end-member abundances, chemistries, and particle size. These parameters are the wavelength position of the reflectance minima around 1 μm and 2 μm, the band centers, and the band area ratio (BAR) which is the ratio of the areas of the second absorption band relative to the first absorption band.

Gaffey (2010) noted that mineralogically diagnostic spectral parameters (band centers, BARs) are "essentially immune to the effects of space weathering observed and modeled to date".

3. Spectral database

The schematic of the M4AST project is given in Fig. 1. The first component is the spectral database. It contains the results of telescopic measurements for the reflectance spectra of different wavelength ranges (V – visible, NIR – near infrared, V+NIR – visible and near infrared) of the asteroids and the observations logs.

3.1. Structure of M4AST database

The information in the database is organized into two type of files: *permanent* and *temporary* files. Additionally, there is a catalog to keep track of the permanent files recorded.

Permanent files are uploaded through a dedicated interface protected by a password. Any new file submitted in this way is recorded in a catalog together with its observation log. The observation log is also kept in the header of the file containing the corresponding spectral data, including IAU designations of the asteroid, the date and hour (UT) of the observation, and the IAU code of the observatory. Additional information could be included such as the investigator name and e-mail address as well as the link to a reference if the spectrum was published.

Each file containing the spectral data includes a header with the observation log and the measurements given in two columns: the first column contains the wavelength in μm, and the second column contains the corresponding reflectance values (normalized to unity at 0.55 μm if the visible part of the spectrum is contained, and otherwise at 1.25 μm). If the dispersions in the measurements are available, they are provided in the third column.

Temporary files are created by the users only for processing the data. They provide a way for the anonymously user to use the applications of M4AST for his own spectral data. Temporary files receive a random name and can be removed by the same user that created them (no administrative rights are required). The application library is fully available for modeling spectral data contained in temporary files. No permanent information is recorded.

3.2. The content

Historically, the database was designed for making available to the scientific community the spectra obtained after observations performed remotely from the Centre d'Observation à Distance en Astronomie à Meudon (CODAM) (Birlan et al. 2004, 2006). The observations were obtained in the 0.8–2.5 μm spectral region using the SpeX/IRTF instrument, located on Mauna Kea, Hawaii. The project now includes around 2,700 permanent spectra (in the V and NIR wavelength regions) of both main belt and near-Earth asteroids.

Along with the spectra obtained via CODAM, the main sources of the project are SMASSI (Xu et al. 1995), SMASII (Bus & Binzel 2002b), and S^3OS^2 (Lazzaro et al. 2004) and de León et al. (2010). Together with our program of asteroid spectroscopic observations, some collaborations are intended in order to enlarge M4AST database.

The purpose of this database is not to duplicate other spectral libraries that already exist, but to offer a unique format for the data, a fast way of applying the existing models, and a rapid comparison of the results.

3.3. M4AST database via the Virtual Observatory

The Virtual Observatory (VO) is an international astronomical community-based initiative. Its aims are to allow global electronic access to the available astronomical data archives of space and ground-based observatories and other sky survey databases and to enable data analysis techniques through a coordinating entity that will provide common standards.

The M4AST spectral database can be accessed via VO-Paris Data Centre[5] using Simple Spectral Access Protocol (Tody 2011). The M4AST spectral data obtained via VO can be retrieved in both *VOTable* format or our native *ASCII* format. A "simple query search" based on asteroid designation correctly returns all the spectra from our database for the corresponding object.

New protocols, dedicated to planetology, (such as table access protocol) will be implemented in the future.

4. The interface

M4AST includes two interfaces, one dedicated to database access and another for running the different applications dedicated to spectral analysis[6]. The access flow starts with the database interface and continues with the modeling tool interface. Figure 1 gives an overview of the M4AST work-flow.

4.1. Database interface

The database interface (Fig. 1), called user input interface, allows the users to access the spectra from the database or upload their own spectra for further processing. The following options are available:

Search spectra in database – the user can search spectra in the database based on a maximum of three keywords. These keywords include object designations, observing date, and the IAU observatory code.

Download file from database – the user can download any spectrum using as input the filename provided by the previous option.

Upload temporary spectrum to database – the anonymously user can upload his own spectral data for further processing. The file with the spectrum should contain two or three columns, the first column containing the wavelengths (given in angstroms, nanometers, or microns), the second column containing the corresponding reflectance. Optionally, the third column may include the dispersion of measurements. The file is given a temporary name over which the user has full control.

Concatenate spectra – spectra in different wavelength regions (V and NIR) can be merged. The procedure consists in the minimization of data into a common spectral region (usually 0.8–0.9 μm). The result is stored in a temporary file and can be further processed.

The results of all these options are displayed at the bottom of each page. These results can be either spectra found in the database or temporary files. The connection with the modeling tools is made using the name of the file containing the spectrum. This filename is provided as a link and a simple click allows us to access the modeling tool interface.

[5] http://voparis-srv.obspm.fr/portal/

[6] http://cardamine.imcce.fr/m4ast/

4.2. Modeling tool interface

The second component of the M4AST project is the set of applications for modeling and analyzing the spectra from the database or any spectrum submitted by the user. The usage of this tool (Fig. 1), called the modeling interface, is based on the name of the file containing the spectral data.

