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Inhomogeneous particle model for light-scattering by cometary dust

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ABSTRACT

We introduce an inhomogeneous irregular-particle model for reproducing the typical light-scattering features of cometary dust such as the negative polarization near the backscattering direction, and the weak increase of the backscattering intensity. The model is based on the hierarchical Voronoi-partitioning and the algorithm provides fast generation of irregular particles with a flexible control of inhomogeneity. The input parameters of the model are refractive indices, their volumetric abundances, and the number of constituents on each level. The light-scattering properties of these particles with parameters relevant to cometary dust are solved by the volume-integral-equation method. The light-scattering features of inhomogeneous particles are compared with the mixtures of homogeneous particles, and particles with the refractive index obtained by the effective-medium approximation. We show that with the inhomogeneity size of order 0.2 μm, the different models produce qualitatively similar scattering features while some quantitative differences are observed which have an effect on the retrieved material composition of dust.

1. Introduction

The degree of linear polarization is one of the key light-scattering parameters in the application of scattering by cometary dust, since it does not depend on the distances of the observer, the target (comet), and the source (the Sun). This means that polarimetric observations made at different epochs are comparable regardless of the observation geometry varying over time. The degree of linear polarization is defined as $P = (I_\perp - I_\parallel)/(I_\perp + I_\parallel)$, where $I_\perp$ and $I_\parallel$ are the intensities of the electric field components $\boldsymbol{I}_k = <\boldsymbol{E}_k \cdot \boldsymbol{E}_k^*>$ perpendicular and parallel to the scattering plane, respectively (the plane spanned by the Sun, the observer, and the comet). The phase angle α is the angle between the incident light onto the comet and the observed light scattered from the comet in the scattering plane.

Electromagnetic scattering by cometary dust particles is known to have some common characteristics such as a weak enhancement of the intensity and a bell-shaped polarization curve with a negative branch near the backscattering direction and the maximum positive polarization near 90° at visible wavelengths. These scattering features have been observed in many different comets regardless of the size or activity of the particular comet. Nevertheless, the deepness of the negative polarization branch and the maximum positive polarization can vary between different comets, and are wavelength dependent (Kolokolova et al., 2004) In addition, the degree of linear polarization may have spatial and temporal variations. Light-scattering properties of dust depend on the size, shape, composition, and density of the dust particles. Since the distances between individual dust particles in the coma are sufficiently large and comae are typically optically thin, scattering by a cloud of dust can be treated as a single-scattering problem, i.e., the electromagnetic coupling between particles can be neglected. Hence, finding a single particle model that reproduces the light-scattering observations, may reveal some important information of the physical composition of comets. However, it is important to keep in mind that the inverse problem of light scattering is ill-posed, and therefore, some restrictions are required for the size, composition, and structure of dust particles to have physically meaningful results (Lumme et al., 2000).

Infrared spectroscopy, *in situ* observations, and analyses of interplanetary dust particles (IDPs) collected from the Earth's stratosphere have revealed that cometary dust particles are porous heterogeneous mixtures of rock-forming elements such as Mg, Si, Ca, Fe, and carbonaceous materials, the so-called CHON-component consisting of light elements: carbon, hydrogen, oxygen, and nitrogen (Hanner et al., 2004). The rock-forming and carbonaceous components are thought to be mixed at sub-micrometer scales (Lawler and Brownlee, 1992). Dust particles may contain micrometer-sized mineral grains coated or glued together by carbonaceous material as suggested by

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the microscopic images of IDPs (Bradley, 2004; Keller et al., 2000) as well as the dust formation model by Greenberg (Li and Greenberg, 1997; Greenberg and Hage, 1990; Greenberg, 1982).

