Journal of Quantitative Spectroscopy & Radiative Transfer 204 (2018) 138–143

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

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

Light scattering by hierarchical aggregates

Ludmilla Kolokolova [a,*], Lev Nagdimunov [a], Daniel Mackowski [b]

[a] University of Maryland, Department of Astronomy, MD, 20742, USA
[b] Auburn University, Mechanical Engineering Department, AL 36849, USA

ARTICLE INFO

Article history:
Received 17 June 2017
Revised 19 September 2017
Accepted 19 September 2017
Available online 21 September 2017

Keywords:
Rosetta spacecraft
Cometary dust
Aggregate
Hierarchical structure
Brightness
Polarization
MSTM modeling

ABSTRACT

Recent *in-situ* studies of the environment of comet 67P/Churyumov–Gerasimenko by the dust instruments onboard the Rosetta spacecraft have indicated a complex structure of cometary dust particles. The majority of those particles appeared to be large aggregates of hierarchical structure, i.e. aggregates of particles, which, in turn, were aggregates of smaller particles. This confirmed an earlier hypothesis that dust particles in protoplanetary disks grow under hierarchical growth process. Thus, it is very likely that hierarchical aggregates are common type of natural dust particles. In this paper, we present results of computer simulations of light scattering by a variety of hierarchical aggregates to determine how their structure affects their brightness and polarization phase curves as well as photometric and polarimetric color, and albedo. The computations were done using Multi-Sphere T-Matrix method. Our results show that the type of hierarchical structure of aggregates, specified by the number of particles at each level of hierarchy, causes variations in their light-scattering characteristics, which noticeably exceed the variations caused by different configuration of monomers in the aggregates of the same hierarchical structure. Although we could not find any regularities in the brightness and polarization dependence on the structure of the aggregates, our results clearly show that not only composition or size of aggregates, but also their specific structure should be carefully examined when light scattering by cometary or any other type of dust is modeled. Specifically, we may need to reconsider modeling the cometary dust particles using simple ballistic particle-cluster and cluster-cluster aggregates.

1. Introduction

The ESA spacecraft Rosetta spent two years, from September 2014 until September 2016, in the vicinity of comet 67P Churyumov–Gerasimenko, studying the cometary nucleus as well as plasma, gas and dust cometary environment. Cometary dust was one of the focuses of Rosetta studies and was accomplished by three dust instruments: GIADA (Grain Impact Analyser and Dust Accumulator), COSIMA (Cometary Secondary Ion Mass Analyser), and MIDAS (Micro-Imaging Dust Analysis System). Additional data about cometary dust was acquired by the Rosetta camera OSIRIS (Optical, Spectroscopic, and Infrared Remote Imaging System) and mass-spectrometer ROSINA (Rosetta Orbiter Spectrometer for Ion and Neutral Analysis). The results by OSIRIS and ROSINA are rather specific: OSIRIS caught images of thick dust jets and very large dust particles [1] and ROSINA observed some spikes in the measurements associated with volatiles that sublimated from dust particles [2]. Since we are interested in the structure of the dust particles, we will focus on the measurements reported by other instruments: GIADA, COSIMA and MIDAS.

GIADA [3] was designed to measure cumulative mass of the dust particles, their size distribution (for sizes larger than 15 µm), velocity distribution, and particle momentum. Indirectly, the instrument team could also estimate the shape and structure of particles. The main result of the GIADA study was a survey of the dust spatial and temporal variations, but in this paper we are mostly interested in the particle properties revealed by GIADA. They were summarized in [4]. It was found that the cometary dust consisted of compact and fluffy particles with the latter forming the bulk of the distribution (~84%). The size of the measured fluffy particles was in the range of 0.2 – 2.5 mm and by comparing the data with laboratory simulations, the GIADA team concluded that they were aggregates of submicron grains with bulk density $< 1\ kg/m^3$.

More detailed information about the structure of cometary dust particles was obtained by COSIMA [5] measurements. This instrument included a dust collector; the particles that were caught by the collector were then placed under a microscope (COSISCOPE)

* Corresponding author.
E-mail address: ludmilla@astro.umd.edu (L. Kolokolova).

https://doi.org/10.1016/j.jqsrt.2017.09.019
0022-4073/

for imaging. COSIMA collected and imaged more than 10,000 cometary particles, which were found to be dominated by clusters (86%). These aggregates differed in their tensile strength and were divided into three types: shattered clusters, glued clusters and rubble piles [6]. The size of particles, studied by COSIMA was in the range of hundreds of microns and the smallest "monomers" of the COSIMA clusters had a size ∼5 µm.

Significant progress in understanding the properties of cometary dust was achieved due to MIDAS [7] measurements. MIDAS was an atomic force microscope studied both the structure and shape of collected dust particles by scanning them with a sharp, needle-like tip located at the end of piezoelectric scanner, which provided a 3D image of the particles. An advantage of MIDAS was that it could work with small, micron-sized, particles and was able to resolve them to a level down to 10 nm. Particles studied by MIDAS also appeared to be aggregates but they were small (∼5 µm) and consisted of monomers of mainly submicron size [8].

The results from GIADA, COSIMA and MIDAS, considered together, allowed characterizing cometary dust particles as hierarchical aggregates, i.e. aggregates of particles, which, in turn, are aggregates of smaller particles. Briefly speaking, the aggregates seen by COSIMA are made up of particles studied by MIDAS; the submicron size of the smallest particles in cometary aggregates is consistent with GIADA findings.

