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## Reflectance spectra of Asteroids and Meteorites: their classifications and statistical comparisons

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**Abstract.** Asteroids have been observed both from the ground and through space missions for decades, which accumulated large amount of their observational data. These data are used to estimate the sizes, orbits, and even possible chemical compositions of asteroids. Even though the



chemical composition is generally difficult to be accurately determined without a sample return or in-situ observation by a spacecraft, asteroids are classified based on their reflectance spectra, which are compared with those of meteorites, which are known to be mostly originated from asteroids. This scheme works reasonably well for some asteroid types, but others, mostly featureless ones in reflectance spectra, remained controversial due to the fact that the observational data of asteroids and measured data of meteorites are different in terms of the data coverage, precision and resolution. Our aim is to connect asteroids with meteorites based on sparse modelling in order to search for the optimal integration scheme for two different databases without relying on preliminary knowledge. For the above purpose, we develop large databases of asteroids and meteorites for easy application of sparse modelling. Through our analyses including principal component analysis, Bayesian spectral deconvolution and dimensionality reduction, we found that our data-driven approach can extract potential information without using empirical knowledge. Our methods show a new type of data handling scheme for asteroid and meteorite data, potentially having a significant contribution for future missions.

## 1. Introduction

Small bodies in the solar system, such as asteroids and comets, are considered as remnants of the early evolution of the solar system [1]. Unlike planets which have experienced large scale melting due to impact and/or radioactive heating, small bodies are considered to have experienced less thermal metamorphism, except for shock heating on the surfaces and initial radioactive heating. Therefore, even today small bodies would likely possess primordial materials which have been lost from planets and large satellites through the evolution of solar system. Thus, understanding the formational histories of asteroids may provide constraints on the physical and chemical conditions of the solar nebula and subsequent evolution [1]. Small bodies are also considered as sources of volatile materials, which provide water and organic materials to the Earth. Thus the distribution of small bodies in the early solar system provide a great influence on the formation of Earth's atmosphere-ocean system and on the origin of life. In order to understand asteroids' formation history, compositions of asteroids are the first clue to infer the initial conditions of asteroids. Asteroids' compositions can be measured with high accuracy and high precision through in-situ observations by spacecraft. Several spacecraft missions have been successfully conducted thus far to explore asteroids, such as Galileo [2], NEAR Shoemaker [3], Rosetta [4] and Dawn [5], as well as sample-return missions such as Stardust [6] and Hayabusa [7]. However, since more than three million asteroids are estimated to exist in the solar system, it is impossible to explore every asteroid with spacecraft. Thus inferring surface compositions of asteroids by ground-based telescopes is vital to complement spacecraft missions. In many cases, observable data of asteroids by ground-based telescopes are limited to orbital characteristics and reflectance spectra. Therefore, comparing asteroids' reflectance spectra with those of meteorites is the most essential approach to infer the composition of asteroids (Figure 1).

Majority of meteorites are considered to originate from asteroids. More than twenty thousand meteorites have been collected to date and their reflectance spectra have been measured. However, direct comparison of reflectance spectra between meteorites and asteroids is not simple because meteorites are classified into more than 70 classes, while asteroids are typically 30 classes. Furthermore, most of ordinary chondrites which are the most common meteorite type is spectrally different with typical S-type asteroids which usually have been assumed as parent bodies of ordinary chondrites [8]. Hayabusa spacecraft resolved this problem by returning surface materials from a S-type asteroid Itokawa, proving that the surface materials of Itokawa are consistent with LL-type ordinary chondrites [7]. This indicates that the spectral difference between ordinary chondrites and S-type asteroids would be originated from the effect of space weathering [9]. The lessons learned from the Hayabusa mission is that studies of high-precision measurement of minor elements and isotope analysis of meteorites can be connected with studies of ground-based observations of asteroids, which cover a wide spatial range with low-precision measurement. Thus ground observations of asteroids reinforced by meteoritical science would greatly improve our understanding of compositional distribution of asteroids.