In light-scattering simulations, cometary dust particles are most often modelled as homogeneous aggregated structures (Lumme and Penttilä, 2011; Zubko et al., 2011; Shen et al., 2009; Kimura et al., 2006; Petrova et al., 2000; Xing and Hanner, 1997; Mukai et al., 1991), in which the refractive index is obtained using the effective-medium approximation or left as a free parameter. Homogenization of complex heterogeneous media with intrinsic microstructure is a sufficient approximation if the inclusions are uniformly distributed and small enough compared to the exciting wavelength. At visible wavelengths, however, the internal composition of cometary dust particles may contain inclusions with sizes comparable to the wavelength. This suggests that these inclusions should be modelled explicitly with an inhomogeneous particle.

There exists only a few models, in which inhomogeneity is explicitly accounted for. In Yanamandra-Fisher and Hanner (1999), the discrete-dipole approximation (DDA) was applied to study scattering by small inhomogeneous aggregates. They, however, considered only small-scale inhomogeneities changing the refractive index in randomly chosen DDA cells. Larger spheroidal inclusions in the host spheroid were considered in Gupta et al. (2006). Both of these attempts failed to reproduce the negative-polarization branch at small phase angles.

An inhomogeneous dust model, based on the core-mantle structure, was studied in Lasue et al. (2009), Levasseur-Regourd et al. (2007) and Lasue and Levasseur-Regourd (2006). This model involves submicrometer-sized silicate cores covered by organic refractory mantles as constituents of the ballistic particle-cluster (BPCA) and ballistic cluster-cluster (BCCA) aggregates, being consistent with the dust-grain formation model (Li and Greenberg, 1997). They concluded that the scattering properties of these grains are similar to those of the pure organic grains assuming that the organic mantles are thick enough. Hence, they used pure organic grains to mimic core-mantle particles. Effects of coating layers were studied in Lindqvist et al. (2009), and they found significant differences in the polarization, but they considered only weakly absorbing particles.

In this paper, we study numerically the influence of inhomogeneity on the light scattering by cometary dust particles. The inhomogeneous particle model is compared with the effective-medium approximation using the Maxwell–Garnett mixing rule as well as mixtures of different homogeneous particles. We use the volume-integral-equation solver in light-scattering computations introduced in Section 2.1, and an irregular inhomogeneous particle model, based on the Voronoi partitioning (also known as Dirichlet tessellation) (Voronoi, 1908; Dirichlet, 1850), described in Section 2.2. Section 3 presents the simulation results, and Section 4 contains discussion and conclusions.

2. Methods and models

In this section, we introduce the numerical procedure used for solving light scattering by irregularly shaped particles, and describe the inhomogeneous irregular particle model for the analysis of light scattering by cometary dust.

2.1. Volume-integral-equation solver

Consider a dielectric object $\mu = \mu_0$ bounded by a volume Ω in a homogeneous background with permittivity ϵ_0. The relative permittivity function $\epsilon_r(\boldsymbol{r})$ (the refractive index is defined as $m = \epsilon_r^2$ when $\mu = \mu_0$) is a function of position $\boldsymbol{r}$. We write a volume-integral-equation formulation for the equivalent electric volumetric (polarization) current $\boldsymbol{J} = -i\omega\epsilon_0(\epsilon_r - 1)\boldsymbol{E}$ as

$$\boldsymbol{J}^{inc} = \boldsymbol{J} - (\bar{\bar{\epsilon}}_r - \bar{\bar{I}})\cdot(\nabla\nabla\cdot + k_0^2)\int_{\Omega} G_0 \boldsymbol{J}\, \mathrm{d}V \tag{1}$$

where G_0 is the Green's function of the background, k_o is the wave number in the background, and $\boldsymbol{J}^{inc} = -i\omega\epsilon_0(\epsilon_r - 1)\boldsymbol{E}^{inc}$ is the incident current due to the incident electric field $\boldsymbol{E}^{inc}$.

