Journal of Quantitative Spectroscopy & Radiative Transfer 204 (2018) 144–151

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

Spectral modeling of meteorites at UV-vis-NIR wavelengths

Julia Martikainen[a,*], Antti Penttilä[a], Maria Gritsevich[a,b], Hannakaisa Lindqvist[c], Karri Muinonen[a,d]

[a] Department of Physics, P.O. Box 64 (Gustaf Hällströmin katu 2a), FI-00014 University of Helsinki, Finland
[b] Institute of Physics and Technology, Ural Federal University, Mira str. 19, 620002 Ekaterinburg, Russia
[c] Finnish Meteorological Institute, Erik Palménin aukio 1, FI-00101 Helsinki, Finland
[d] Finnish Geospatial Research Institute FGI, National Land Survey of Finland, Geodeetinrinne 2, FI-02430 Masala, Finland

ARTICLE INFO

Article history:
Received 16 June 2017
Revised 11 September 2017
Accepted 11 September 2017
Available online 15 September 2017

Keywords:
Asteroids
Meteorites
Reflectance spectroscopy
Light scattering
Spectral modeling

ABSTRACT

We present a novel simulation framework for assessing the spectral properties of meteorite specimens. The framework utilizes a ray-optics code, which simulates light scattering by Gaussian-random-sphere particles large compared to the wavelength of the incident light and accounts for internal diffuse scatterers. The code uses incoherent input and computes phase matrices by utilizing incoherent scattering matrices. Reflectance spectra are modeled by introducing a combination of olivine, pyroxene, and iron, the most common materials present in meteorites that dominate their spectral features. The complex refractive indices of olivine and iron are obtained from existing databases. The refractive indices of pyroxene are derived using an optimization that utilizes our ray-optics code and the measured spectrum of the material. We demonstrate our approach by applying it on the measured meteorite reflectance spectra obtained with the University of Helsinki integrating-sphere UV–vis-NIR spectrometer.

1. Introduction

Every year approximately $3.7 - 7.8 \times 10^7$ kg of extraterrestrial material bombard the Earth's atmosphere [1]. This material mostly consists of small dust particles that fully ablate in the atmosphere. Nevertheless, some of them survive atmospheric entry and reach the ground [2]. These are called meteorites, our free samples of the Solar System.

Asteroids remain mostly the same for the past 4.5 billion years. They provide us information on the origin, evolution, and current state of the Solar System. Meteorites and asteroids can be linked by matching their respective reflectance spectra. However, this is difficult because the spectral features depend strongly on the surface properties [3]. Asteroid surfaces are usually covered with a regolith, which is a layer of loose material, such as dust and rock. On the other hand, meteorites are free of the regolith. To better interpret the spectra, we need to gain more knowledge of the light-scattering physics involved.

The strength of meteorites imposes a selection effect on those meteorites that survive entry into the atmosphere [4]. It is thought that there is also a dependence on the size. Smaller objects are more easily transported out of the asteroid main belt due to the Yarkovsky effect [5] than the large objects. These in turn are from a few locations near resonant orbits with Jupiter. Finally, it is also thought that meteorites sample the inner main belt [6], although it is possible that meteorites can be transported from further out [7]. The metamorphic evolution of asteroids is preserved within the meteorite collection and can give us information on differentiated asteroids such as in the case of Vesta with the HED group of meteorites [8].

Some good matches have been made between individual meteorite spectra and Near-Earth Asteroids (NEAs) [9] as well as between meteorite spectra and large main belt asteroids (MBAs) [10]. The principal properties of the spectra used to identify possible matches between meteorites and asteroids are the band minimum location and Band Area Ratio (BAR). The band minimum is the wavelength of an absorption band in the spectra. The BAR is the ratio between the area of the bands in the spectra. These properties are diagnostic of the object's mineralogy and, to a lesser extend, of other physical properties such as surface roughness and grain size [11]. The spectra of meteorites and asteroids are also dependent on observational conditions such as the phase angle between the line connecting the light source (e.g., the Sun) with the target and the line connecting the target with the observer. This is a key effect that needs to be understood to help improve matches between meteorites and asteroids, as this phase angle, when observing asteroids, varies due to the ever changing orbital positions of the viewer and the target. Variations in the band depths, band

