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Optical Properties of Fluffy Particles

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Abstract. For particles grown in the two limiting cases of coagulation (ballistic particle-cluster agglomeration and ballistic cluster-cluster agglomeration), lower and upper limits of the extinction at wavelengths from 1 μm to 1 mm are derived. The particle sizes are in the Rayleigh limit and the number of constituent grains in each particle is constant. Effective medium theories, the discrete dipole approximation and the discrete multipole method are applied to compute the optical behaviour of the coagulated particles. The spectral representation for inhomogeneous media is employed to investigate topology effects systematically.

1. Introduction

The question of how fluffy particles behave in their interaction with electromagnetic radiation is of interest for many different fields in physical, biological, medical, and also environmental sciences. For the different branches of astrophysics, the optical properties of fluffy particles are of topical interest, because almost all observations of processes where interplanetary or interstellar dust is involved are "optical" observations. That the interplanetary as well as the interstellar dust grains are inhomogeneous and have irregular shapes/structures is widely accepted for theoretical reasons and proved by in-situ observations of interplanetary dust particles collected in the upper earth atmosphere.

The theoretical modeling of the optical properties of inhomogeneous and irregular dust grains is quite complicated. Nevertheless, the progress in that field made in the last two decades is encouraging. Now, several methods are available all of which have their range of applicability. We tested the methods which should be well suited to calculate the extinction of small dust aggregates consisting of spherical sub-grains touching each other at one point. The test particles were grown in the two limiting cases of coagulation: ballistic particle-cluster agglomeration (BPCA; which results in rather spherical aggregates with dense cores) and ballistic cluster-cluster agglomeration (BCCA; which results in very fluffy aggregates with an open structure). In addition, we derived upper and lower limits for the extinction of "real" aggregates, i.e. aggregates where the sub-grains contact each other at finite areas.

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2. Methods

Here, we outline the basics of the spectral representation for inhomogeneous media. This method allows the study of the influence of the dust grain morphology on the optical properties in a systematic way. In doing this, we only touch on the other methods which are used to calculate the optical behaviour of the aggregates. For more details and also for the characterization of the aggregates, we refer to Stognienko et al. (1995) and Henning et al. (1995).

In the concept of effective medium theories (EMTs) an aggregate with its complicated morphology is thought to be replaced by a homogeneous spherical grain with a effective dielectric function ϵ_{eff}. In the so called differential effective medium theory (DEMT) ϵ_{eff} is considered to be radius dependent. The replacement can be considered as an orientation or ensemble average for the aggregates and is justified if the scale of inhomogeneity within the aggregates is small compared to the wavelength. The quantity ϵ_{eff} is often defined by the requirement that the forward scattering amplitude, i.e. the extinction, of the the "effective" particle mimics the extinction of the aggregates. This leads to the well-known Garnett mixing rule (often incorrectly called Maxwell-Garnett) and the Bruggeman mixing formula (denoted by EMT in the following). Both rules contain the volume filling factor of the aggregate material and its dielectric function. These rules can also be applied locally, i.e. for radially varying filling factors.

The spectral representation (Bergman 1978) relates ϵ_{eff} of a two-component system to the dielectric functions ϵ_i of the components, their filling factors f_i (with $f_1 + f_2 = 1$), and the spectral functions g_i in a rigorous way:

$$\epsilon_{\text{eff}} = \epsilon_2 \left(1 - f_1 \int_0^1 \frac{g_1(n)}{t-n} \, dn \right), \qquad t = \frac{1}{1 - \epsilon_1/\epsilon_2}, \tag{1}$$

which can also be formulated with the spectral function g_2 for the second component. The functions g_i also have to obey the two moment-equations $\int_0^1 g_i(n)\, dn = 1$ and $\int_0^1 n g_i(n)\, dn = (1 - f_i)/3$.

The interpretation of Eq. 1 is as follows: All possible geometric resonances of a two-phase composite (e.g. the aggregate matter and vacuum) occur if the complex quantity t assumes only real values with the real part in the interval [0,1]. With the integration over n, one scans all possible resonance positions. Whether a resonance occurs or not is determined by the spectral function $g_i(n)$ which carries all topological information. Therefore, the spectral representation clearly distinguishes between the influence of the geometrical quantities and that of the dielectric properties of the components on the effective behaviour of the system.