The following applications are currently available in this interface:

Plot spectrum – plot the reflectance as a function of wavelength. Additional information related to the selected spectrum (the observing log) are also given.

Taxonomy – classify the spectrum according to different taxonomies. Taxonomic systems that can be selected are Bus-DeMeo (DeMeo et al. 2009), G13 (Birlan et al. 1996), and G9 (Fulchignoni et al. 2000). The methods behind these classifications are outlined in Sect. 5. The results of this application consist in the first three classes that match the asteroid spectrum, together with some matching quantitative values (coefficients). In addition, the asteroid spectrum is plotted together with standard spectra corresponding to the best matches.

Search matching with spectra from the Relab database – performs spectral comparison with spectra from Relab database. In general, only the meteorite spectra are of interest, thus an option for selecting between all spectra and only meteorite spectra is included. However, the "all spectra" option includes spectral measurements for mixtures (olivine/pyroxene) prepared in the laboratory that can be considered when analyzing asteroid spectra. Four methods are available for the spectral matching. Their description is given in Sect. 5. This application provides the first 50 laboratory spectra that matched the spectrum (in order of the matching coefficient). These results are given in a table, along with a link to visualize a comparative plot of laboratory spectra and asteroid spectra. The table includes all the information regarding the spectral measurements and the sample characteristics.

Space weathering effects – uses the space weathering model defined by Brunetto et al. (2006). The results consists in computing the parameters of the model and de-reddening the spectrum. The de-reddening (removal of space weathering effects) is done by dividing the spectrum by its continuum. The spectrum obtained can be further analyzed, being provided in a temporary file.

Band parameters and mineralogical analysis – computes the spectral parameters defined by Cloutis et al. (1986). If only the infrared part of the spectrum is given, the algorithm computes the band minima. If the spectrum contains both V and NIR regions, all the parameters described in Sect. 2.4 are calculated. Along with the results, the plots required to interpret these parameters are also provided.

After each computation made in M4AST, the results are displayed at the bottom of the page. It must be noted that some of these applications provides meaningfully results only for certain types of spectra. Their applicability is indicated in the publications describing the models. The reference to the relevant publications is also available via the web interface.

4.3. Updating the database

Permanent spectra can be added into the database via a dedicated interface – update database (Fig. 1) – that requires administrative rights. The information needed to add a new permanent file with spectral data are asteroid designations (an additional utility is provided to check the designations), information about the observation (date, investigator, and IAU code of the observatory), and information about the uploaded file containing the measurements. Each record submitted to the database can be removed only from this interface.

5. Algorithms – the mathematical approach

This section describes the algorithms used to analyze the different types of spectra.

5.1. Taxonomic classification

We used different approaches for the three taxonomies types proposed in M4AST.

To classify a spectrum in the Bus-DeMeo taxonomy, we determine how closely this asteroid spectrum is fitted by the standard spectrum of each class using a curve matching approach. This approach involves first fitting the spectrum with a polynomial curve and then comparing this curve to the standard spectrum at the wavelengths given in the taxonomy. We select the taxonomic classes producing the smallest standard deviation in the error (see Eq. (5)).

For G-mode taxonomy, we used the algorithm defined in Fulchignoni et al. (2000). This comprises the computation of the g parameter, which gives the statistical distance of a new sample, characterized by $\{x_i\}$ from the taxonomic class s

$$g_s = \sqrt{2\,R_s\,\sum_i^M\left(\frac{x_i-\overline{x}_{is}}{\sigma_{is}}\right)^2} - \sqrt{2\,R_s\,M-1}, \qquad (1)$$

where M is the number of points and $i = \overline{1...M}$. The G-mode method defines for each taxonomic class s the mean values $\{\overline{x}_{is}\}$, the standard deviations $\{\sigma_{is}\}$, and a statistical indicator R_s. We select the classes that have the lowest g_s, the ideal case being $g_s = -\sqrt{2\,R_s\,M-1}$.

The taxonomic classes are defined depending on the taxonomy in different wavelength intervals (0.45–2.45 μm for Bus-DeMeo taxonomy, 0.337–2.359 μm for G13 taxonomy, and 0.337–1.041 and for G9 taxonomy) and some of them also using the albedo. The curve matching or g factor computation can be made across a smaller wavelength interval (depending on the available wavelength range of the asteroid spectrum) but with a lower confidence, thus a reliability criterion is required (Popescu et al. 2011)

$$Reliability = \frac{card\left([\lambda_{\rm m},\lambda_{\rm M}]\bigcap\{\lambda_1^T,\lambda_2^T,...,\lambda_N^T\}\right)}{N}, \qquad (2)$$

where $[\lambda_{\rm m},\lambda_{\rm M}]$ is the spectral interval between the minimum wavelength and the maximum wavelength in the asteroid spectrum, $\lambda_1^T,\lambda_2^T,...,{\lambda_N}^T$ are the N wavelengths for which the standard spectra of the taxonomy are given, and $card()$ represents the number of elements of a discrete set.

5.2. Curve matching

The methods for taxonomic classification and comparison with meteorite spectra are based on curve matching. These procedures involve minimizing a quantity (usually called Φ) in order to determine the best estimates for a given asteroid spectrum.

