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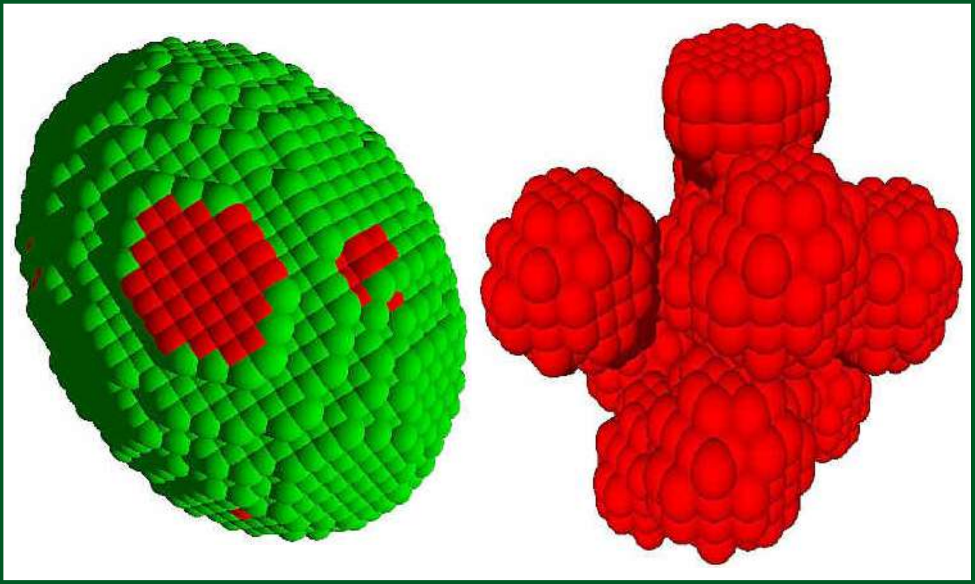

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Effect of grain shape on extinction using effective medium theory

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Apart from the size of the dust grains in the interstellar medium, their shape too can cause different scattering and absorption efficiencies. The grains in space could also be a composite formed from different materials. The scattering and absorption for each material is different depending on their dielectric constant or refractive index. Effective medium theory (EMT) is used to obtain an effective dielectric constant that replaces the consideration of different materials in a particular grain, thus reducing the computational effort. The dependence of EMT on the shape of the dust grain is studied in the present work. The grains are considered to be composed of 20% carbon and 80% silicate clustered into compact or loose non-spherical shapes. Various extinction efficiencies in the visible electromagnetic spectrum are computed and compared with other methods.

Keywords: Dust grains, Interstellar medium, Dielectric constant, Electromagnetic spectrum, Extinction efficiencies

1 Introduction

The dust in Interstellar medium (ISM) or in comets are not spherical. In general they are even far from any regular or symmetrical shape. The interaction of electromagnetic radiation with dust grains depends on the dielectric constant, size and shape of the grain material. The attenuation of radiation by grains, which includes scattering and absorption, has a solution for spherical grains [1-3]. This solution 'Mie theory' is relied upon by various authors for sphere, coated sphere [4-7] and even for multilayered grains [8]. Approximate methods that are not restricted to spherical shapes include T-matrix [9,10], used mainly for symmetrical particles, and Discrete Dipole Approximation (DDA) method [11,12], which can ideally be used for any arbitrary shape. The DDA method is computationally time consuming but the development of fast computing has made it popular.

The dust grains in the ISM are formed in extreme physical conditions and are likely to be of random shapes and also complex composites of different types of materials. The gas ejected from evolved stars cool and sublimate into solid grains, whose properties depend on the elemental abundances in the circumstellar shells. The possibility of different types of material in the same random shaped grains complicates the computation of interstellar extinction. Models that derive average dielectric permeability for heterogeneous grains are useful in this regard. Such effective medium theories (EMT) [13] approximate a single dielectric constant and make computation of extinction simpler.

