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Porous and Fluffy Grains in the Regions of Anomalous Extinction

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Abstract. It has long been established that the ratio of total to selective extinction is anomalously large (≥ 5) in certain regions of the interstellar medium. In these regions of anomalous extinction the dust grains are likely to be irregular in shape and fluffy in structure. Using discrete dipole approximation (DDA) we calculate the extinction for porous and fluffy grains. We apply DDA first to solid spheroidal particles assumed to be made of a certain (large) number of dipoles. Then we systematically reduce the number of dipoles to model the porous grains. The aggregates of these particles are suggested to form the fluffy grains. We study the extinction for these particles as a function of grain size, porosity and wavelength. We apply these calculations to interpret the observed extinction data in the regions of star formation (e.g. the Orion complex).

Key words. Interstellar dust—extinction—porous grains—anomalous extinction.

1. Introduction

The ratio (R) of the total to the selective extinction ($= A_\upsilon/E(B - V)$) depends upon the environment along the line of sight. A direction through a low density interstellar medium (diffuse ISM) usually has a value of $R \sim 3.1$. However, a line of sight penetrating into a dense cloud, such as the Ophiuchus or the Taurus molecular clouds has $4 \leq R \leq 6$ (Mathis 1990). Also several studies of visual and infrared colors of the Orion stars have found large value of $R \sim 5.2$ (Breger *et al.* 1981; Cardelli & Clayton 1988). These large values of R have been attributed to large grain sizes (≥ 0.2 μm) in these regions. These grains could have grown larger than normal size through either accretion or coagulation (Mathis 1990). If the grains have grown large due to accretion of the material, then the core mantle grain models would be appropriate in these regions, as suggested earlier (Leger *et al.* 1983; Vaidya & Anandarao 1993). The other possibility is that the grains have grown large due to coagulation as shown by Jura (1980) to interpret the observations of extinction toward ρ Oph. In the case of coagulation a single grain consists of an assembly of small particles stuck together loosely; i.e., the particles are porous and fluffy. Hence, there is a need for models of electromagnetic scattering by porous and fluffy grains. Exact solutions to Maxwell's equations are known to calculate absorption, scattering and extinction of electromagnetic waves by homogeneous spheres (Van de Hulst 1981), spheroids (Asano &

Yamamoto 1975) and infinite cylinders (Greenberg 1960). However, in order to calculate the scattering, absorption and extinction of irregularly shaped and inhomogeneous (i.e. porous and fluffy) particles approximate methods are required. The discrete dipole approximation (DDA) is one such method. We apply DDA first to the spheroidal solid grains assumed to be made of a large number of dipoles. Then we systematically reduce the number of dipoles (by decreasing the packing density) to model the porous grains (Vaidya & Gupta 1997). Recently, Lumme & Rahola (1994) have used DDA to study the light scattering properties (angular distribution of the scattered intensity and polarization) of porous dust particles. Wolff *et al.* (1994) have used DDA to model the porous and fluffy grains. They have studied the extinction properties of the astronomical silicate grains and have compared their results with those obtained using the effective medium theory (EMT). In EMT the inhomogeneous particle is replaced by a homogeneous one with some averaged 'effective' dielectric function, which is obtained by using the classical Bruggeman and Maxwell-Garnet mixing rules (for discussion on EMT see, e.g., Bohren & Huffman 1983). However, the effects related to the fluctuations of the dielectric function within the inhomogeneous structures such as surface roughness and special distributions of the components can not be treated by the averaging approach of the EMT's. The DDA is a direct finite element technique and it allows the consideration of irregular shape effects and special distributions of the components in the particles. In the present study we have chosen the DDA method to take into account the influence of the internal structures (porosity) of the grains (including the non-Rayleigh structures, i.e., structure size large compared to the wavelength), which may not be possible by using the other methods (Wolff *et al.* 1994). Henning & Stognienko (1993) have used the DDA to study the polarization by porous silicate grains. Vaidya & Desai (1996) have used the porous grain model with the code 'ddscat.4b. 1' (Draine & Flatau 1994a) to calculate the angular distribution of the scattered intensity and polarization for the astronomical silicate particles. They have used the porous grain model to explain the low density and low albedo observed in the dust coma of the comet Halley.