Despite the success of sample-return missions represented by Hayabusa, there still remains a few major issues to connect asteroids with meteorites. One of the largest obstacles is that the classification scheme between asteroids and meteorites are fundamentally different. Asteroids are classified mainly based on the shape of their reflectance spectra and orbital parameters [10], while meteorites are classified by detailed petrology and mineralogy [11]. In addition, reflectance spectra of asteroids are greatly influenced by surface properties (e.g. roughness, particle size) and space weathering effect. Reflectance spectra of meteorites are also significantly influenced by various terrestrial weathering and contamination. Sampling bias of meteorites is another major problem because some of the meteorites, such as iron meteorites, can more frequently survive destruction by aerodynamic heating during entry. Such meteorites are also easy to be discovered on the ground because of their pronounced colors compared with other type of meteorites. From the perspective of data science, the above problems can be described as (1) choosing the optimal integration scheme for two databases with significantly different accuracies and certainties, and (2) extracting appropriate base functions to explain different kinds of physical models. Previous spectra analyses, for example, have focused on certain wavelength regions or intensity ratios based on preliminary knowledge given by petrology or meteoritics. By using sparse modelling, however, we could extract optimal base functions without relying on preliminary knowledge. Sparse modelling is also strongly required for automatic analyses of big data in the present situation, where amount of observation data is dramatically increasing. In this paper we report our attempt to connect asteroids with meteorites using statistical scheme based on sparse modelling.

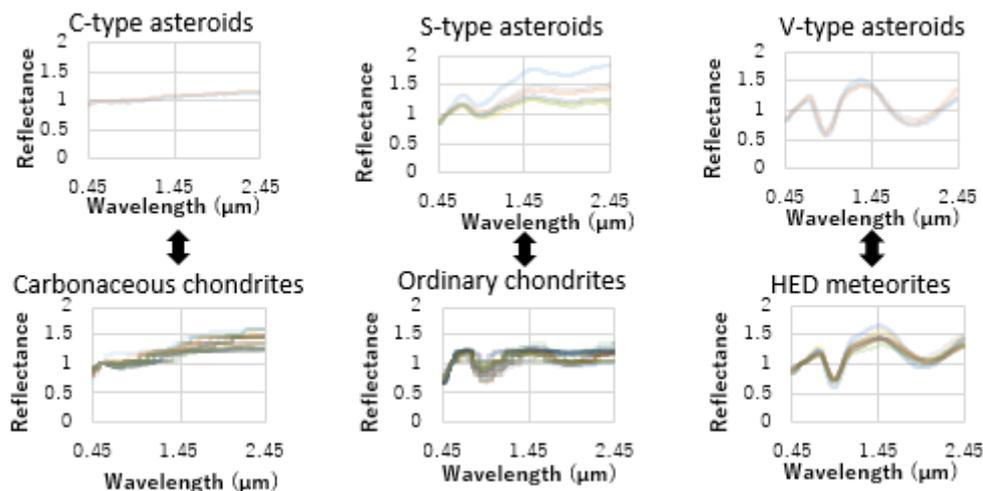


Figure 1. Typical reflectance spectra for asteroids (C-type, S-type, and V-type) and their presumably-corresponding meteorites (C chondrites, O chondrites, and HED).

## 2. Cluster analysis of the bulk elemental compositions of meteorites

Identifications of the corresponding meteorite types of the targeted bodies of asteroid missions are among the major goals of asteroid missions. Besides such scientific importance, rapid identification of the surface materials during the reconnaissance phase is also critically important. Modern spacecraft carry cameras/spectrometers in the visible to infrared wavelengths, which can identify surface materials. However, irradiation by cosmic rays and solar wind as well as bombardment by interplanetary dust particles modify the surfaces of airless bodies through processes known as space weathering. Impact events also mix materials on the surface of the body. These processes may flatten or change the absorption characteristics of reflectance spectra. Therefore, elemental compositions, which can be measured by X and gamma-ray spectrometers, may be useful for the above purpose. However, it has not been investigated extensively how well we can classify these planetary materials based on elemental composition alone.

We perform principal component and cluster analyses on 12 major and minor elements of the bulk compositions of 500 meteorites reported in the NIPR database [12]. Our analyses, including hierarchical cluster analysis, indicate that meteorites can be classified into about 10 groups solely by their bulk elemental compositions. We suggest that Si, Fe, Mg, Ca, and Na are the optimal set of elements, as this set has been used successfully to classify meteorites of the NIPR database with more than 94% accuracy. Principal components analysis indicates that elemental compositions of meteorites form 8 clusters in the three-dimensional space of the components. Three major principal components (PC1, PC2, and PC3) can be interpreted as degree of differentiations of the source body (i.e., primitive vs. differentiated), degree of thermal effects, and degree of chemical fractionation, respectively. Although the exact ranges of elements of each cluster could suffer from the systematic intra-laboratory error, realized through comparing our results with those of another elemental composition database, our new method shows promise in the classification of the surface materials of a small body into a known group of meteorites, having a significant importance in future reconnaissance.