A quantity commonly used to test whether any given points are well-described by some hypothesized function is chi-square (χ^2), the determination being called the chi-square test for goodness of the fit (Bevington & Robinson 1992).

The classical definition for the χ^2 is:

$$\chi^2 = \sum_i^N \frac{(x_i-\mu_i)^2}{\sigma_i^2}, \qquad (3)$$

where there are N variables x_i normally distributed with the mean μ_i and variance σ_i^2. If σ_i^2 are correctly estimated, the data are well-described by the values μ_i when $\Phi = \chi^2 \to 0$.

We denote by $\{e_i\}$ the error between the data (asteroid spectrum) and the curve that was fitted

$$e_i = (x_i - \mu_i). \qquad (4)$$

Our first approach to curve matching, derived from chi-square fitting, is based on the formula

$$\Phi_{std} = \frac{1}{N}\sqrt{\sum_i^N (e_i-\overline{e})^2}, \qquad (5)$$

where we have denoted with $\overline{e}$ the mean value of the set $\{e_i\}$ (Eq. (4)).

The quantity to minimize in this case is the standard deviation of the errors. To apply this procedure, we smooth our asteroid spectrum by a polynomial curve (using the $polyfit$ function from the Octave3.2 computation environment). This step is required to eliminate the outlier points produced by the incomplete removal of telluric absorption lines.

We used this type of curve matching to find the taxonomic class of the asteroid in the Bus-DeMeo taxonomy and to compare with laboratory spectra. In the latter case, we determine how well the asteroid spectrum is fitted by different laboratory spectra, and select the closest 50 fits, in ascending order of Φ.

A second approach to curve matching can be made using χ^2 with the definition (Nedelcu et al. 2007):

$$\chi^2 = \frac{1}{N}\sum_i^N \frac{(x_i-\mu_i)^2}{x_i}, \qquad (6)$$

where x_i are the values of a polynomial fit to the asteroid spectrum and μ_i are the reflectance values for the meteorite spectrum. The meaning of this formula is that of a relative error at each wavelength (N being the number of wavelengths on which the comparison is made).

The third approach to curve fitting is based on the correlation coefficient

$$\rho_{X,M} = \frac{cov(X,M)}{\sigma_X\,\sigma_M}, \qquad (7)$$

where, $X = \{x_i\}$ is the spectrum of the asteroid and $M = \{\mu_i\}$ is the laboratory spectrum. The correlation coefficient detects linear dependences between two variables. If the variables are independent (i.e. the asteroid and laboratory spectra), then the correlation coefficient is zero. A unitary value for the correlation coefficient indicates that the variables are in a perfect linear relationship, though in this case we search for laboratory spectra that match the desired asteroid spectrum with the highest $\rho_{X,M}$.

Finally, we concluded that a good fitting can be achieved by combining the standard deviation method and correlation coefficient method. Thus, the fourth coefficient we propose is

$$\Phi_{\rm comb} = \frac{\rho_{X,M}}{\Phi_{\rm std}}, \qquad (8)$$

where $\rho_{X,M}$ was defined in Eq. (7) and Φ_{std} was defined in Eq. (5). In this case, the laboratory spectra that match the asteroid spectrum are those with the highest value of Φ_{comb}.

5.3. Computing the space weathering effects

Our approach to computing space weathering effects applies the model proposed by Brunetto et al. (2006). On the basis of laboratory experiments, they concluded that a weathered spectrum can be obtained by multiplying the spectrum of the unaltered sample by an exponential function (see Eq. (9)) that depends on the precise parameter C_s.

By fitting the asteroid spectral curve with an exponential function using a least-square error algorithm, we can compute the C_s parameter

$$W(\lambda) = K \times \exp\left(\frac{Cs}{\lambda}\right) \tag{9}$$

Brunetto & Strazzulla (2005) demonstrated that ion-induced spectral reddening is related to the formation of displacements, with the C_s parameter being correlated with the number of displacements per cm^2 (named damage parameter – d). Brunetto et al. (2006) obtained an empirical relation between C_s and the number of displacements per cm^2

$$C_s = \alpha \times \ln(\beta \times d + 1), \tag{10}$$

where $\alpha = -0.33\ \mu$m and $\beta = 1.1 \times 10^{19}$ cm^2. M4AST applies Eq. (10) to compute the damage parameter d.

This model for the space weathering effects describes the effects of solar-wind ion irradiation. While this is not the only active weathering process, it seems to be the most efficient at 1 AU (Vernazza et al. 2009; Brunetto et al. 2006).

The removal of space weathering effects is made in M4AST by dividing the asteroid spectrum by $W(\lambda)$ at each wavelength.

5.4. Application of the Cloutis model

Cloutis et al. (1986) proposed a method for the mineralogical analysis of spectra showing absorption bands. We implemented an application to compute the spectral parameters defined by this method. The computation of all the parameters described in Sect. 4.2 is done for spectra that contains the V + NIR wavelength regions. If only the NIR region is given, then only the band minima can be computed.