---

[*] Corresponding author.
E-mail address: julia.martikainen@helsinki.fi (J. Martikainen).

http://dx.doi.org/10.1016/j.jqsrt.2017.09.017
0022-4073/© 2017 Elsevier Ltd. All rights reserved.

minimum locations, the band area ratio, and spectral slope have been noted to vary with phase angle and have been characterized [12]. Although this effect does not seem to affect the mineralogical analysis very much, it is important for understanding optical effects and their relationship to physical properties such as surface roughness and grain size.

When it comes to spectral modeling, Hapke's radiative transfer model has been utilized in most of the studies: S. J. Lawrence and P. G. Lucey used Hapke mixing models to model asteroid mineralogy [13], whereas B. E. Clark modeled S-type asteroid spectra [14]. In this study, we abandoned the Hapke model and utilized a ray-optics code that accounts for internal diffuse scatterers, to derive the refractive indices for both clinopyroxene and bronzite, and to further model the reflectance spectra of three meteorites. The corresponding measured meteorite reflectance spectra were obtained with the University of Helsinki integrating-sphere UV-vis-NIR spectrometer. The details of the model are described in Section 4.1 and the modeling results are presented in Section 5.2.

2. Light scattering

2.1. Ray optics

The size of the particle can be described as a size parameter $x = ka$, where k is the wave number and a is the mean radius of the particle. In geometric optics, a Stokes parameter vector is related to every ray. At a boundary surface, refraction and reflection take place according to Snel's law and Fresnel's reflection and refraction matrices.

In the ray optics approximation [15]:

$$\sigma_{\text{ext}} = \sigma_{\text{abs}} + \sigma_{\text{sca}} \tag{1}$$

where σ_{ext} and σ_{abs} are extinction and absorption cross sections.

The single-scattering albedo $\tilde{\omega}$ is defined as [16]:

$$\tilde{\omega} = \frac{\sigma_{\text{sca}}}{\sigma_{\text{ext}}}. \tag{2}$$

The phase matrix P can be obtained from:

$$\mathbf{P} = \frac{4\pi}{k^2 \sigma_{\text{sca}}} S, \tag{3}$$

where S is the 4×4 element scattering matrix describing the scattering event in terms of angular dependence, and links the Stokes parameters of the incident and scattered fields [16]:

$$[I_{\text{sca}}, Q_{\text{sca}}, U_{\text{sca}}, V_{\text{sca}}]^T = \frac{1}{k^2 r^2} S [I_{\text{inc}}, Q_{\text{inc}}, U_{\text{inc}}, V_{\text{inc}}]^T. \tag{4}$$

The ray optics with diffuse and specular interactions (RODS) method, which uses the scattering phase matrix $\mathbf{P}$, single-scattering albedo $\tilde{\omega}$, and extinction mean free-path length l_0 to account for internal inhomogeneities, was utilized to model the reflectance spectra of meteorites. In this method, the diffuse scatterers are distributed inside an isotropic and homogenous medium that has a complex refractive index m. The extinction mean free-path length l_0, which describes the average distance traveled by the ray, can be obtained from [15]

$$l_o = \frac{1}{k_0}, \tag{5}$$

where k_0 is the extinction coefficient and can be written as

$$k_0 = n_0 q_{\text{ext}} \pi a^2 = \frac{3\nu_0 q_{\text{ext}}}{4a}, \tag{6}$$

where q_{ext} is the extinction efficiency, a is the mean radius of the particle, n_0 is the number density, and ν_0 is the volume density.

