THE ULTRAVIOLET EXTINCTION BY HOLLOW SPHERICAL
PARTICLES OF GRAPHITE

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(Received 25 September, 1990)

Abstract. Using the discrete dipole approximation, we have calculated the extinction efficiency of hollow spherical particles of graphite as a possible constituent of interstellar grains. The particles had a shell structure with the basal plane perpendicular to the radius. The calculations were made on the particles having the outer radius \( R_0 = 10 \) and 5 nm in the wave number region from 0.8 to 8.0 \( \mu \text{m}^{-1} \) using the anisotropic optical constants. It was found that the hollow particles with the inner radius \( R_I \approx 0.65 R_0 \) yield an extinction feature at 4.6 \( \mu \text{m}^{-1} \), which fits fairly well to one observed in the interstellar extinction.

1. Introduction

For many years, graphite particles have been considered one of plausible constituents of interstellar grains responsible for the feature at 4.6 \( \mu \text{m}^{-1} \) observed in the interstellar extinction. Extensive studies have been made on the extinction properties of graphite particles in the visible to the ultraviolet region (Day and Huffman, 1973; Mathis et al., 1977; Draine and Lee, 1984).

Graphite is highly anisotropic in the crystalline structure and, hence, in the optical property. Consequently, the theoretical treatments hitherto made have suffered from two major limitations. One was that most calculations of the extinction properties have been made on particles in a spherical shape using the Mie theory. Since graphite crystal is in a layered structure, such an idealized particle shape is unrealistic. The second one was that, since no rigorous theory has been developed for calculating the extinction properties of particles with the anisotropic optical property, extinction by graphite particles was approximated by one obtained for a mixture of two different types of fictitious isotropic particles: \( \frac{2}{3} \) have a dielectric function \( \varepsilon_\perp \) and the other \( \frac{1}{3} \) has a dielectric function \( \varepsilon_\parallel \), where \( \varepsilon_\perp \) and \( \varepsilon_\parallel \) are the dielectric functions for graphite for incident photons with the electric field perpendicular and parallel to the \( c \)-crystal axis, respectively. This approximation is not valid except in the limit \( x \to 0 \), where \( x \) is the size parameter given by \( x = 2\pi R/\lambda \) using the particle radius \( R \) and the wavelength \( \lambda \) of the incident photon (Draine and Lee, 1984).

Recently, new model of 'astronomical' graphite, whose particle shapes are nearly spherical, have been proposed. Kroto et al. (1985) have found experimentally that a carbon cluster \( C_{60} \) may be produced preferentially under a certain condition by the technique of laser irradiation of graphite surface under a stream of helium gas. It is speculated that the cluster has a structure of truncated icosahedron just like a soccer

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ball. The diameter is $\sim 0.7$ nm, providing an inner cavity, and the graphitic basal planes are perpendicular to the radius. Rabilizirov (1986) has calculated extinction efficiency of the $C_{60}$ cluster. It was found that the cluster gives an extinction peak at $4.6 \mu m^{-1}$ if the inner cavity has a diameter $\sim 0.35$ nm and is filled with matter whose refractive index value is 1.4. However, no explanation was given concerning how the optical anisotropy of the graphitic layer producing an icosahedron structure has been treated in the calculations.

Kroto and McKay (1988) have proposed another model of spherical graphite particles, which are somewhat similar in structure to but are much larger in size than the cluster $C_{60}$. The particles (the Kroto-spheres) are quasi-single crystals of concentric shell structure made of graphitic multi-layers. Such particles have originally been found by Iijima (1980) in arc-evaporated carbon films using a high-resolution electron microscope. The particles are usually smaller than 10 nm in diameter, and have an inner cavity of various sizes. Extinction efficiencies of the Kroto-spheres without an inner cavity (the filled Kroto-spheres) have been recently studied by Wright (1988). To treat the optical anisotropy properly, he has employed the discrete dipole approximation (DDA) due to Purcell and Pennypacker (1973). It was found that a sphere with a radius $\sim 25$ nm gives an extinction peak at $4.6 \mu m^{-1}$. However, the peak is nearly twice wider than one observed in the interstellar extinction. It was concluded, therefore, that the filled Kroto-spheres cannot be a major constituent of the interstellar grains. Here we report that the Kroto-spheres with an inner cavity (the hollow Kroto-spheres) yield an extinction peak at $4.6 \mu m^{-1}$, whose width does not differ much from one observed in the interstellar extinction.

2. Discrete Dipole Model

Since we are primarily interested in changes in the extinction curve of the Kroto-sphere caused by the presence of the inner cavity, we have calculated the extinction efficiencies for both the filled and the hollow spheres using the DDA with exactly the same model geometry. In the DDA, a particle is represented by an assembly of discrete dipoles placed usually on a simple cubic lattice. A cross-sectional view of such a dipole assembly representing a hollow Kroto-sphere is depicted in Figure 1, where each circle represents a discrete dipole used in the calculation and a line drawn through each circle denotes the orientation of the graphitic basal plane.

For the filled spheres, we have used $N = 208$ discrete dipoles. For a given outer radius $R_o$, a volume $v$ given by

$$(4/3)\pi R_o^3 = N_v$$

was assigned to each dipole. The inner cavity was introduced by removing $N'$ discrete dipoles from the central part of the sphere. The radius of the cavity $R_1$ was then determined from

$$(4/3)\pi R_1^3 = N'v.$$