### **3. Automatic deconvolution method for Modified Gaussian model using the exchange Monte Carlo method**

Deconvolution analysis of reflectance spectra has been a useful method to infer mineral composition and crystal structure for major rock forming minerals, including olivine and pyroxene. Clinopyroxene is one of the most important mineral groups due to both its rich abundance on solid bodies in the solar system and distinguished absorption features. The band centers of visible to near-infrared spectra of clinopyroxene are known to vary due to total iron and calcium content. Visible/near infrared spectra of synthetic clinopyroxene are characterized based on a modified Gaussian Model (MGM) [13]. The numerical algorithm of the widely used MGM, however, utilizes the steepest descent method, which has a local minima problem [14]. With bad initial parameters, the steepest descent method converges into a local minimum, thus one needs to manually adjust initial parameters and calculate the model repeatedly to obtain the desired solution.

In order to avoid the local minimum problem, we analyzed visible/near infrared spectra of clinopyroxene using Bayesian spectral deconvolution with the exchange Monte Carlo method [15]. This method is an improved algorithm of the Markov chain Monte Carlo method, aimed to both avoid local minima traps and remove the arbitrariness originated from initial parameters [16]. We used the visible/near infrared spectra of clinopyroxene, measured at 5 nm intervals over the wavelength range of 0.3-2.6  $\mu\text{m}$  [13]. We chose only sieved powder samples whose grain sizes are smaller than 45  $\mu\text{m}$  with individual grains about 15-25  $\mu\text{m}$  in size. We collected 31 clinopyroxene spectra from published database with wide ranging Ca, Mg, Fe compositions (8-52%, 0-52% and 3-90%, respectively). We found that: (1) 1  $\mu\text{m}$  band shifts regularly to longer wavelengths with an increase of Ca content; (2) 1  $\mu\text{m}$  band shifts to shorter wavelengths with an increase of Fe content, although the variance is larger than that of orthopyroxene; (3) for Ca contents < 30%, 2  $\mu\text{m}$  band shifts to longer wavelength as a function of Ca, while for Ca contents > 30%, the center of 2  $\mu\text{m}$  band remains almost constant at  $\sim 2.4$   $\mu\text{m}$ ; and (4) the center of 2  $\mu\text{m}$  band of augites (Ca <  $\sim 20\%$ ) does not depend on Fe content significantly, while the center of 2  $\mu\text{m}$  band of pigeonites (Ca >  $\sim 20\%$ ) shifts to longer wavelengths as a function of Fe content. These results are consistent with the previous study [13], suggesting that the exchange Monte Carlo method can yield the same results obtained by conventional MGM analysis, which is important to remove issues of local minima and arbitrariness of initial parameters. The successful application of the exchange Monte Carlo method to a wide range of clinopyroxene would pave the way for further deconvolution analysis of reflectance spectra of mineral mixtures, such as olivine, orthopyroxene, and clinopyroxene.

### **4. Relationship between reflectance spectra of asteroids and meteorites**

#### *4.1. Albedo and reflectance spectra*

Asteroids have been classified into several types based on principal component analysis of reflectance spectra [10]. Different types of meteorite samples, however, can yield similar reflectance spectra such as black ordinary chondrites and carbonaceous chondrites [17]. Thus the degeneracy of reflectance spectra may suggest that there is an application limit of the classification scheme based solely on reflectance spectra. Albedo data also have been accumulated, however, their relationship with reflectance spectra are not fully understood [18]. Our objective is to combine albedo with reflectance spectra in an attempt of improving asteroid classification.