In this paper first we show how the porous particles are generated. Then we calculate the extinction efficiencies of porous silicate grains at several wavelengths between 0.30 μm and 3.4 μm. In section 2 we describe the DDA, the validity criteria for DDA and the porous models. We present the results in section 3 and apply these results to interpret the observed extinction towards the Orion region of star formation. In section 4 we give the conclusions of the present study.

2. The DDA and the porous grains

The DDA is a very useful technique to study the scattering and absorption properties of the particles of arbitrary shape. It was first used by Purcell & Pennypacker (1973) and later developed by Draine (1988). The DDA replaces a solid particle by a 3-dimensional array of N point dipoles. We use the DDA program 'ddscat.4b.l' developed by Draine & Flatau (1994a) to generate porous grains. There are two validity criteria for DDA (Draine & Flatau 1994b): viz., (i) $mkd \leq 1$, where m is the complex refractive index, $k = \pi/\lambda$, and d is the lattice dispersion spacing and (ii) d should be small enough (N should be large enough) to describe the shape of the target satisfactorily. In this program it is also assumed that the dipoles are located on a cubic lattice. Initially we assume the number of dipoles N_x, N_y, N_z along the axis x, y, z for the spheroidal target grain. This would result in a certain number N of dipoles in the spheroidal target grain, e.g., for $N_x = 24$, $N_y = 18$, $N_z = 18$; we get $N \sim 4088$ (Draine & Flatau 1994a). Then we reduce N_x, N_y, N_z to generate the porous grains (viz., 16, 12, 12; 8, 6, 6 and so on). The assumed shape of the grain is a prolate spheroid with the axial ratio of 1.3. If the semi-major and semi-minor axes of the prolate spheroids are denoted by $x/2$ and $y/2$ respectively then we have $a^3 = (x/2) \times (y/2)^2$; where a is the radius of a sphere whose volume is the same as that of a spheroid. Hence, e.g., for a spheroid with $N_x = 16$, $N_y = 12$ and $N_z = 12$, the program 'ddscat.4b.l' (Draine & Flatau 1994a) will yield $N \sim 4/3 \times \pi \times (x/2) \times (y/2)^2 \sim 4/3 \times \pi \times 8 \times (6)^2 \sim 1184$ (Vaidya & Gupta 1997). Depending upon the number of dipoles N in the grain the porosity P varies between $0 \leq P \leq 1$ (Greenberg 1990). In the present work P varies between (close to) 0 (for very large N, e.g. 4088) and 0.75 (for $N = 152$). We know that $N = 4088$ is not very large but it is sufficiently large for the grain sizes and the wavelength range considered in the present study. Fig. 1 shows the plots of the lattice dispersion *mkd* as a function of grain size a at two wavelengths, viz. 0.70 μm and 3.4 μm for the porous silicate grains. These curves indicate validity criteria for DDA (viz. $mkd < 1$) at these two wavelengths for the porous ($N = 152$,