The volume of the scatterer is divided into tetrahedral elements T_k, and the unknown function $\boldsymbol{J}$ is expanded with piecewise constant basis functions $\boldsymbol{b}_k^i$ as

$$\boldsymbol{J} \approx \sum_{k,i} c_k^i \boldsymbol{b}_k^i = \sum_{k=1}^{N_{tet}} \Pi_k \left(c_k^x \hat{\boldsymbol{e}}_x + c_k^y \hat{\boldsymbol{e}}_y + c_k^z \hat{\boldsymbol{e}}_z \right) / \sqrt{V_k}, \tag{2}$$

where c_k^i are the unknown coefficient, $\hat{\boldsymbol{e}}_{x,y,z}$ are the basis vectors in the Cartesian coordinate system, and V_k is the volume of the tetrahedron T_k. Π_k is the step function, i.e., its value is one inside T_k and zero otherwise. The continuous integral equation is converted into a system of linear equations by Galerkin's technique, i.e., testing $\boldsymbol{t}_m^i$ and basis functions $\boldsymbol{b}_n^j$ are identical. To reduce the singularity of the kernel, the derivatives are moved into the testing and basis functions. And using the divergence theorem, the expression for the elements of the system matrix reads as

$$\begin{aligned} A_{mn}^{ij} = &\int_{T_m} \boldsymbol{t}_m^i\cdot\boldsymbol{b}_m^j \,\mathrm{d}V \\ &+ \int_{\partial T_m} \boldsymbol{n}_m\cdot(\bar{\bar{\tau}}^T\cdot\boldsymbol{t}_m^i)\cdot \int_{\partial T_n} G_0\, \boldsymbol{n}_n'\cdot\boldsymbol{b}_n^j \,\mathrm{d}S'\,\mathrm{d}S \\ &- \int_{T_m} \boldsymbol{t}_m^i\cdot\bar{\bar{\tau}}\cdot k_0^2\bar{\bar{I}}\cdot \int_{T_n} G_0 \boldsymbol{b}_n^j \,\mathrm{d}V'\,\mathrm{d}V, \end{aligned} \tag{3}$$

in which $\bar{\bar{\tau}} = (\epsilon_r - 1)\bar{\bar{I}}$, $\boldsymbol{n}_m$ is the unit normal vector of the element T_m, and ∂T_m is a closed surface of the tetrahedron T_m. The integrals are computed by the Gauss–Legendre quadrature in combination with the singularity extraction method Järvenpää et al. (2003). The elements of the force vector read as

$$f_m^i = \int_{T_m} \boldsymbol{t}_m^i \cdot \boldsymbol{J}^{inc}\,\mathrm{d}V. \tag{4}$$

More details of the method can be found in Markkanen et al. (2012). The resulting system is solved iteratively by the GMRES method, in which the matrix-vector multiplications are accelerated by the precorrected-FFT algorithm (Phillips and White, 1997). The main advantage of this formulation over the widely used DDA method is that the testing functions span the proper finite-dimensional vector space, hence, the boundary conditions across material interfaces are well-tested.

The method has computational complexity of $O(N_{iter}N \log N)$ for time and $O(N)$ for memory where N is the number of unknowns and N_{iter} is the number of iterations required to solve the system. N_{iter} is generally much smaller than N and it depends on the refractive index, size, and shape of the particle (Markkanen, 2014). The asymptotical complexity of this method is, therefore, the same as in the DDA.

2.2. Particle model

We model cometary dust as irregularly shaped inhomogeneous particles consisting of carbonaceous materials and silicate minerals which are generally considered to be the most abundant components in comets (see, e.g., Hanner et al., 2004 and references therein). Silicates can be associated with weakly absorbing materials with the refractive index between $m = 1.5 + 0i$ and $1.7 + 0.01i$ at wavelengths of visible light, and in this work, we assume silicate minerals to consist of Mg-rich pyroxene with the constant refractive index $m = 1.63 + 0.003i$ (Dorschner et al., 1995). Carbonaceous components are associated with highly