The following steps are made: we first compute the minima and maxima of the spectrum. This is done by starting with the assumption that there is a maximum around 0.7 μm followed by a minimum around 1 μm, then a maximum between 1.3–1.7 μm and a minimum around 2 μm. The spectrum is fitted around these regions by a polynomial function. The order of the polynomial is selected to be between three to eight, in order to obtain the smallest least square residuals. The minima and the maxima are the points where the first derivative of the fitted polynomial functions is zero.

In the second step, using the wavelengths and the reflectance at the two maxima and at the end of the spectrum (around 2.5 μm), we compute two linear continua, tangential to the spectral curve. The continuum part is removed by dividing the spectrum by the two tangential lines (in the corresponding regions). The band centers are computed following a method similar to that applied to the band minima, but after the removal of the continuum.

The last step consists in computing the two absorption-band areas. The first absorption band is located around 1 μm and between the first and second maxima. The second absorption band is located around 2 μm, between the second maximum and the end of the spectrum. The area is computed using a simple integration method. This method consists in computing the area between two consecutive points in the spectrum defined by a trapezoid and summing all these small areas corresponding to the absorption band.

$$\frac{OPX}{OPX + OL} = 0.4187 \times \left(\frac{BII}{BI} + 0.125\right). \tag{11}$$

The ratio of the areas of the second to the first absorption band ($BAR = \frac{BII}{BI}$) gives the relative abundance orthopyroxene vs. olivine presented in Eq. (11) (Fornasier et al. 2003).

6. Results and discussions

The functionality of M4AST is now exemplified by the analysis of three spectra available in the database that were previously discussed by Popescu et al. (2012), Binzel et al. (2009), and de León et al. (2011). Our selection here covers a wide variety of spectra: (9147) Kourakuen is a vestoid with deep absorption features, (99 942) Apophis is an Sq type asteroid with moderate features, and (175 706) 1996 FG3 is a primitive type with featureless spectra.

The discussion of the taxonomic type of each object is made with reference to both Fig. 2 for Bus-DeMeo taxonomy and Fig. 3 for G-mode taxonomies. Table 1 summarizes the comparison of asteroid spectra with spectra from the Relab database. The corresponding plots are given in Fig. 4.

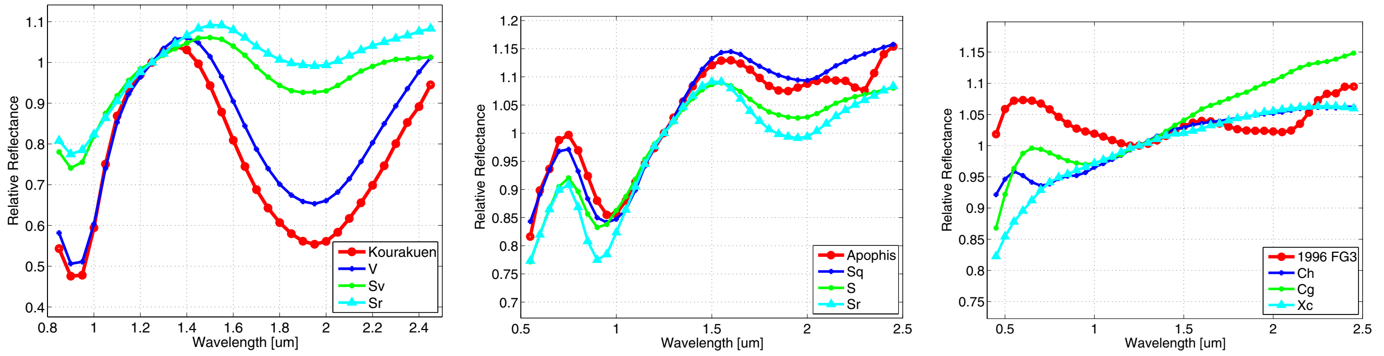
6.1. Results

The spectrum of (9147) Kourakuen has the characteristics of a V-type asteroid. In Bus-DeMeo taxonomy, V-type asteroids are characterized by a very strong and very narrow 1 μm absorption and a strong 2 μm absorption feature (DeMeo et al. 2009). M4AST undoubtedly classify this spectrum as V-type. This agrees with the classification made via the MIT-SMASS online tool[7]. The next two matches (the programs always returns the first three matches) of Sv and Sr types have larger matching errors (Fig. 2(a)).

The solution given by all four methods for comparison with laboratory spectra shows that the spectrum of (9147) Kourakuen is almost identical to the spectrum of a sample from the Pavlovka meteorite (Fig. 4(a)), which is a howardite achondrite meteorite. The second best match corresponds to the spectrum of a a man-made mixture of pyroxene hypersthene plagioclase bytownite ilmenite (Fig. 4(b)). This man-made mixture reproduces quite well the natural composition of volcanic rocks or melting rock of volcanic beds, and is consistent to the V-type mineralogical composition of asteroids. The majority of the laboratory spectra proposed by M4AST as good matches to this asteroid corresponds to Howardite-Eucrite-Diogenite (HED) achondrites, which are meteorites that come from asteroid (4) Vesta. This agrees with the the classification of a V-type asteroid.