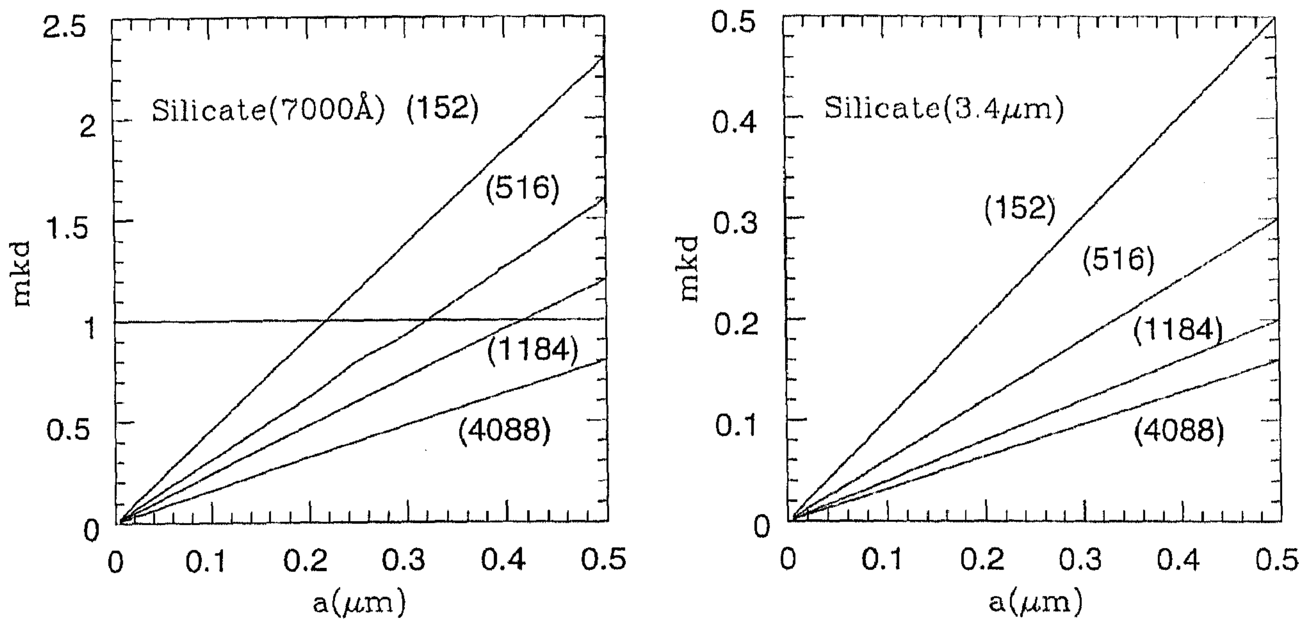

Figure 1. Lattice dispersion relation *mkd* as a function of grain size at two wavelengths for the porous silicate grains.

Table 1. Maximum grain size satisfying the DDA validity criteria.

Wavelength (μm)	$N = 152$ a(μm)	$N = 516$ a(μm)	$N = 1184$ a(μm)	$N = 4088$ a(μm)
0.3000	0.090	0.105	0.19	0.25
0.4400	0.134	0.195	0.27	0.40
0.5500	0.170	0.255	0.35	0.50
0.7000	0.215	0.305	0.42	0.63
1.0000	0.308	0.446	0.64	0.92
2.2000	0.678	1.050	1.34	2.03
3.4000	1.000	1.500	2.08	3.12

516, 1184 and 4088) silicate grains; similar curves at other wavelengths can be drawn from the *mkd* values obtained using the 'ddscat.4b.1' program (Draine & Flatau 1994a). Table 1 shows the maximum grain size satisfying the DDA validity criteria. It is seen from this table that as the wavelength increases the maximum grain size that satisfies the DDA validity criteria also increases. It varies between about 0.1 and 1.0 μm for N = 152 and from 0.25 to 3.0 μm for N = 4088.

3. Results and discussion

Using the 'ddscat.4b.1' program we have obtained the extinction efficiency factor Q_{ext}, the ratio of the cross section of the extinction to the geometrical cross section for the porous astronomical silicate grains (i.e., N = 152, 516, 1184 and 4088). These efficiencies are calculated using the optical constants given by Draine (1985, 1987). The prolate spheroidal grains are assumed to be randomly oriented and the