In geometric optics, there are no interference effect among the fields scattered by the particles in the system, and thus the scattered electromagnetic field can be considered incoherent. The incoherent scattered electromagnetic field $\mathbf{E}^s_{i,ic}$ is obtained by subtracting the coherent field $\mathbf{E}^s_c$ from the free-space scattered field of a specific volume element $\mathbf{E}^s_i$ [17,18]:

$$\mathbf{E}^s_{i,ic} = \mathbf{E}^s_i - \mathbf{E}^s_c. \tag{7}$$

The coherent scattered electromagnetic field can be obtained by ensemble averaging the field scattered by individual realizations for finite volumes of spherical particles [19]:

$$\mathbf{E}^s_c = \frac{1}{N_r} \sum_{i=1}^{N_r} \mathbf{E}^s_i, \tag{8}$$

where N_r is the number of realizations. Geometric optics input is incoherent a priori and the scattering phase matrix $\mathbf{P}$ is computed using the incoherent scattering matrices.

For our spectral model, we combine olivine and pyroxene particles that contain micro iron scatterers by averaging their single-scattering albedos $\tilde{\omega}$, mean free-path lengths l_o, and phase matrices $\mathbf{P}$. The averaged single-scattering albedo $\tilde{\omega}_{\text{avg}}$ is obtained by dividing the averaged scattering cross section $\sigma_{\text{sca,avg}}$ with the averaged extinction cross section $\sigma_{\text{ext,avg}}$:

$$\tilde{\omega}_{\text{avg}} = \frac{\sigma_{\text{sca,avg}}}{\sigma_{\text{ext,avg}}}. \tag{9}$$

The averaged scattering cross section is calculated by adding up scattering cross sections for olivine and pyroxene particles and weighting them based on their ratio in the meteorite. The averaged extinction cross section is calculated similarly using extinction cross sections of both olivine and pyroxene particles. The phase matrices are averaged by first averaging the scattering matrices using weights and then converting the averaged scattering matrix back to a phase matrix by utilizing the averaged scattering cross section in Eq. (3). The averaged mean free-path length can be obtained from

$$l_0 = \frac{1}{\kappa_{\text{ext,tot}}}, \tag{10}$$

where $\kappa_{\text{ext,tot}}$ is a weighted sum of the averaged κ_{ext} for olivine and pyroxene particles. In a volume element δV, the ensemble average of total extinction cross section is $\langle \sigma^{\text{tot}}_{\text{ext}} \rangle$. In this volume, the particles occupy an averaged volume $\langle V^{\text{tot}}_{\text{ext}} \rangle$. When the corresponding quantities for one particle are $\langle \sigma^1_{\text{ext}} \rangle$ and $\langle V^1_{\text{ext}} \rangle$, κ_{ext} can be obtained [20]:

$$\begin{aligned}
\kappa_{\text{ext}} &= \frac{\langle \sigma^{\text{tot}}_{\text{ext}} \rangle}{\delta V} \\
&= \frac{\langle \sigma^{\text{tot}}_{\text{ext}} \rangle}{\langle V^{\text{tot}}_{\text{ext}} \rangle} \frac{\langle V^{\text{tot}}_{\text{ext}} \rangle}{\delta V} \\
&= \frac{\langle \sigma^{\text{tot}}_{\text{ext}} \rangle}{\langle V^{\text{tot}}_{\text{ext}} \rangle} \nu_0 \\
&= \nu_0 \frac{\langle \sigma^1_{\text{ext}} \rangle}{\langle V^1_{\text{ext}} \rangle} \\
&= \nu_0 \frac{3 \langle \sigma^1_{\text{ext}} \rangle}{4\pi a^3 \exp(3\beta^2)} \\
&= 3\nu_0 \frac{\langle \sigma^1_{\text{ext}} \rangle}{4\pi a^3_{\text{vol}}} \\
&= 3\nu_0 \frac{\langle q^1_{\text{ext}} \pi a^2_{\text{perp}} \rangle}{4\pi a^3_{\text{vol}}} \\
&= 3\nu_0 \frac{\langle q^1_{\text{ext}} a^2_{\text{perp}} \rangle}{4\pi a^3_{\text{vol}}},
\end{aligned} \tag{11}$$