In the present work, EMT is used to compute the scattering and absorption efficiencies for grains that have both carbonaceous and silicate components. Comparison with 'Mie theory' is performed for coated sphere and also for arbitrary shapes that may grow through clustering. The effective dielectric constant depends on the ratio of the volumes of the different components. The effect of shape of the dust agglomerate in extinction computation using EMT is studied and compared with other methods. The grain evolution methods have their important role in formation of different types of grains, which affect the scattering and absorption efficiencies [14]. Two different categories of shapes, compact and loose aggregates of grains, are considered. The Garnett mixing rule [15] is used for obtaining the effective dielectric permeability in the study. The study is performed in the 0.3 - 3.0 μm wavelength range. In order to study only the shape effect, refractive indices are considered to be independent of wavelength.

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2 The aggregation models

Two kinds of aggregation models akin to kinetic colloidal formation [16] are used to simulate the astrophysical composite dust particles. Each small particle is considered to be having a core and a mantle. The chemical composition is further assumed to be 80% silicates, which are essentially transparent, and 20% of carbon, which is strongly absorbing. However, the distribution of the two components inside a dust particle depends on the model, i.e. on the physical conditions of the ISM.

2.1 Disordered compact coated particles

In this model the first step corresponds to seed particles traveling fast through low-density, cold, cloud of small compact grains made of only one compound. The physical conditions of the cloud are such that the small compound grains are almost motionless with respect to one another and do not stick together. The small grains collide and condensate onto the fast moving seed particles through the Reaction-limited Particle-Cluster Aggregation process (RPCA) [14]. These clusters are compact with rough surface. In the second process the cluster passes through a cloud of second particle and acquires a coating in a similar RPCA process.

For the simulation of the cluster formation a cubic lattice is considered. Each point has six possible bonds and sticking occurs randomly on to these bonds. Upon each particle attachment there is one site less and five new ones appear. The process continues until the expected number of grains in the aggregate is reached. Five such compact clusters are used in the calculations and shown in Fig 1. The compact clusters CMP 1 through 5 are in the order of increasing oblateness.