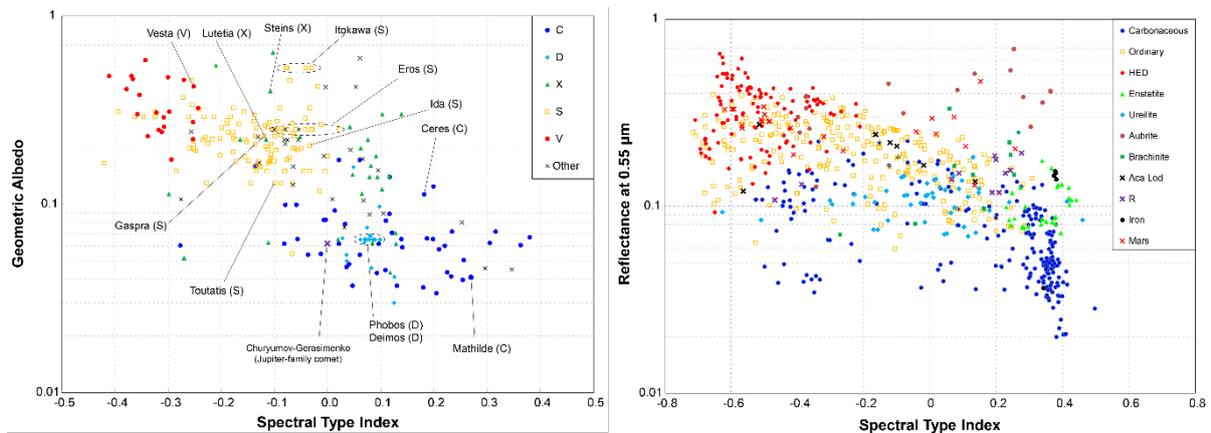
We compiled visible/infrared reflectance spectra within the region of 0.45 to 2.45  $\mu\text{m}$  based on published databases. All the spectra were sampled with cubic spline fits at a wavelength interval of 0.05  $\mu\text{m}$ , resulting in 41 data points. Each spectrum was subtracted by its mean. Using the reduced spectrum, we defined the spectral type index  $R$ , which is the difference between correlation coefficients with average S and C-type spectra as follows:

$$R = \frac{\mathbf{t} \cdot \mathbf{r}_c}{\|\mathbf{t}\| \|\mathbf{r}_c\|} - \frac{\mathbf{t} \cdot \mathbf{r}_s}{\|\mathbf{t}\| \|\mathbf{r}_s\|}$$

where  $\mathbf{t}$ ,  $\mathbf{r}_c$ , and  $\mathbf{r}_s$  are the reduced target spectrum, average C-type, and average S-type spectra, respectively. Positive  $R$  values more closely approximate C-type spectra, while negative  $R$  values S-type. We also compiled asteroids' geometric albedo data mostly from Supplemental IRAS Minor Planet Survey [19].

The albedo-spectra map indicates that there is a general trend in the distribution of asteroid types (Figure 2). V-type, C-type and S-type asteroids are distinctly separated from each other on the albedo-spectra map. The variance of each cluster appears to increase in the order of V-type, S-type and C-type. The reflectance-spectra map for meteorites also shows a trend in the distribution of meteorite types. HED meteorites distribute at the top left, carbonaceous chondrites distribute at the bottom right, and ordinary chondrites distribute between HED meteorites and carbonaceous chondrites (Figure 2). It appears that geometric albedo or reflectance plays a significant role in the resulting spectral signature. There are many possible factors which could influence albedo, such as (1) mineral and/or elemental composition, (2) fragmented particle size, (3) space weathering and (4) crystal size. We consider, however, crystal size to be the primary factor in the resultant albedo-spectra map because: (1) based on the analyses of meteorites, there is no significant difference between ordinary and carbonaceous chondrites in terms of carbon content or modal composition, (2) smaller particles tend to yield higher albedo, though not enough to explain the significant albedo difference observed among asteroids, and (3) spectral darkening due to space weathering requires reduced Fe (noting that there is no clear evidence that C-type asteroids, which are significantly darker than S-type or V-type asteroids, have higher Fe abundances). With the above consideration, we discuss the crystal size in the context of thermal processes of asteroids to help explain albedo-spectra map.

Smaller crystals generally result in darker reflectance. V-type asteroids are believed to have experienced differentiation and magmatism, as evidenced by the analyses of HED meteorites. Thus the crystals would become coarser due to a slow cooling rate, resulting in brighter and more pyroxene-rich surface spectra. On the other hand, S- and C-types would be undifferentiated chondrite asteroids, believed to correspond to ordinary and carbonaceous chondrites, respectively. Those meteorites preserve chondrules generally having finer crystals due to rapid cooling in the presolar nebula [20]. This would result in dark featureless surface spectra of C-types. S-type asteroids have experienced moderate thermal metamorphism after their accretion, causing recrystallization which results in larger crystals and in more evident pyroxene signals than C-type.



