Infrared extinction by aggregates of SiC particles: 
Comparison of different theoretical approaches

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\section{Abstract}

Particle shape and aggregation have a strong influence on the spectral profiles of infrared phonon bands of solid dust grains. In this paper, we use a discrete dipole approximation (DDSCAT; \cite{1}), a cluster-of-spheres code following the Gérardy-Ausloos approach (MQAGGR; \cite{2}) and a T-matrix method (SCSMTM; \cite{3}) for calculating IR extinction spectra of aggregates of spherical silicon carbide (SiC) particles. We compare the results obtained with the three different methods and discuss differences in the band profiles.

\section{Introduction}

Grain growth by aggregation is an important process in dense cosmic environments as well as in the earth’s atmosphere. Besides influencing dynamic properties it also changes the absorption and scattering properties of the solid dust particles for electromagnetic radiation (e.g. \cite{4}). This is especially true in spectral regions where resonant absorption occurs, such as the phonon bands in the infrared. It is quite well known that shape and aggregation effects actually determine the band profiles of such absorption and emission bands, which hinders e.g. the identification of particulate materials by their IR bands, but detailed investigations especially of the influence of grain aggregation are still lacking. We plan to set up a spectroscopic experiment (see Tamanai et al., this volume) for measuring aggregation effects on IR extinction by dust particles dispersed in air and, simultaneously, have started to use light scattering theory in order to predict numerically the band profiles for different aggregation states.

Figure 1: The clusters frac7, lin9 and sc8.
3 Structure of the clusters

We consider three-dimensional clusters of identical touching spherical particles arranged in three different geometries: fractal, cubic, and linear. For a high precision of the calculations, we restrict the number of particles per cluster to less than 10. Therefore, we have selected only three geometries, namely a “snowflake 1st-order prefractal” cluster (fractal dimension $D = \ln 7 / \ln 3 = 1.77$, [5]), where one sphere is surrounded by six others along the positive and negative cartesian axes, a cluster of eight spheres arranged as a cube and a linear chain of nine spheres. All of the clusters (Fig. 1) consist of spheres with radii $R = 10$ nm and are embedded in vacuum (or air).

For the optical constants of the particle we have chosen the data of $\beta$-SiC in the wavelength range 10-13$\mu$m, calculated from a Lorentzian oscillator-type dielectric function describing the phonon resonance in this wavelength range (see [6]). On the one hand, this phonon resonance is of practical importance since it is observed as an emission band from dust particles in carbon star envelopes. On the other hand, depending on the resonance damping parameter, it represents a model material of a very high complex refractive index with $|m| > 10$ and sharp surface resonances in the wavelength range between the LO and TO frequencies.

4 Computational approaches

4.1 The DDA method

The discrete dipole approximation (DDA) method is one of several discretisation methods (e.g. [7], [8]) for solving scattering problems in the presence of a target with arbitrary geometry. In this work we use the DDSCAT code version 6.1 [9], which is very popular among astrophysicists. In DDSCAT the considered grain/cluster is replaced by a cubic array of point dipoles of certain polarizabilities [10]. The cubic array has numerical advantages because the conjugate gradient
method can be efficiently applied to solve the matrix equation describing the dipole interactions. By specifying an appropriate grid resolution, calculations of the scattering and absorption of light by inhomogeneous media such as particle aggregates can be carried out to in principle whatever accuracy is required. For the sc8 cluster we used a grid of $36 \times 36 \times 36$ dipole, which provides 23752 dipoles in the cluster, while for the lin9 cluster a grid of $64 \times 64 \times 64$ dipole was used providing 1676 dipoles in the cluster. The program performs orientational averaging of the clusters.

4.2 The clusters-of-spheres method

The clusters-of-spheres calculations have been performed using (1) the program developed by M. Quinten (MQAGGR, commercially available) based on the theoretical approach by [10] and (2) using the T-matrix code by D.W. Mackowski (SCSMTM) calculating the random-orientation scattering matrix for an ensemble of spheres [3]. Both programs aim at solving the scattering problem in an exact way by treating the superposition of incident and all scattered fields, developed into a series of vector spherical harmonics. Available computer power, however, forces to truncate the series at a certain maximum multipole order $npol_{\text{max}}$, which in both programs can be specified explicitly. Furthermore, both programs perform an orientational average of the cluster, the resolution of which was set to 15 degrees in MQAGGR and 10 degrees in...
SCSMTM for theta (the scattering angle). The variation in the azimuthal angle is not specified in SCSMTM. In MQAGGR it is varied between 0 and 360 degrees, again with a resolution of 15 degrees.

5 Results and discussion

The extinction profiles shown in Fig. 3 display the results obtained for two cluster geometries and three different codes. The profiles obtained with the two clusters-of-spheres codes at the same multipolar order (13 for the linear chain and 15 for the cubic cluster) give quasi-identical results in the case of the linear chain but differences for the cubic cluster. SCSMTM gave less resonances than MQAGGR, which is true for all lower maximum multipolar orders as well. The reason for that could possibly be different ways of orientational averaging. This is not completely understood yet. Generally speaking, both codes didn’t converge up to the multipolar orders tried (up to 2h of CPU time per wavelength point).

DDSCAT at the maximum resolution used (1676 dipoles in the linear cluster, 23752 dipoles in the cubic one) gave much smoother profiles, i.e. with less distinct resonances. DDSCAT possesses limitations for large refractive indices ([11]). On the other hand, the resonances produced by the clusters-of-spheres codes depend so much on the maximum multipolar order that it seems reasonable to assume that the (unreached) converged spectrum would show a more smooth profile as well. Results with lower dipole resolution tend to show sharp resonances as well.

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References

[1] B.T. Draine, P.J. Flatau, “User guide for the discrete dipole approximation code DDSCAT 6.1”, http://arxiv.org/abs/astro-ph/030969 (2004).
[2] M. Quinten, U. Kreibig, “Absorption and elastic scattering of light by particle aggregates”, Appl. Opt. 32, 6173–6182 (1993).
[3] D.W. Mackowski, M.I. Mishchenko, “Calculation of the T matrix and scattering matrix for ensembles of spheres”, J. Opt. Soc. Amer. A 13, 266–2278 (1996).
[4] R. Stognienko, Th. Henning, V. Ossenkopf, “Optical properties of coagulated particles”, Astron. Astrophys. 296, 797–809 (1995).
[5] T. Vicsek, “Fractal models for diffusion controlled aggregation”, J. Phys. A 16, L647–L652 (1983).
[6] H. Mutschke, A.C. Andersen, D. Clément, Th. Henning, G. Peiter, “Infrared properties of SiC particles”, Astron. Astrophys. 345, 187–202 (1999).
[7] B.T. Draine, “The discrete-dipole approximation and its application to interstellar graphite grains”, Astrophys. J. 333, 848–872 (1988).
[8] J.I. Hage, J.M. Greenberg, “A model for the optical properties of porous grains”, Astrophys. J. 361, 251–259 (1990).
[9] J.J. Goodman, B.T. Draine, P.J. Flatau, “Application of FFT techniques to the discrete dipole approximation”, Opt. Lett. 16, 1198–1200 (1991).

[10] J.M. Gérardy, M. Ausloos, “Absorption spectrum of clusters of spheres from the general solution of Maxwell’s equations. II. Optical properties of aggregated metal spheres”, Phys. Rev. B 25, 4204–4229 (1982)

[11] B.T. Draine, J.J. Goodman, “Beyond Clausius-Mossotti - Wave propagation on a polarizable point lattice and the discrete dipole approximation”, Astrophys. J. 405, 685–697 (1993).