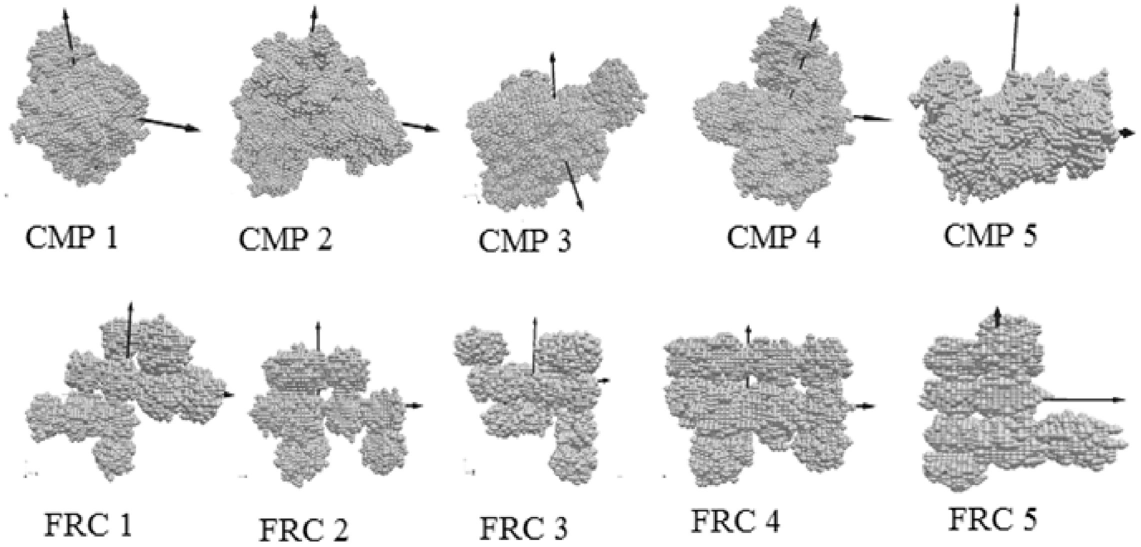

Fig 1. Examples of different shapes used in calculations

2.2 Loose fractal aggregation model

In this model, the first step of the aggregation process is changed. The initial process is started with grains colliding and sticking together in a high-density, cold, cloud. The clusters are random and essentially anisotropic without any alignment mechanism. As the clusters move freely this process generates Reaction-limited Cluster-Cluster Aggregation (RCCA) fractal particles [17]. In the next step the particles pass through a cloud of second particle and acquire coating as in the RPCA process. Finally making a disordered fractal core of chosen material coated with secondary material.

For the simulation N identical grains are considered for initial aggregation. As the system evolves a grain site of one cluster randomly attaches to a site on the other cluster. The fractal loose aggregates generated that are used in the calculations FRC 1 through 5 are shown in Fig 1.

3 Calculations

The dust grains that are generated by the aggregation models use silicates and carbonaceous materials. The core-mantle grains have either carbon core with silicate mantle or silicate core with carbon mantle. In either case carbon is considered to be only 20% by volume and remaining 80% are silicates. The extinction and absorption efficiency calculations are done in the wavelength range 0.3 to 3.0 µm for particle size 10 nm. To study only the effect of shape, the grain size is fixed. This size is in Rayleigh limit as size parameter $x = 2\pi a, \lambda << 1$, where a is radius and λ is wavelength. Thus the field is weakly attenuated in the particle and wave travelling time in the particle is much smaller than inverse frequency [18,19]. Under these considerations one obtains the extinction efficiency $Q_{ext} \propto x$ and scattering efficiency $Q_{\mathrm{sca}} \propto x^4$ for small sphere of radius 'a' and refractive index $m = n + i\,k$ or dielectric constant $\varepsilon = \varepsilon_1 + i\,\varepsilon_2$ at wavelength λ. Similar results are expected for small non-spherical particles. Accordingly Q_{ext} is linear with a and λ^{-1}. For smaller particles nearly all the extinction is due to absorption and shape does not matter much. The refractive indices of the two materials silicates and carbon chosen for study are taken to be independent of wavelength. For silicates $m_{\mathrm{si}} = 1.55 + i10^{-3}$ (negligible absorption) and for carbonaceous matter $m_{\mathrm{c}} = 1.9 + i\,0.5$ (strongly absorbing).

Several discussions on dust formation mechanisms in different circumstellar and interstellar regions have been made that include layered grains and core-mantle type systems [20-24]. Observations and modeling of cometary dust also suggest that the particles may be compact or loose aggregates of random shape [25-27]. Thus the model generated compact (CMP) and loose fractal (FRC) grain shapes (Fig 1) are close to realistic dust grains in astrophysical environments.

The calculations for spherical shape coated sphere are done using Mie theory [3] and for all non-spherical shapes DDSCAT 7.2 [28] is employed. The DDSCAT validity criteria, $|m|\ kd \leq 1$, where m is complex refractive index, k is $2\pi/\lambda$ and d is inter dipole separation, is well followed in the studied wavelength range.

3.1 Effective medium approximation

The aim of the work is to evaluate the usefulness of EMT in extinction calculations for different shapes by comparing the calculations with methods where independent dielectric constant for each material is considered. It has been shown that for compact spheroidal particles component mixing can reproduce the observed optical properties with refractive indices ranging between $n = 1.6 - 1.7$ and $k = 0.05 - 0.1$ [29]. The EMT have been attempted to consider heterogeneous cometary grains, treating aggregates as mixture of constituent particles with inclusions and voids [30-32].