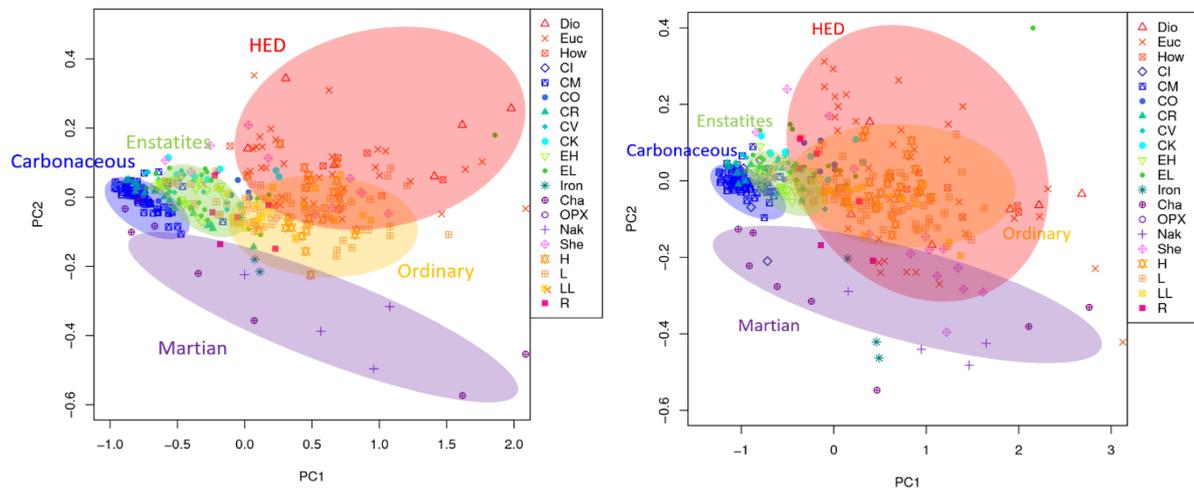
**Figure 2.** (left) Relationship between geometric albedo and visible/near infrared spectral type for asteroids. Also shown are the names of asteroids that have been explored by spacecraft. (right) Relationship between reflectance at  $0.55\ \mu\text{m}$  and visible/near infrared spectral type for meteorites.

#### 4.2. Principal component analysis including $3\ \mu\text{m}$ wavelength region

In order to better understand the compositions of asteroids, mineralogical relationship between asteroids and meteorites have been studied based on reflectance spectra obtained by ground- and space-based telescope. Their relationship, however, remains poorly constrained except for a S-type asteroid Itokawa and LL chondrites [7]. Although spectral similarities have been suggested between V-type asteroids and HED meteorites and between carbonaceous chondrites and C- and/or D-type asteroids, detailed relationship is not well constrained. The major obstacle to compare asteroids and meteorites is that the classification scheme between asteroids and meteorites are fundamentally different. Asteroids are classified mainly based on the shape of their reflectance spectra and orbital parameters [10], while meteorites are classified by detailed petrology and mineralogy [11]. Based on principal component analysis, Britt et al. (1992) [17] compare reflectance spectra of asteroids with those of meteorites. In this pioneer work, they pointed out some offsets remain between meteorites and asteroids, which might be due to the fact that they used eight color spectra within visible wavelength from  $0.35$  to  $1.0\ \mu\text{m}$ . Since characteristic absorptions are observed in the near-infrared range, including pyroxene ( $2\ \mu\text{m}$ ) and hydrated silicates ( $3\ \mu\text{m}$ ), using reflectance spectra with a wider wavelength range could result in a better spectral matching between asteroids and meteorites. In this study, we developed a database of reflectance spectra for asteroids and meteorites with wavelengths ranging from  $0.3$  to  $4\ \mu\text{m}$  and perform multivariate analysis.