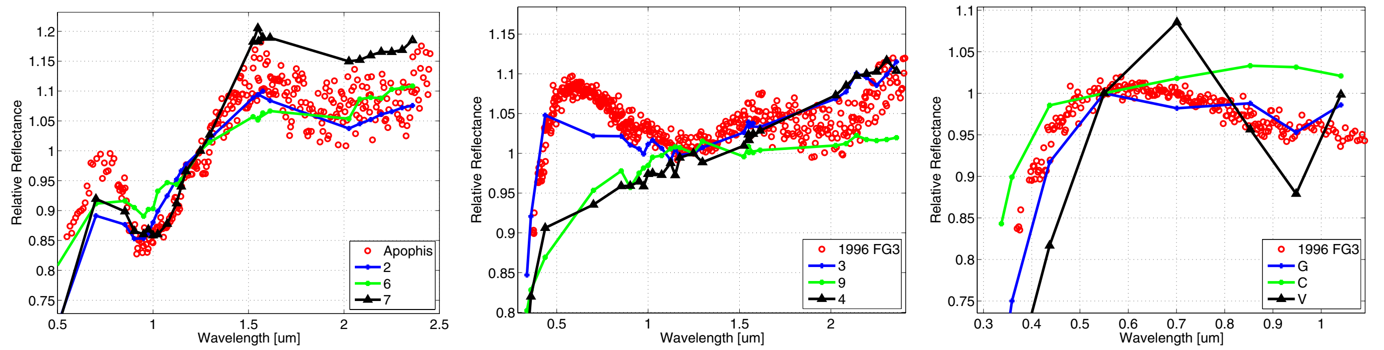
While the standard deviation measures the overall matching between the two spectra, the correlation coefficient find the spectra for which the spectral features positions and shapes are very close. In the case of spectrum of (9147) Kourakuen, a very high

[7] http://smass.mit.edu/busdemeoclass.html



(a) (b) (c)

Fig. 2. Classification in Bus-DeMeo taxonomical system for: **a)** (9147) Kourakuen; **b)** (99 942) Apophis; and **c)** (175 706) 1996 FG3. All the spectra are normalized to 1.25 μm.



(a) (b) (c)

Fig. 3. Classification in the G-mode taxonomical system for: **a)** (99 942) Apophis using G13 taxonomy; **b)** (175 706) 1996 FG3 using G13 taxonomy; and **c)** (175 706) 1996 FG3 using G9 taxonomy. All the spectra are normalized either to 1.25 μm (*left and central panel*), or to 0.55 μm (**c**)).

Table 1. Summary of the results obtained by matching the asteroids spectra with spectra from the Relab database.

Spectrum	Std. dev.	Corr. coef.	Meteorite/Sample	Sample ID	Type	Texture
(9147)	0.01884	0.99477	Pavlovka	MR-MJG-094	Achondrite(AHOW)	–
	0.02244	0.99207	Mixture	SC-EAC-039	Pyrox Hyper Plagi Bytow Ilmen	Particulate
(99 942)	0.01756	0.98013	Simulant	CM-CMP-001-B	Soil/Lunar	Particulate
	0.01970	0.98224	Hamlet	OC-TXH-002-C	OC-LL4	Particulate
(99 942)	0.01539	0.96245	Cherokee Springs	TB-TJM-090	OC-LL6	Particulate
de-reddened	0.01609	0.97272	Cat Mountain	MB-DTB-035-A	OC-L5	Particulate
(175 706)	0.01219	0.90546	Sete Lagoas	MH-JFB-021	OC-H4	Slab
	0.01504	0.85366	Murchison heated 1000 °C	MB-TXH-064-G	CC-CM2	Particulate

Notes. For each asteroid, we show the best two matches, obtained by measuring the standard deviation (std. dev.) and the correlation coefficient (corr. coef.).

correlation coefficient (more than 0.99) characterizes the first matching solutions (Table 1).

Since only the NIR part of the spectrum is available, we can only compute the band minima. The high signal to noise ratio of this spectrum ensures that there is a small error in computing the band minima. The first minimum is at 0.9217 ± 0.0005 μm and the second minimum is at 1.9517 ± 0.0062 μm, which imply a band separation of 1.03 μm. The band separation provides a way of estimating the iron content. Cloutis et al. (1990) noted that the band separation is a linear function of the BII minimum for orthopyroxenes and that both parameters increase with the iron content. If we refer to the relation obtained by de Sanctis et al. (2011), the parameters that we found match their formula $y = 0.801 * x - 0.536$, where y is the band separation and x is the BII minimum. These parameters corresponds to an iron content of around 40 wt%. However, the laboratory calibrations suggest that the correspondence is true for a number of low aluminum orthopyroxenes but invalid for mixtures of olivine, metal, and both ortho- and clino-pyroxenes (de Sanctis et al. 2011).

The second spectrum we consider to exemplify the M4AST routines is that of the potential hazardous asteroid (99 942) Apophis (Binzel et al. 2009). On the basis of this spectrum this asteroid was found to be an Sq type, and has a composition that closely resemble those of LL ordinary chondrite meteorites.