In spite of the elegance of the spectral representation, there exists no general way to compute the spectral function for a given system. Only for certain topologies was a determination of the spectral function performed. The discrete multipole method (DMM) in the formulation by Hinsen (1992) results in the spectral functions for hard-sphere systems. The DMM is the static limit version of the generalized Mie theory (see e.g. Xu & Gustafson 1996) and includes multipole-orders as high as possible for the expansion of the potential outside the spheres. The DMM is, therefore, superior to the discrete dipole approximation (DDA) which is often used in the literature to model aggregates of spheres by replacing each sphere with one dipole (see e.g. Kozasa et al. 1992).

Because Eq. 1 relates the volume filling factors and the dielectric functions to ϵ_{eff}, analytic expressions for $g(n)$ for a given mixing rule can be derived. Therefore, we are able to compare the spectral functions which correspond to the mixing rules with the spectral functions computed with the DMM.

A detailed comparison is, however, not necessary, because of the denominator in the integrand of Eq. 1. If the complex quantity t has a value far from the real interval [0,1] in the complex plane, Eq. 1 reduces to $\epsilon_{\text{eff}} = f_1\epsilon_1 + (1 - f_1)\epsilon_2$ and, therefore, the spectral functions, i.e. the morphology of the aggregates or the used mixing rules, are of no interest. This is just the situation we have for many astrophysically interesting materials. Only some metals or materials like amorphous carbon and graphite have $|t| \approx 0$ at far infrared and sub-mm wavelengths. In this case, only the behaviour of the spectral functions at $n \approx 0$ is of interest.

The special surface mode at $n = 0$ describes the so called percolation of the system. The percolation strength g_0 is defined by the decomposition of $g(n)$ into $g_{\text{r}}(n) + g_0\delta(n)$. The quantity g_0 can be considered as the fraction of the component that contributes to the dc conductivity of the system if the component is a conductor and the second component an insulator. The EMT and the DMM give $g_0 = 0$ which is correct for the considered aggregates because they consist of sub-grains touching each other at *one point* only. However, this is not very realistic because we know that the sub-grains in "real" aggregates are physically percolated, i.e. the sub-grains contact each other at *finite areas*.

Ossenkopf (1991) models the percolation of "real" aggregates by introducing effective shape factors into various mixing rules. We denote this modified rules with an appended "-O". For another modeling of g_0 we refer to Henning & Stognienko (1996). Including an upper limit of g_0 into $g(n)$ obtained with the DMM leads to the modified spectral function (MSF).

3. Results

The results of our calculations are shown in Fig. 1, where ϵ_{eff} was estimated with various mixing rules and with Eq. 1 using the MSF and the spectral function obtained with the DMM. The extinction cross section per compact volume is calculated as $3k\,\text{Im}[\frac{\epsilon_{\text{eff}}-1}{\epsilon_{\text{eff}}+2}]$, where $k = 2\pi/\lambda$ is the wavenumber. The (averaged) radius of the aggregates was assumed to be $a = 0.1\ \mu$m.

In the computations by the DDA and the DMM, averages are taken over eight clusters and three perpendicular directions of each cluster with respect to the incoming wave. Three perpendicular orientations gives the correct extinction value in the static limit ($k \rightarrow 0$) and are sufficient for the DDA calculations, because the aggregate sizes are well within the Rayleigh limit ($ka \ll 1$). The radially varying as well as the averaged filling factors are obtained for the same eight aggregates and used in the DEMT and the EMT calculations, respectively.

We found that the extinction limits (denoted by the DMM and the MSF graphs) strongly depend on the refractive indices used and on the topology of the aggregates and that the porosity of the particles is not the most important parameter.

