

Interstellar extinction by fractal polycrystalline graphite clusters?

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Abstract

Certain dust particles in space are expected to appear as clusters of individual grains. The morphology of these clusters could be fractal or compact. To determine how these structural features would affect the interpretation of the observed interstellar extinction peak at $\sim 4.6 \mu\text{m}$, we have calculated the extinction by compact and fractal polycrystalline graphite clusters consisting of touching identical spheres. We compare three general methods for computing the extinction of the clusters, namely, a rigorous solution [1] and two different discrete-dipole approximation methods – MarCODES [2] and DDSCAT [3].

1 Introduction

The shape of many interstellar grains are expected to be non-spherical and maybe even highly irregular. One way to deal with irregular particles and clusters of dust grains is to assume that they consist of touching spheres. With such an assumption it is possible to construct a variety of morphologies which can then be compared with observations.

Fitzpatrick & Massa [4] studied the interstellar extinction in the direction of 45 reddened stars, and found that it displays a peak whose central wavelength λ_0 is remarkably constant ($\lambda_0 = 2174.4 \pm 17 \text{ \AA}$), even though its full width at half maximum (FWHM) varies considerably from 360 to 600 \AA ; they also found no apparent correlation between the small variation in λ_0 and the large variation in the FWHM. These characteristics have since been known as the “2200 \AA peak”. Graphite is a very promising though controversial candidate for explaining the 2200 \AA peak [5, 6, 7].

2 Method

We investigate the effect of cluster shape in the extinction of clusters of spherical polycrystalline graphite particles. Table 1 shows all the clusters we have used in this work; they are either sparse or compact, and small or large. Their extinction is computed using a rigorous solution (GA) [1] as well as two DDA implementations – MarCODES [2] and DDSCAT [3] – this allows us to test how well the DDA performs when applied to clusters of different geometries.

The three dimensional clusters of 7, 49, 343 ($7^n, n = 1, 2, 3$) particles correspond to the first three stages in the recursive building of the snowflake fractal. The dimension of this fractal is $D = \ln 7 / \ln 3 = 1.77$ [8]. Although such a deterministic structure is not expected to occur in nature, its fractal dimension is close to that of more realistic random cluster-cluster aggregation models. In particular, small particles in space may move in straight, ballistic trajectories and form larger aggregates upon collisions. Numerical simulation of this process yields that the fractal dimension of the resulting aggregates is around 1.9 [9] and this value has also been confirmed by

Table 1: The clusters presented in this paper have three different geometries: fractal (frac; $D= 1.77$), face-center-cubic (fcc) and simple-cubic (sc).

Structure	frac	frac	frac	fcc	fcc	fcc	fcc	sc	sc
# particles	7	49	343	4	32	49	108	8	27
Designation	frac7	frac49	frac343	fcc4	fcc32	fcc49	fcc108	sc8	sc27

experimental results [10]. Moreover, optical properties of fractal clusters with $D < 2$ are predicted to be significantly different from those with $D > 2$ [11]; hence we consider it important to use a realistic fractal dimension in our computations.

Theoretical computation of absorption and scattering by graphite particles is difficult because graphite is a semi-metal with high anisotropy ($\epsilon_{\parallel}, \epsilon_{\perp}$). In this work we use the dielectric functions ϵ_{\perp} and ϵ_{\parallel} derived by [12], and we deal with the anisotropy of graphite by assuming that in all our clusters, each individual particle is polycrystalline having a dielectric function ϵ_{ave} given by the arithmetic average of ϵ_{\parallel} and ϵ_{\perp} , namely $\epsilon_{\text{ave}} = \frac{1}{3}\epsilon_{\parallel} + \frac{2}{3}\epsilon_{\perp}$. By contrast, the usual “1/3–2/3” approximation, treats individual particles as mono-crystalline - 1/3 of the cluster particles are assumed to have dielectric function ϵ_{\parallel} and the remaining 2/3 to have dielectric function ϵ_{\perp} . Considering grain formation and grain growth in stellar environments [13], polycrystalline particles seems to be a better choice than mono-crystalline ones.

A rigorous and complete solution to the multi-sphere light scattering problem has been given by Gérardy & Ausloos (GA) [1]. It is based on the exact solution of Maxwell’s equations for arbitrary cluster geometries, polarisation and incidence direction of the light. This gives a system of $2NL(L + 2)$ equations whose solution is the 2^L -polar approximation to the electro-magnetic response of the cluster. The smallest L needed for the convergence of the extinction will be different in different spectral regions. In the UV-visible range it is enough to use $L = 7$ for open clusters, or $L = 9$ for compact ones, to compute the extinction with an accuracy of 1%; this holds for clusters of up to a few tens of particles.

The discrete dipole approximation (DDA), on the other hand is one of several discretisation methods for solving scattering problems in the presence of targets of arbitrary geometry. In this work we use the DDSCAT code version 5a10 [3] and MarCoDES [2].

3 Results

The results from the three methods for the frac7, frac49, sc8 and sc 27 cluster can be seen in Fig. 1 and 2. It is clear that there are significant differences between the results of the three codes. MarCoDES uses one dipole per particle, and the difference from the GA results is due to the neglect of higher order terms, $L \geq 2$. Even in the DDSCAT computations the number of dipoles used per particle (977 for frac7, 2103 for sc8, 35 for frac49 and 622 for sc27) was probably not enough to ensure full convergence of the result.