We obtained reflectance spectra for meteorites and asteroids from RELAB [21] and the database of Planetary Spectroscopy at MIT [22], respectively. Asteroid spectra for  $3\ \mu\text{m}$  band are obtained from previous studies [e.g., 23]. All the spectra were sampled with cubic spline fits at a wavelength interval of  $0.05\ \mu\text{m}$ . Meteorite spectra are chosen based on the following criteria: (1) particulate sample, (2) phase angle is  $30^\circ$ , (3) sample is from valid/known meteorite, (4) not heated/laser-irradiated, inclusion or impact melt sample, (5) not moon sample or lunar meteorite. The developed database includes 534 meteorite spectra and 369 asteroid spectra. We performed principal component analysis on the database and measure how well each meteorite group and asteroid group is separated on the principal component space (Figure 3). Our analyses show that using spectra from  $0.4$  to  $2.5\ \mu\text{m}$ , accuracy of separation among ordinary chondrites, carbonaceous chondrites, HED meteorites is significantly improved compared with the case using spectra from  $0.4$  to  $1.0\ \mu\text{m}$ . In fact, cluster analysis (Ward's method) on asteroid spectra show that including  $2.5\ \mu\text{m}$  improve accuracy of classification from  $65\%$  to  $75\%$ . On the other hand, we found that the accuracy of separation is not significantly improved when using meteorite spectra from  $0.4$  to  $4\ \mu\text{m}$  compared with the case using spectra from  $0.4$  to  $2.5\ \mu\text{m}$ . This suggests that  $3\ \mu\text{m}$  band may not be useful for classification of some meteorites, because  $3\ \mu\text{m}$  band is widely observed among chondrites and achondrites. Our analysis also revealed that an inherent spectral difference exist between

asteroids and meteorites. This may be attributed to space weathering effect. Or it may be originated from the difference of observation target, in which reflectance spectroscopy of asteroids measure surface compositions while reflectance spectroscopy of meteorites measure bulk compositions.