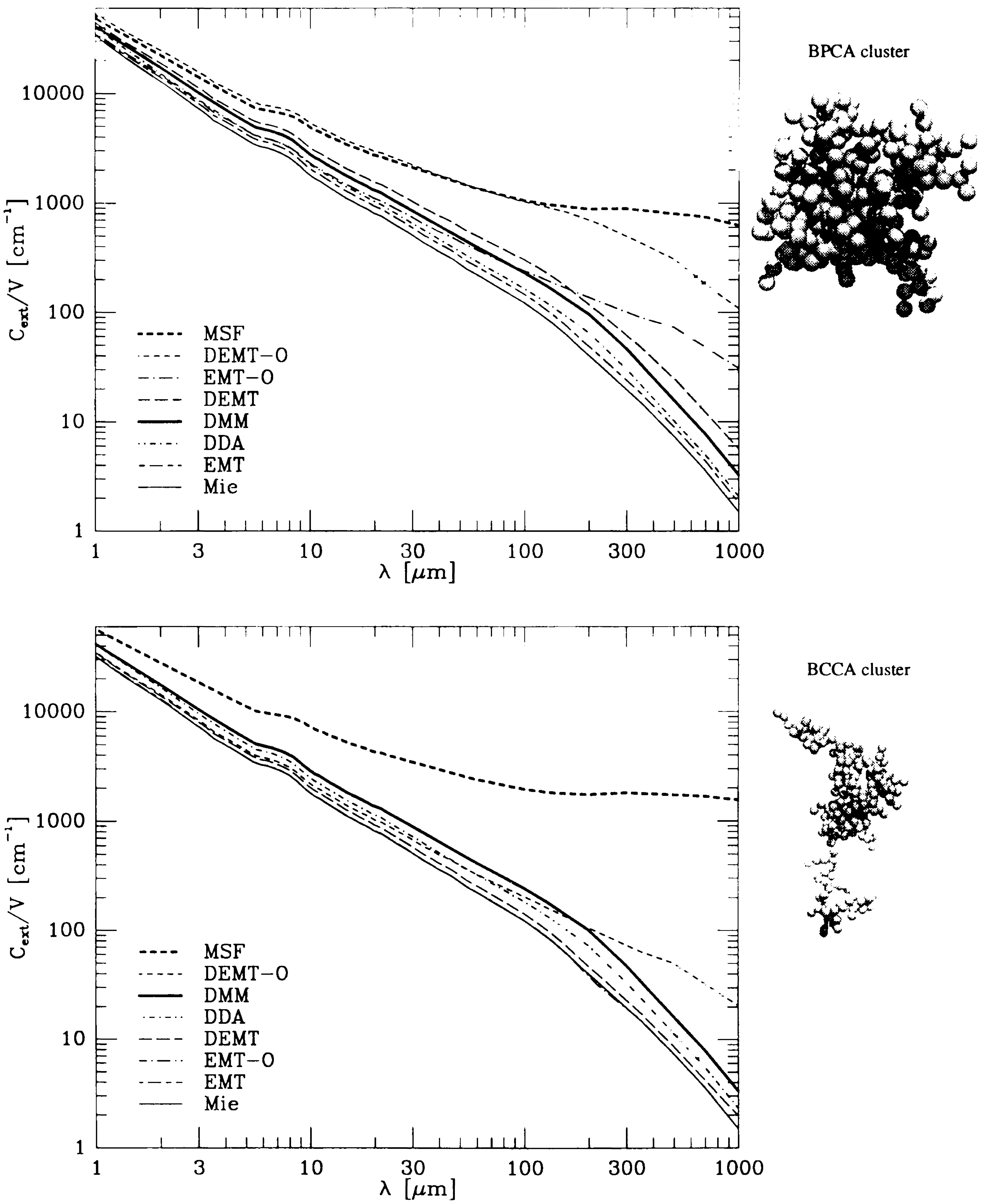

Figure 1. Extinction cross section per compact volume for two types of aggregates (see sample aggregates in the margin) consisting of amorphous carbon (optical constants after Preibisch et al. 1993) computed with different EMTs, the DDA, DMM, and MSF. The curves are listed in the same order as they appear at 1000 μm. Note that the graphs labeled with Mie correspond to the Garnett mixing rule *and* to homogeneous compact spheres with the same mass as the aggregates.

For particles composed of amorphous carbon, the enhancement of the extinction with respect to the extinction value for compact spheres of the same mass is between 2 and 1000 at 1 mm wavelength. For silicate particles (not shown), the enhancement of the extinction is in the range 1.5–3.5 at 1 mm wavelength.

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