There are many mixing rules available in literature to obtain the average dielectric permeability in a composite material [33,34]. In the present work the Maxwell-Garnett mixing rule [15,18] is applied, which gives the effective dielectric as:

$$\varepsilon_{eff} = \varepsilon_m \left[\frac{1 + 2 f_i \dfrac{\varepsilon_i - \varepsilon_m}{\varepsilon_i + 2\varepsilon_m}}{1 - f_i \dfrac{\varepsilon_i - \varepsilon_m}{\varepsilon_i + 2\varepsilon_m}} \right] = \left[1 + \frac{3 f_i \dfrac{\varepsilon_i - \varepsilon_m}{\varepsilon_i + 2\varepsilon_m}}{1 - f_i \dfrac{\varepsilon_i - \varepsilon_m}{\varepsilon_i + 2\varepsilon_m}} \right]$$

where inclusion (by suffix i) is to be associated with matrix (suffix m). The matrix and inclusions need to be carefully considered as per the model, in this case 20% is carbon and 80% is silicate.

4 Results

The extinction efficiency for all the simulated shapes is performed using DDSCAT [28]. The core-mantle systems are considered to have (i) carbon core with silicate mantle and (ii) silicate core with carbon mantle. In both the cases carbon is considered to be 20% by volume and silicates are 80%. Considering (i) and compact CMP shapes the obtained extinction is plotted in Fig 2. The extinction efficiencies for all compact shapes, i.e. CMP 1 to CMP 5, overlap. This implies that extinction efficiency is independent of the grain shape. The same result is obtained for all fractal loose aggregate FRC grain shapes. The extinction, which is a result of scattering and absorption, is different for carbon and silicates independently. But in the coated aggregates of type (i) the resultant extinction depends only on the volume fraction of the two components and not on the clustering process.

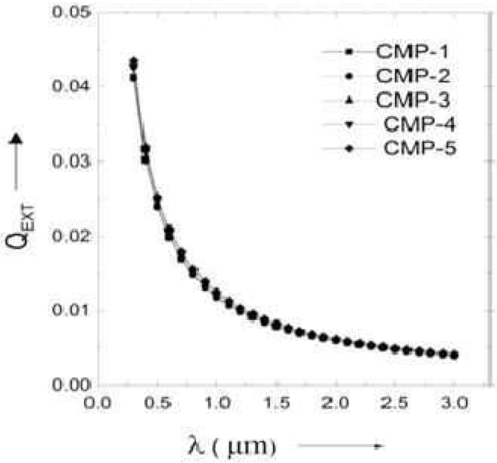

Fig 2. Q_{ext} for compact shapes with C core and silicate coating

A comparison of the extinction for random shapes computed by approximate methods is made with the spherical shape computed using Mie theory. In Fig 3 this ratio is plotted and it indicates that Q_{ext} for random shapes is larger by 7.5% with respect to Mie sphere calculations. The figure also shows the comparison with only the scattering component Q_{sca}, which is only 3% larger. As $Q_{ext} = Q_{abs} + Q_{sca}$, the larger Q_{ext} is primarily due to Q_{abs}. Except in the small wavelength regime the ratio with Mie sphere is a constant. This indicates small increase in extinction due to departure from spherical shape.

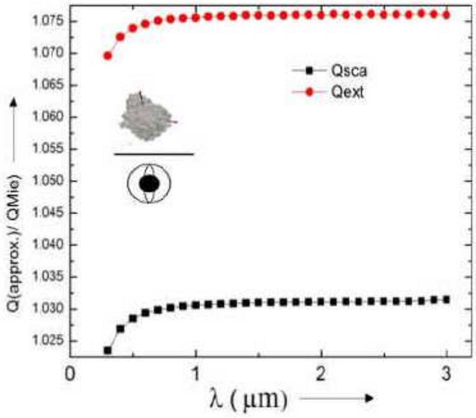

Fig 3. Comparison with coated Mie sphere

The aggregates of type (ii) that have silicate core and carbon mantle also have no effect of shape on the extinction efficiencies, as shown in Fig 4, for five generated shapes. Carbon having larger imaginary component of refractive index is highly absorbing. Bringing it to the mantle in the same volume makes a thinner coating and decreases the absorption. The total extinction efficiency in this case is smaller than when the carbon goes into the core. Thus the grain material and its percentage in total volume are more important than the shape of the dust agglomerates. The extinction also remains unchanged when one goes from compact to loose aggregates.