M4AST classifies this spectrum in the Bus-DeMeo taxonomy as an Sq-type (Fig. 2(b)). The next two types, S and Sr,

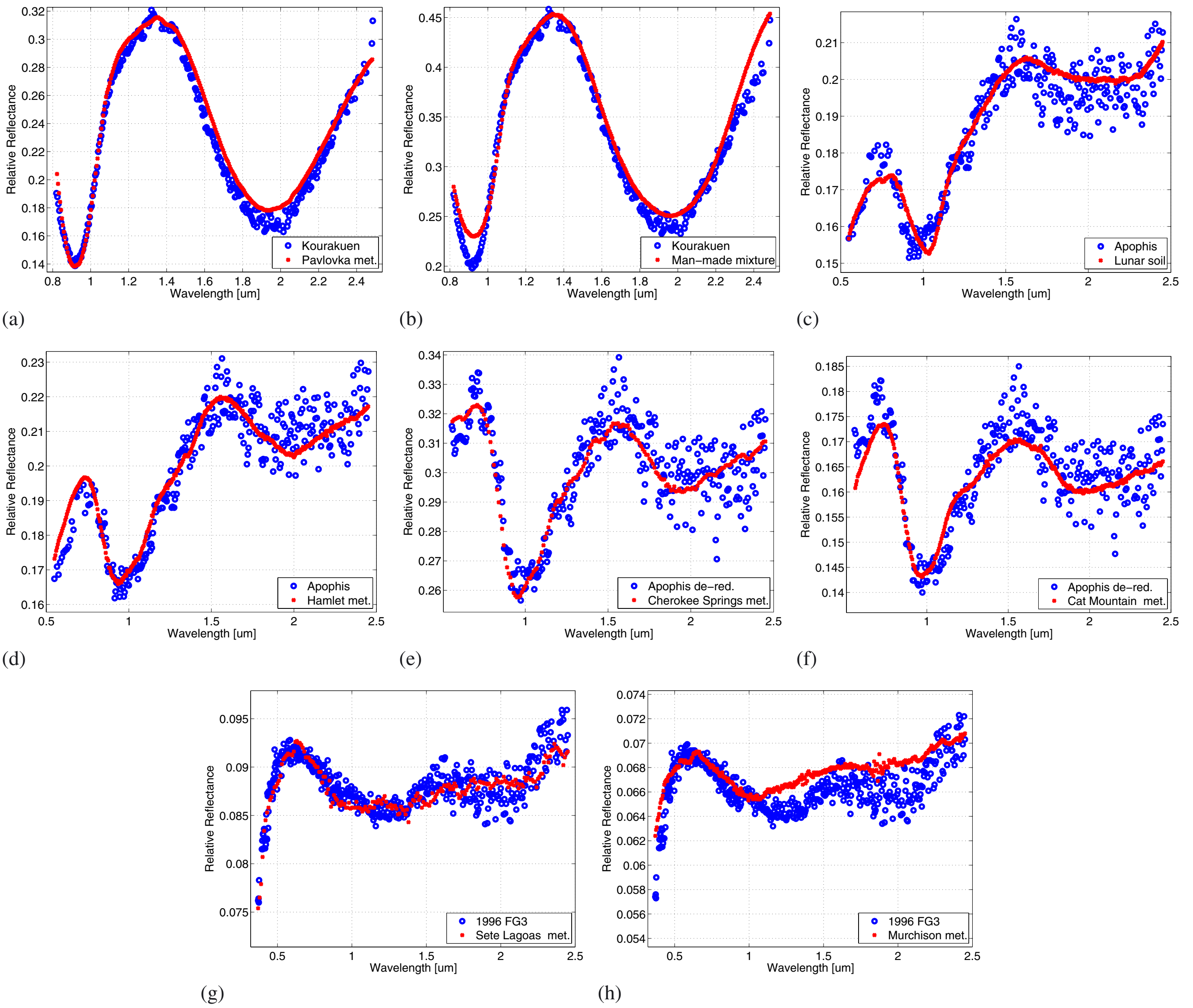


Fig. 4. Asteroid spectra and the best two matches derived from a comparison with laboratory spectra: **a)** spectrum of Kourakuen and the spectrum of a sample from Pavlovka; **b)** spectrum of Kourakuen and the spectrum of a mixture of pyroxene hypersthene plagioclase bytownite ilmenite; **c)** spectrum of Apophis and the spectrum of a simulant Lunar soil; **d)** spectrum of Apophis and the spectrum of a particulate sample from the Hamlet meteorite; **e)** de-reddened spectrum of Apophis and the spectrum of a particulate sample from the Cherokee Springs meteorite; **f)** de-reddened spectrum of Apophis and the spectrum of a particulate sample from the Cat Mountain meteorite; **g)** spectrum of 1996 FG3 and the spectrum of a sample from the meteorite Sete Lagoas; and **h)** spectrum of 1996 FG3 and the spectrum of a sample from the Murchison meteorite heated to 1000 °C.

are relatively good matches, but have larger errors. Applying the G13 taxonomy, M4AST classifies this asteroid as being in class 2 (Fig. 3(a)). Two other classes (namely 6 and 7) are relatively close in terms of g factor (Fig. 3, upper plot). Class 2 has the representative members (7) Iris and (11) Parthenope, which are S- and S-q type asteroids according to DeMeo et al. (2009). The classes 2, 6, and 7 are equivalent to the S profile.