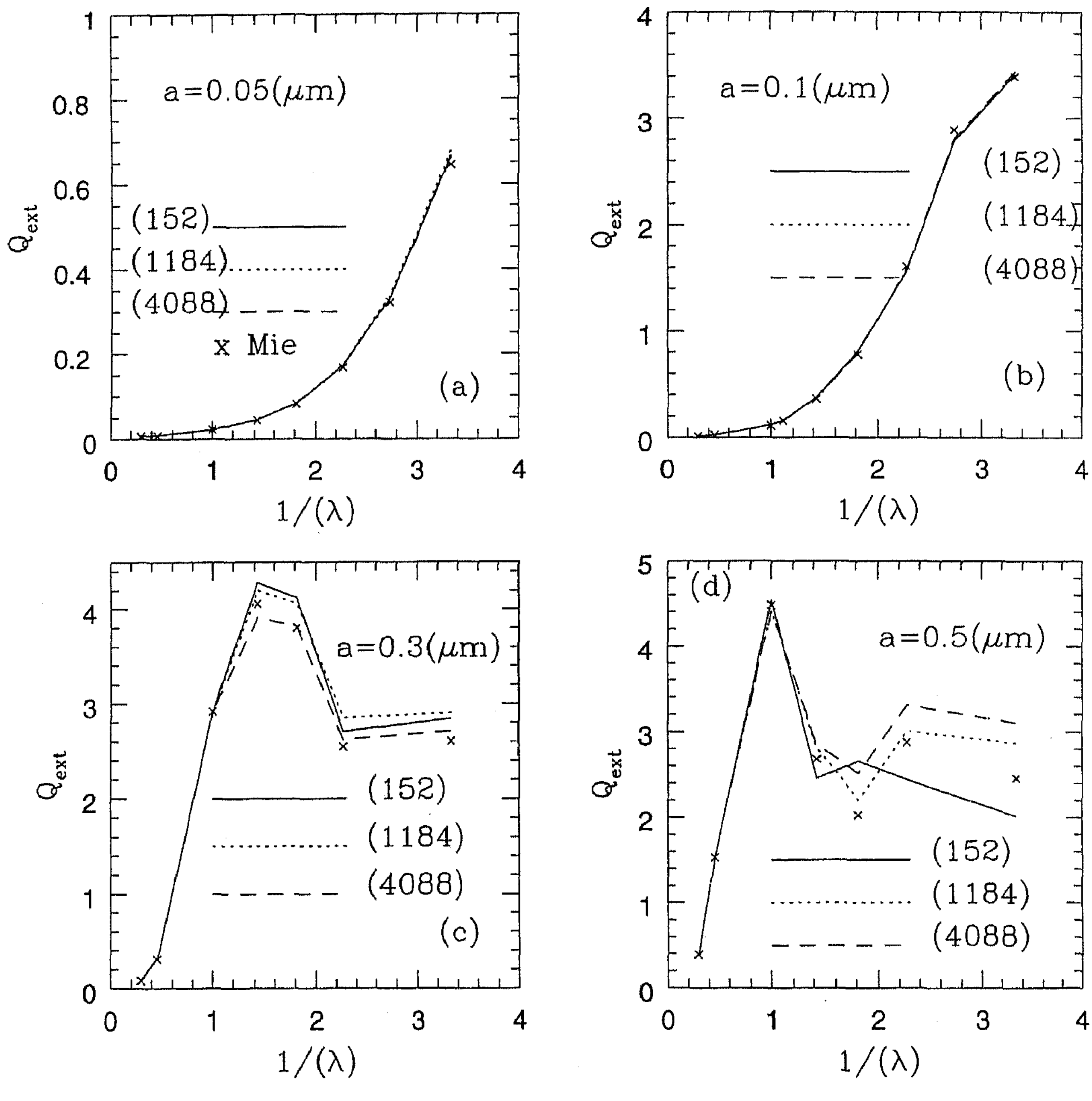

Figure 2. Extinction efficiencies Q_{ext} for porous silicate grains of four different sizes.

geometrical cross section of these prolate grains is taken to be $\pi \times (y/2)^2$, where y is the semi-major axis of the prolate spheroid. Fig. 2(a–d) show plots of the extinction efficiency Q_{ext} against $1/\lambda$ for the porous (N = 152, 1184 and 4088) silicate grains in the wavelength range of 0.30 μm–3.4 μm for the grain size a equal to (a) 0.05 (b) 0.10 (c) 0.30 and (d) 0.50 μm. For the solid grains the extinction efficiency factors Q_{ext} are obtained using Mie theory. The crosses in the figure show the extinction efficiency factors for the solid particles (Mie values). It is seen from these plots that for small grains (i.e., a = 0.05 μm and 0.10 μm) there is no significant variation in the extinction efficiencies for the porous grains. However, for grains with $a \geq 0.1$ μm the extinction is modified considerably (Fig. 2(c)). The extinction for the porous grains is enhanced (i.e., the extinction for the grains with N = 152 is more than that which is obtained for N = 1184, N = 4088 and solid grains (Mie values)). For grains with a = 0.5 μm (Fig. 2(d)) the extinction for the porous grains is enhanced; however, one notes that beyond 0.40 μm, the effect of porosity on the extinction is not very clear. This could be due to the number of dipoles N is not large enough for the grain size a = 0.5 μm in the wavelength range 0.40–0.30 μm. We use these results on the extinction by porous grains and the power law grain size distribution (Mathis, Rumpl & Nordsieck 1977), $n(a) \sim a^{-3.5}$, with the size range of 0.005–0.300 μm, to reproduce the observed interstellar extinction curve, viz. $E(\lambda - V)/E(B - V)$ vs $1/\lambda$ for the star