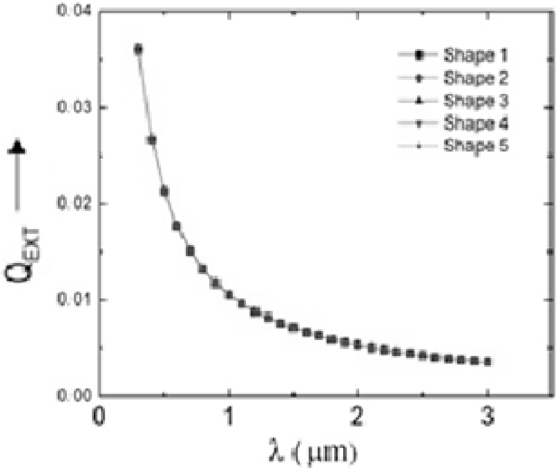

Fig 4. Q_{ext} for different shapes with silicate core and carbon coating

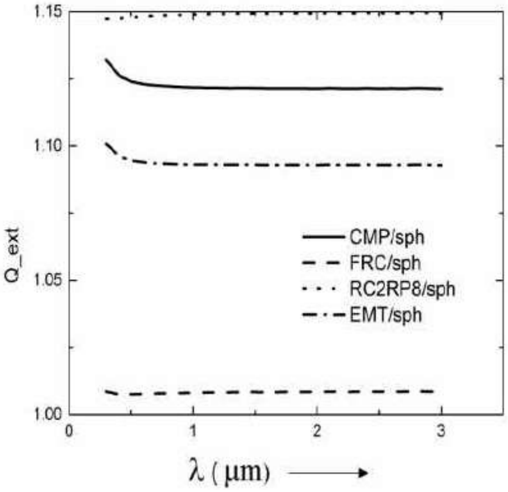

Fig 5. Comparison of different grain types and EMT

The calculations using EMT and the Maxwell-Garnet mixing scheme give similar shape independence. In order to make a close comparison ratio of extinction with Mie coated sphere is plotted in Fig 5 for different types of grains and using EMT. The fractal FRC shapes having carbon coated grains matches best with the coated Mie sphere (FRC/sph in figure). Considering the RCCA aggregation with carbon as core gives nearly 15% higher extinction (RC2RP8/sph in figure) than a similar coated sphere. The EMT calculations are for compact shapes (EMT/sph in figure) and result in lower extinction than that obtained using two refractive indices for the two components (CMP/sph in figure). It is evident from Fig 5 that compact shapes have nearly 12 % higher values than coated sphere, while EMT calculation for the same shape is lower.

5 Conclusions

Two kinds of aggregation models RPCA and RCCA are used to simulate astrophysical composite dust particles. Only a two components composition is considered with 20% carbon and 80% silicates by volume. Each grain is considered to be having a core and a mantle. Both the possibilities, i.e. carbon core with silicate mantle and silicate core with carbon mantle, are considered. The distribution of the two components will in general depend on the physical conditions of the ISM. For nanometer sized particles it is seen that there is hardly any shape effect. EMT also applies very suitably for such a distribution of grains.

A very restricted set of parameters were considered in the study but a detailed study is indicated. In particular the variation of the composition needs special consideration. Multi component grains that may include ices need to be studied. It will be of interest to see if an effective dielectric constant can be generated when three or more components make up heterogeneous grains. As the results change when the core material is changed, laboratory and observations should put better constraints on the likelihood of carbon being in core or as mantle.

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