Being an Sq type, for this asteroid spectrum we can apply the space weathering model proposed by Brunetto et al. (2006). Thus, fitting the spectrum with an exponential continuum we found $C_s = -0.196$ μm, corresponding to a moderate spectral reddening. The result obtained by Binzel et al. (2009) is $C_s = -0.17 \pm 0.01$ μm. This difference could be caused by the different method that they used: their "best fit was performed as an integral part of the overall minimum RMS solution". The C_s value gives the number of displacements per cm^2, $d = 0.74 \times 10^{19}$ displacements/cm^2. We analyze both the original spectrum and the de-reddened spectrum.

Comparing the original spectrum of (99 942) Apophis with all laboratory spectra from Relab, M4AST found matches with some ordinary chondrite meteorites (L and LL subtypes, and petrologic classes from 3 to 6) and some lunar soils (Figs. 4(c) and 4(d)). Referring to standard deviation and to correlation coefficient, the closest matches were those of particulate lunar soils and some spectra from the Hamlet meteorite which is particulate with grain sizes smaller than 500 μm. The meteorite Hamlet is an ordinary chondrite, subtype LL4.

In the case of the de-reddened spectrum, the majority of solutions correspond to ordinary chondrite meteorites, of subtype

L and LL, with petrologic classes from 4 to 6. The best matches were those of the Cherokee Springs meteorite (an LL6 ordinary chondrite, Fig. 4(e)) and the Cat Mountain meteorite (an L5 ordinary chondrite, Fig. 4(e)). From spectral modeling of mixtures of olivine, orthopyroxene, and clinopyroxene, Binzel et al. (2009) correlate the spectrum of (99 942) Apophis with the spectra of LL meteorites. This results agrees with the spectral matching solutions found by M4AST.

No significant differences between the Cloutis model parameters computed for original and de-reddened spectrum are found. The application found the first band center at $0.9721 \pm 0.0143\,\mu$m ($0.9755 \pm 0.0144\,\mu$m for the de-reddened spectrum), the second band center at $1.8200 \pm 0.0679\,\mu$m ($1.8404 \pm 0.0591\,\mu$m for the de-reddened spectrum), and the band area ratio 0.4059 ± 0.0047 (0.3886 ± 0.0015 for the de-reddened spectrum). These parameters correspond to an ordinary chondrite with an $OPX/(OPX + OL)$ ratio of 0.222 (0.215 for the de-reddened spectrum). This ratio agrees with the compatibility relation between NEA and LL ordinary chondrites found by Vernazza et al. (2008), which is similarly consistent with the spectral matching we found.

This value means that the ordinary chondrite consist of 78% olivine, which is consistent with an LL ordinary chondrite. And this result agrees with the spectral matching.

The dark primitive asteroid (175 706) 1996 FG3 is the primary target of the ESA Marco Polo-R mission. Some papers were dedicated to this object, namely de León et al. (2011), Wolters et al. (2011), Rivkin et al. (2012), and Walsh et al. (2012). There are few spectra published in both V and NIR. In the M4AST database, we included the spectra from the MIT-UH-IRTF (MINUS) survey[8] and the spectrum of de León et al. (2011).

On the basis of different spectra, the asteroid has been classified as belonging to primitive types (C, B, or X), but there is no consensus on its classification in the literature (de León et al. 2011; Walsh et al. 2012). In addition some spectral matchings have been noted with meteorites ranging from ordinary chondrite H-type to both CM2 and CV3 carbonaceous chondrite (de León et al. 2011; Rivkin et al. 2012).

To exemplify the applications of M4AST, we used the spectrum obtained on March 30, 2009 by MIT-UH-IRTF (MINUS). The classification in the Bus-DeMeo taxonomy returned the Ch, Cg, and Xc taxonomic types (Fig. 2(c)). The scores obtained for the classes Ch, Cg, Xc, C, and Cgh are very similar. This object has neither the absorption band centered at 0.7 μm typical of Ch-type, nor the redder spectral slope of Xk-types (de León et al. 2011). In addition, the slope in the NIR part of the spectrum, that is of Cg type does not corresponds to the spectrum of (175 706) 1996 FG3.

Classifying this spectrum of (175 706) 1996 FG3 using the G13 taxonomy, we obtain with high confidence ($g_s = -1.237$) the type corresponding to class 3. The other two types (classes 9 and 4) have greater g_s coefficients (Fig. 3(b)). Groups 3 and 4 are the equivalents for the C-type asteroids. As representative members of the class 3, there are (1) Ceres and (10) Hygiea, which are both primitive asteroids. The classification in the G9 taxonomy (Fig. 3(c)) confirms the classification as a primitive type, suggesting as the first options the classes G and C, while the third option (V) could be ignored because it has a larger g_s.

Considering these three classifications, the solution on which the applications of M4AST seems to converge is that the spectrum of (175 706) 1996 FG3 is of a Cg taxonomic type.