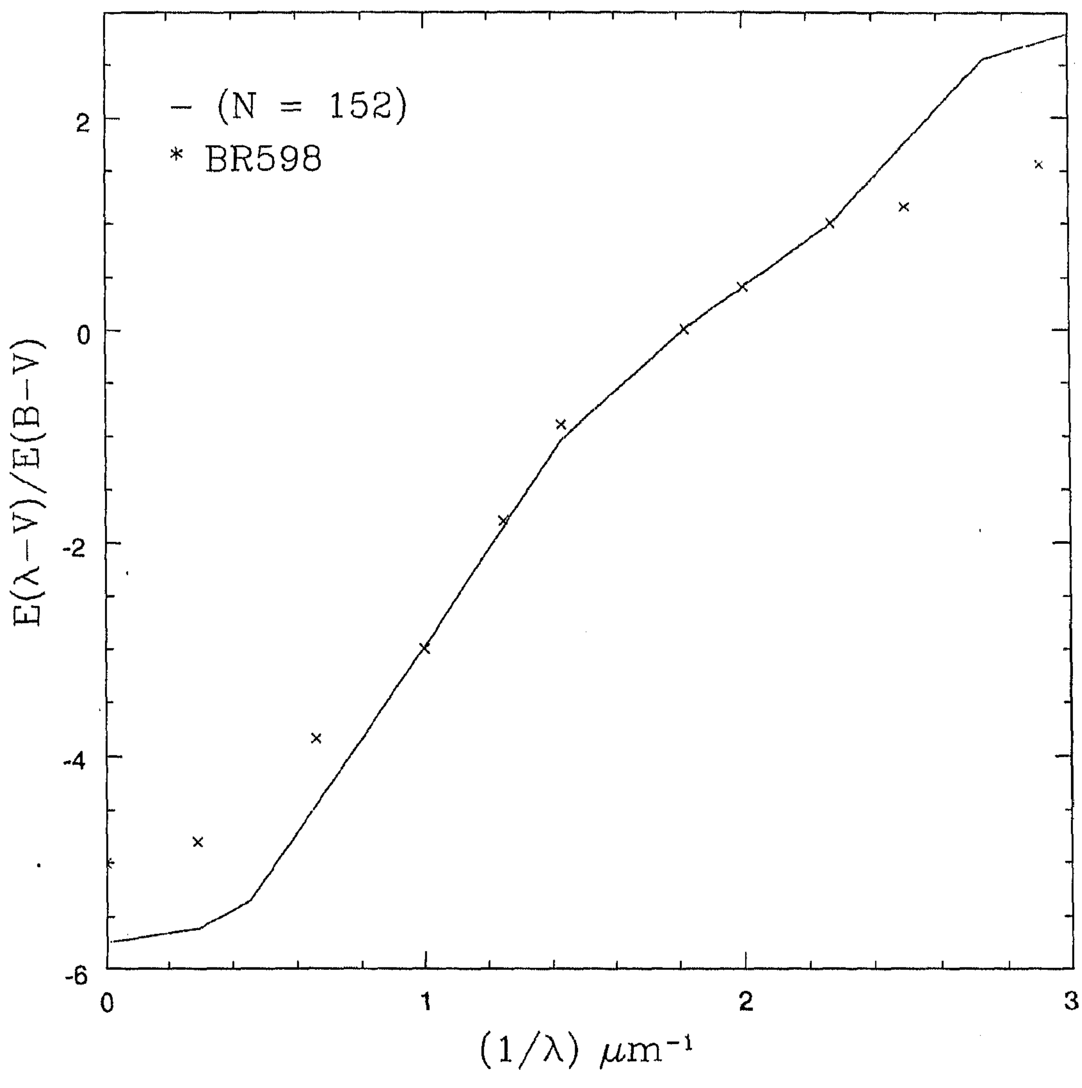

Figure 3. Comparison of the observed extinction curve with the porous silicate grains with N = 152.

BR598 (Breger *et al.* 1981) in the Orion. The ratio R of the total to the selective extinction is also evaluated for these porous grains. It is to be noted here that the maximum size for the porous grains required to obtain $R \sim 5.2$ is 0.30 μm whereas for the solid grains the maximum size required would be ≥ 0.500 (Leger *et al.* 1983; Vaidya & Anandarao 1993). Figs. 3, 4, 5 and 6 show the observed interstellar extinction curve with the model curve of porous silicate grains with $N = 152$, $N = 516$, $N = 1184$ and $N = 4088$ respectively. It is seen that models with $N = 1184$ and $N = 4088$ reproduce the observed extinction for this star reasonably well. A comparison of Figs. 3–6 shows that the model for $N = 152$ deviates considerably from the observed curve especially in the U band and in the IR. One also notes that the model $N = 152$ does not satisfy the validity criteria for DDA (Table 1, Fig. 1) for the large grain sizes (i.e., ≥ 0.1 μm). Grain models with $N = 516$ also do not fit well in the IR region. Among the other two possible models, however, one does not find much difference. This means that the porous grains with about 40% porosity ($N = 1184$) would fit the observed curve reasonably well and increasing the number of dipoles N (e.g., 4088) would not improve the fit. The only possible criterion, therefore, to choose a particular model suitable for a given observation is by considering the total amount of matter locked up in grains (small for high porosity). Hence measurements in metallic abundances in the interstellar medium should be taken as a handle to select a particular model as the best fit for extinction observations

