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

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1 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; [1]), a commercially available cluster-of-spheres code following the Gerardy-Ausloos approach (MQAGGR; [3]) and a T-matrix method (SCSMTM; [2]) for calculating IR extinction spectra of aggregates of spherical silicon carbide (SiC) particles. We compare the results obtained with the three different methods and kindly ask the community to help us in understanding them better.

2 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. [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 hinderes e.g. the identification of solid 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.

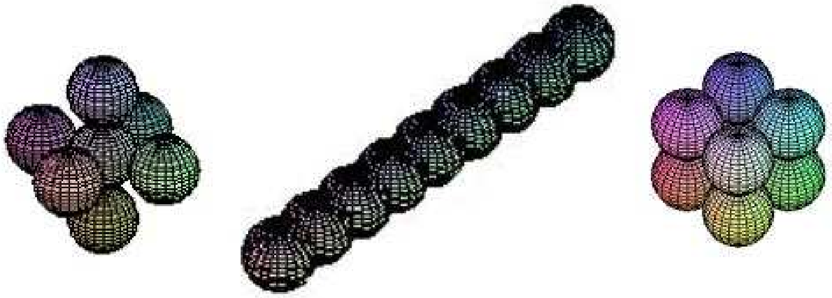

Figure 1: The clusters frac7, lin9 and sc8.

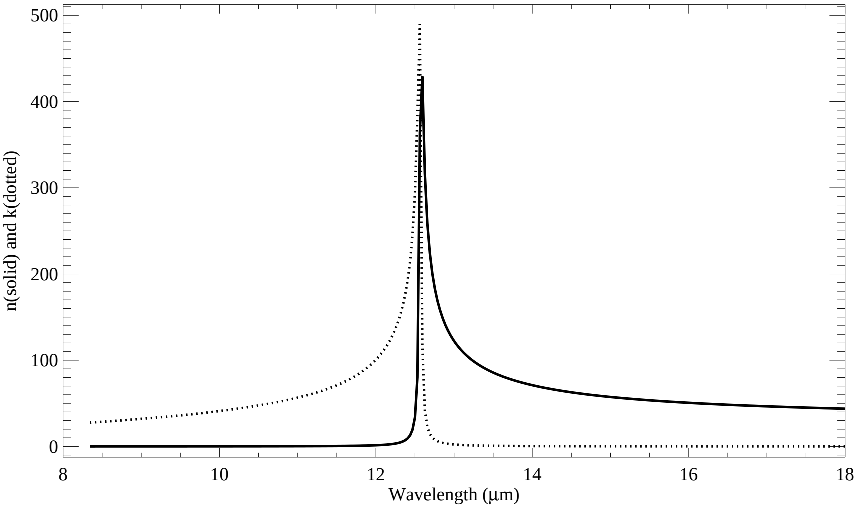

Figure 2: The refractive index for β-SiC with the damping constant $gamma = 2$. The damping constant γ (inverse proportional to the phonon life time) is an "ad hoc" introduced parameter, which in a perfect crystal reflects the anharmocnicity of the potential curve. High-quality SiC is characterized by damping constants of 1–3 cm1.

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 1'st–order prefractal" cluster (fractal dimension $D = \ln 7/\ln 3 = 1.77$, Vicsek 1983), 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 β-SiC in the wavelength range 10-13μm, calculated from a Lorentzian oscillator-type dielectric function describing the phonon resonance in this wavelength range (see [5]). 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 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) - also known as the coupled dipole approximation - method is one of several discretisation methods (e.g. [6], [7]) for solving scattering problems in the presence of a target with arbitrary geometry.

In this work we use the DDSCAT code version 6.1 [1]. In DDSCAT the considered grain/cluster is replaced by a cubic array of point dipoles. The cubic array has numerical advantages because the conjugate gradient method can be efficiently applied to solve the matrix equation describing the dipole interactions [8]. When knowing the dipole strength of each cell in the particle it is

Figure 3: Clusteres with g=2.

possible to compute the optical properties of arbitrary dust configurations.

5 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 [2]. 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_{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 betwen 0 and 360 degrees, again with a resolution of 15 degrees.

6 Results and discussion

For materials with large refractive index ($|m| > 2$), [9] show that especially the absorption is overestimated by DDA. The limitation in DDSCAT is set by the use of the lattice dispersion relation (LDR) for electromagnetic waves propagating on an infinite cubic lattice of point dipoles of polarisability α_i and spacing d. According to [9], the LDR prescription for α_i gives fair accuracy for scattering but poorer results for absorption. When $|m - 1|$ is large the continuum material is effective at screening the external field: in the limit $|m - 1| \to \infty$ the internal field generated by the polarisation would exactly cancel the incident field, so that the continuum material in the interior of the target would be subjected to zero field. In the case of a discrete dipole array, the dipoles in the interior will also be effectively shielded, while the dipoles located on the target surface are not fully shielded and, as a result, absorb energy from the external field at an excessive rate. This error can be reduced to any desired level by increasing the number

N of dipoles, thereby minimising the fraction $N^{-1/3}$ of the dipoles which are at surface sites, but very large values of N are required when $|m|$ is large [9].

Acknowledgment

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