[8] http://smass.mit.edu/minus.html

Comparing the spectrum of (175 706) 1996 FG3 to the laboratory spectra, we obtain a good match to a sample of the meteorite Sete Lagoas (Fig. 4(g)). Other matches are the spectrum of a sample from meteorite Murchison heated to 1000 °C (Fig. 4(h)), the spectrum of a sample from the Dhofar 225 meteorite, and the spectrum of a sample from Ozona. This is puzzling, since both the Sete Lagoas and Ozona meteorites are ordinary chondrites (H4 and H6, respectively), and both Murchinson and Dhofar 225 are carbonaceous chondrites. However, we note that the majority of matching solutions are spectra of carbonaceous chondrite meteorites (CM type). If additionally, we take into account the asteroid albedo[9], then the spectrum of Dhofar 225 (sample ID: MA-LXM-078) and Murchison heated to 1000 °C (sample ID: MB-TXH-064-G) seems to be the most probable analogs of this asteroid spectrum.

With the results of M4AST in agreement with those already published, we conclude that the routines of M4AST work correctly and their implementation is robust.

6.2. Discussions regarding misinterpretations of spectra

Applying the correct methods for interpreting asteroid spectra can reveal a lot of information about the physical properties of these objects. However, each method has its own limitations which in general are well-described in the corresponding paper, and using the methods beyond their limits may of course lead to incorrect results.

The first misinterpretation that may occur is related to space weathering. As Gaffey (2008) noted, "space weathering is commonly invoked to reconcile observational data to the incorrect expectation that ordinary chondrite assemblage are common in the asteroid belt". While space weathering for the lunar samples has been well-documented using the samples returned from the Apollo missions, it has been observed that different models are required to interpret the space weathering processes that acted on different asteroid surfaces.

The model we applied for space weathering was based on laboratory experiments that consist in ion irradiation (Ar^+) of olivine and pyroxene powders. This model is suitable for asteroids that seems to consist of olivine and pyroxene, such as those from the S complex.

According to these experiments, the reddening in the infrared part of spectra due to solar-wind ion irradiation can be removed, by dividing the spectrum by an exponential function. However, there are several other effects that can modulate the spectra, such as either thermal influence (Rivkin et al. 2005) or the debated phase-angle effect (Veverka et al. 2000).

The second misinterpretation that may occur is related to the spectral matches with laboratory spectra (Gaffey 2008). Curve matching can provide clues to the nature of the asteroid surface composition. The efficiency of this method can be clearly observed in the case of asteroids that have strong spectral features, such as the vestoids. Misinterpretations can occur when the asteroid surface is modified by space weathering effects, while the meteorite can be modified by terrestrial influences.

The four methods we proposed take into account different characteristics of the spectra: spectral slope, band depths, and the various feature positions. In the context of taxonomic classification, albedo value, space-weathering effects, and similar solutions obtained from all four matching methods, we believe that

[9] The geometric albedo was found as 0.039 ± 0.012 by Walsh et al. (2012).

spectral matches with laboratory spectra provide valuable constraints of the asteroid surface nature.

By applying the methods of M4AST, we observed that a good solution for interpreting the asteroid spectrum is found when all the methods converge to the same mineralogical interpretation. For example, when the spectrum of (99 942) Apophis was processed, despite the poor signal to noise ratio in the infrared part of its spectrum, we obtained the classification Sq in the Bus-DeMeo taxonomy and an analog of this class in the G13 taxonomy. We then found that the spectra of ordinary chondrite meteorites (L, LL subtypes) match this spectrum. These two results were confirmed and developed by applying the Cloutis model: the fraction of olivine-orthopyroxene is 22%, and the associated parameters are equivalent to those of an ordinary chondrite. This conclusion is in general valid for all the spectra we analyzed via M4AST.

7. Conclusions and perspectives

Spectroscopy plays a key role in determining the chemical composition and physical processes that took place and modified the surface of atmosphere-less bodies in the solar system. The development of telescopic instruments (such as SpeX on IRTF, NICS on TNG etc.) and the possibility to access them remotely has led to an increasing number of asteroid spectral measurements. In this context, the exploitation of spectral measurements becomes one of the important means of developing minor planet science. During the past few decades, several methods have been developed to analyze asteroid spectra in order to reveal the physical and chemical properties of these objects. These methods comprise taxonomic classifications, band analyses and comparative mineralogy.

In this paper, we have described M4AST (Modeling for Asteroids), which is a software project dedicated to asteroid spectra. It consists of an asteroid spectral database and a set of applications for analyzing the spectra. The M4AST spectral database has around 2700 asteroid spectra obtained from our observing program and different collaborations. The spectra from the database are in a standard format and are fully available for download.

The M4AST applications cover aspects related to taxonomy, curve matching with laboratory spectra, space weatherin models, and diagnostic spectral parameters.

M4AST was conceived to be fully available via a web interface and can be used by the scientific community. We have presented the interfaces available to access this software tool and the algorithms behind each method used to perform the spectral analysis. The applications have been exemplified with three different types of spectra. The robustness of the routines has been demonstrated by the solutions found for the asteroid spectra of (9147) Kourakuen, a V-type asteroid, (99 942) Apophis an Sq asteroid, and (175 706) 1996 FG3 a Cg type asteroid and a target of *Marco Polo* – R mission. The results agree with and complement those previously published for these objects.

Future developments of this project will include increasing the number of spectra in the database, additional methods for analyzing the spectra (such as mineralogical charts – Birlan et al. 2011), and a more friendly interface.

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