Table 2 lists the extinction’s peak position and width for all the clusters, as computed with the GA method; the polar order at which the GA calculation was truncated is also indicated. The width was determined as the FWHM. For the asymmetric compact cluster fcc49 we have investigated the importance of the orientation of the cluster and it was found that the peak position was shifted less than $0.1 \mu\text{m}^{-1}$ while its width remained the same. The clusters considered by [7] all had peak positions at higher wavenumber than the 2200 Å peak while our clusters all have peak position at lower wavenumbers. The main difference between our study and the one in [7] is the way we deal

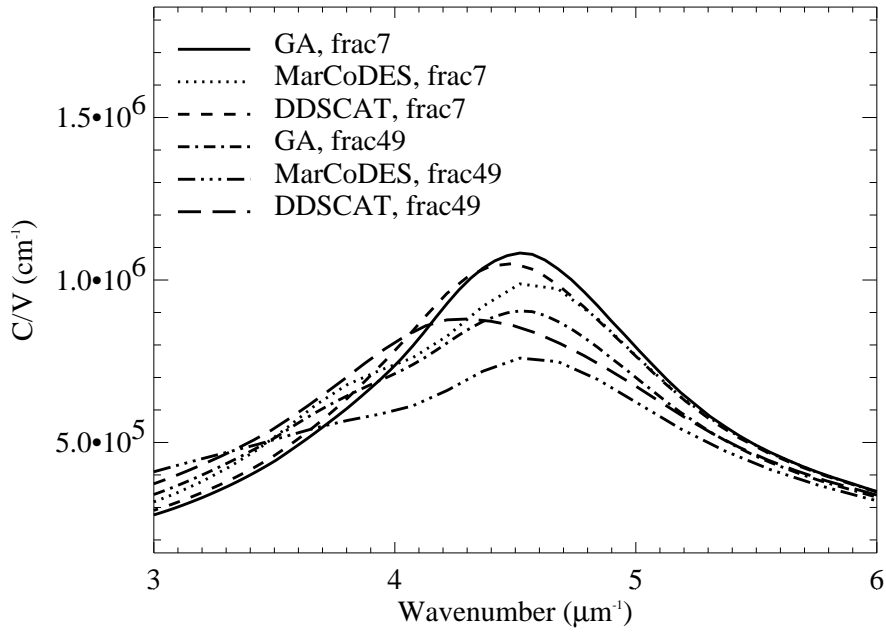


Figure 1: The extinction efficiency for the two fractal clusters, frac7 and frac49, as calculated with the exact GA solution and the two DDA codes: DDSCAT and MarCoDES.

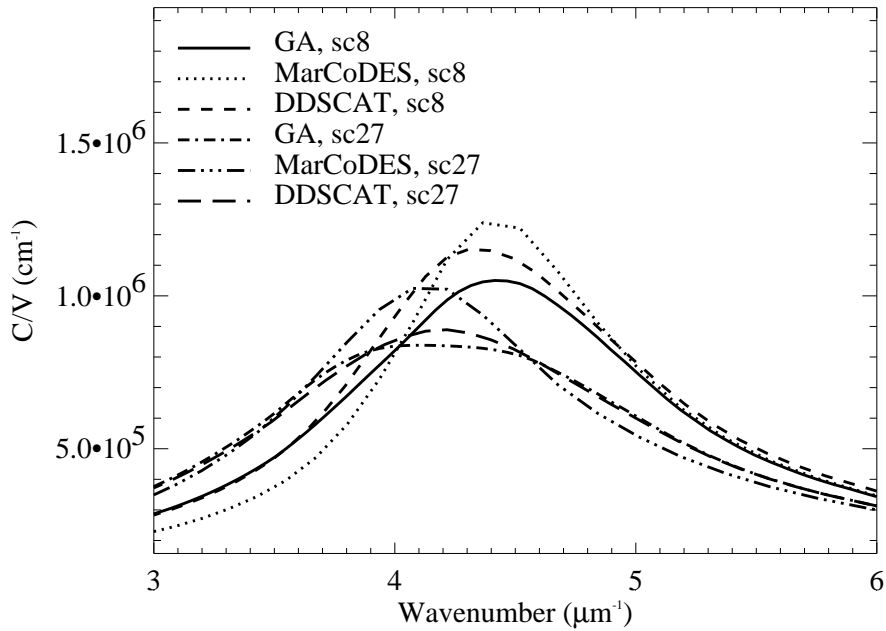


Figure 2: The extinction efficiency for the two compact clusters, sc8 and sc27, as calculated with the exact GA solution and the two DDA codes: DDSCAT and MarCoDES.

Table 2: Peak position [μm^{-1}] and FWHM [μm^{-1}] of different clusters, as calculated with the GA method. The value of L indicates at which polar order the GA calculations were truncated.

Cluster	frac7	frac49	frac343	sphere	fcc4	fcc32	fcc 49	fcc108	sc8	sc27
L	11	6	2	3	11	7	6	3	11	7
Peak	4.52	4.52	4.42	4.62	4.43	3.98	3.71	3.98	4.41	4.12
FWHM	1.17	1.33	1.27	0.96	1.15	1.43	1.52	2.01	1.27	1.62

with the anisotropy of the graphite grains. They [7] used the usual “ $1/3 - 2/3$ ” approximation. The frac7 and frac49 clusters come close (peak position is off by $0.04 - 0.08 \mu\text{m}^{-1}$) to the observational constrains. This indicates that small ($N \sim 5 - 100$) fractal clusters ought to be investigated in more detail to determine if fractal clusters with low fractal dimension have a stable peak position around $4.6 \mu\text{m}^{-1}$ and produce a variable width depending on the number of particles in the cluster.

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