It is interesting that hierarchical structure of cometary dust particles was predicted, for example, in [9], where such a structure allowed the authors to model thermophysical properties of the upper layers of cometary nuclei. Moreover, Dominik [10] showed that hierarchical growth of dust is the most efficient type of dust particles formation in protoplanetary disks, where said dust aggregates then agglomerate to planetesimals and cometary nuclei.

These new developments in studying cometary dust motivated us to investigate the differences in light scattering characteristics of hierarchical structure aggregates from the properties of regular ballistic aggregates, usually used to model cometary dust (see Section 2]).

In this paper we present results of our study. The aggregates we consider were built using a model, developed by co-author Nagdimunov, which is described in Section 2. In Section 3, we present and analyse the results of our computer simulations of light scattering by a variety of hierarchical aggregates made of comet-like material and of ice. The computations were done with Multi-Sphere T-Matrix code by Mackowski and Mishchenko [11,12].

2. Model of hierarchical aggregates

The first step in our modeling was to create the ability to build hierarchical aggregates of various yet controlled structure. For this, we employed a ballistic approach. Introduced by Meakin [13] in 1984, it was then widely used in light-scattering simulations for building Ballistic Particle-Cluster Aggregates (BPCA) and Ballistic Cluster-Cluster Aggregates (BCCA), see, e.g., [14–21]. This approach supposes that units, whether particle or cluster, travel in random straight trajectories until they collide with an aggregate that started from a single monomer with the coordinates (0, 0, 0). Here, as well as in the papers listed above, "collision" means that the unit touches, but not overlaps, with one or more monomers of the central aggregate and sticks to them at the point(s) of touching. It should be emphasized that the described procedure is not based on any physics of the realistic processes responsible for the formation of cosmic, including cometary, aggregates. This is just a convenient algorithm for generating porous particles whose structure resembles the structure of real cometary dust particles.

For building hierarchical aggregates, we stratified the procedure described above. The first step in the procedure was building the first-level aggregates, i.e. aggregates made of individual spheres of a given size; these are built using a ballistic-particles approach, i.e. they are BPCAs. At each higher level of aggregation, the clusters of the previous level collide with a central cluster; again, this is identical to the BPCA process at each level, except that the units of collision are increasingly larger aggregates. We incorporated this procedure into an IDL code that can build hierarchical aggregates of an unlimited number of the aggregation levels. Its parameters are the size of the first-level spheres, where all spheres have an identical size, and the number of units (i.e. lower level aggregates) at each level. If we build a two-level aggregate of N clusters, consisting of M spheres each, the code first builds N different randomly built BPCAs of M spheres, and then ballistically combines them into a larger aggregate as described above. In this paper, in order to be consistent with the Rosetta findings described in the previous section, we mainly consider two-level aggregates. We also consider some examples of 3-level aggregates where the first level is presented by clusters of two spheres. This use of bispheres brings our model closer to the MIDAS results, which showed that the cometary monomers are spheroids of aspect ratio ∼2.8 [8]. Spheroids with the axes ratio of 2 were also suggested in [22] based on the dust growth processes in molecular clouds, and were successfully used in simulations of polarimetric observations of comets in [16,17].

The second step in the preparation of the model for computations was the selection of the monomer size. We tried to be as consistent as possible with the grain size in cometary aggregated particles for this step. MIDAS results showed that the basic units ("monomers") were polydisperse, with an average size (diameter) around 1.36–1.48 µm [23]. However, the size distribution was very much skewed in the direction of smaller grains, covering the sizes from 0.1 to 1.61 µm; thus, a large number of the grains in the MIDAS particles were of submicron size. The submicron size of the grains is also consistent with the GIADA results [4] and Stardust findings [24]; IDPs are also described as "aggregates of submicrometer-to-nanometer sized crystalline and amorphous grains" [25]. Modeling photopolarimetric and thermal infrared characteristics of the cometary dust showed that the best fit could be achieved with monomers of diameter 0.2 µm (see a review [21] and references therein); this size is also consistent with modeling of aggregated dust particle formation in the protosolar nebula [26]. Similar reasons were used in [27] where the diameter of spherical monomers equal to 0.2 µm was selected. In our study, we also selected 0.2 µm for the spherical monomer diameter; this defined the size 0.4 µm for the monomers presented as bispheres (see above). A secondary reason for selecting this size of monomers was the limitations of the computing resources, where larger sizes of monomers would not allow us to perform light-scattering modeling for an aggregate sufficiently large to exhibit a well-developed hierarchical structure. The largest aggregates we could consider were composed of 1024 monomers. This means that in the case of a 2-level aggregate we built ∼1 µm sized first level clusters; then those clusters collided to form second level aggregates of size ∼10 µm. Although the aggregate-generating code can create larger particles by using larger first level clusters, or a larger number of clusters at any level, or by having more levels of aggregation, in this study we are limited to aggregates with sizes of tens of microns.

For our simulations presented in the next section, we built three aggregates of each type (three configurations of the same structure) to be sure that the differences between the light scattering properties of the aggregates are due to the type of their hierarchical structure, and not caused by a random variations in different configurations of the aggregates of the same hierarchical structure.