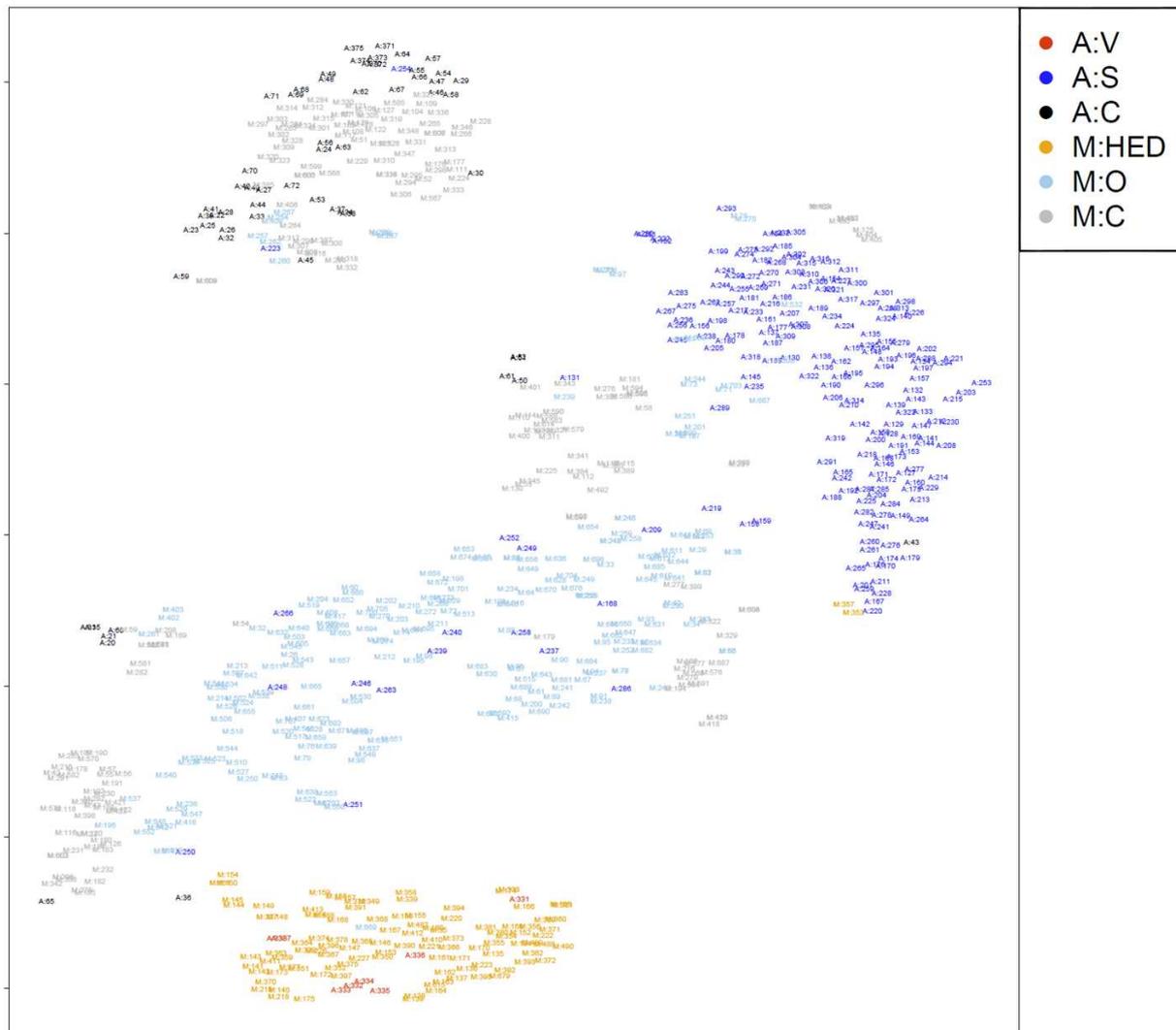


**Figure 3.** (left) Principal components of meteorites' spectra from 0.3 to 2.5  $\mu\text{m}$ . (right) Principal components of meteorites' spectra from 0.3 to 4  $\mu\text{m}$ .

#### 4.3. Spectral relationship visualized by correlation distance and t-SNE

Statistical classifications of spectral types without detailed interpretation of spectral shapes can be useful to overview the variation and relationships within a spectral data set, even though there are known difficulties of comminution, melting, mixing, and space weathering. For example, as discussed in section 4.2, simple scheme such as principal component analysis cannot overcome the inherent spectral difference between asteroids and meteorites.

Thus we expand our analysis by applying to a wider and denser datasets of reflectance spectra for both meteorites and asteroids based on mathematically more advanced methods. We analyse sixteen kinds of distance of spectra including Partial Autocorrelation, Dynamic Time Warping, Pearson Correlation, and Euclidean distance. The distances are visualized by using six kinds of schemes including t-SNE (t-Stochastic Neighbor Embedding) [24]. We find that correlations of both meteorites and asteroids are generally good by this simple scheme. Preliminary results (Figure 4) indicate that (1) V-type asteroids generally match HED meteorites, (2) S-type asteroids locate near ordinary chondrites but they do not entirely match each other, which may reflect the effect of space weathering as discussed in the previous section (3) C-type asteroids match carbonaceous chondrites and they are separated into a few sub clusters. We consider that our unique approach is the first to quantitatively visualize the corresponding relationship between asteroid and meteorite spectra, which could obtain potential base functions to physically describe reflectance spectra in the future.



**Figure 4.** Correlation distance of asteroid and meteorite spectra visualized by t-SNE.

## 5. Summary

We have examined the relationship between asteroid and meteorite data by sparse modelling. These two kinds of data have significantly different spatial coverage and different precision and accuracy. By using sparse modelling, we aim to analyze asteroid and meteorite data without relying on preliminary knowledge and to perform automatic analysis of big data. We summarize our works as follows.

1. Building database of meteorites' elemental compositions (section 2)
2. Developing classification scheme for meteorites solely based on bulk elemental compositions (section 2)
3. Developing automatic deconvolution method of reflectance spectra for major rock-forming minerals based on the exchange Monte Carlo method (section 3)
4. Building database of reflectance spectra of asteroids and meteorites (section 4)
5. Visualization of albedo-spectra relationship of asteroids and meteorites (section 4.1)
6. Comparison between asteroids and meteorites spectra in PCA space using improved database (section 4.2)
7. Developing successful visualization scheme to compare asteroids' spectra with those of meteorites (section 4.3)

Since we have tested our method on relatively simple problems, we are now extending our analysis to more challenging problems. One is to develop a method to analyze dark featureless flat spectra, such as C-type asteroid and carbonaceous chondrites. These spectra are very important because they are often observed on small bodies which are expected to possess primordial materials. In addition, some of these bodies are the target for future space missions, including Hayabusa-2 and OSIRIS-Rex. Another project is to compare asteroids spectra with meteorites' spectra and elemental compositions. Through supervised learning, adding elemental compositions to the classification of reflectance spectra could improve the accuracy of comparison. Finally, spectral deconvolution without preliminary knowledge on mixtures of minerals is also an important, because an appropriate handling scheme for big data would be required for future remote sensing observations.

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