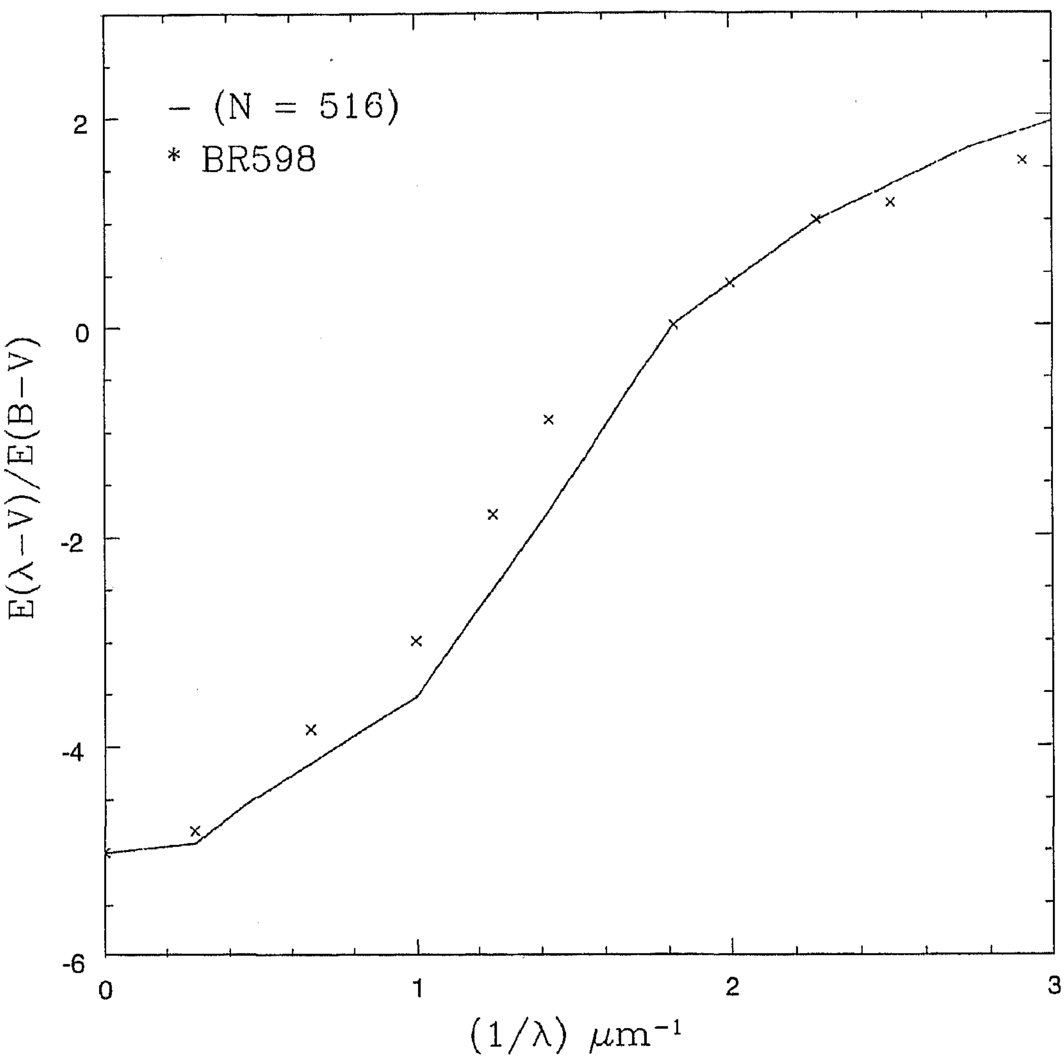

Figure 4. Same as Fig. 3 but with $N = 516$.

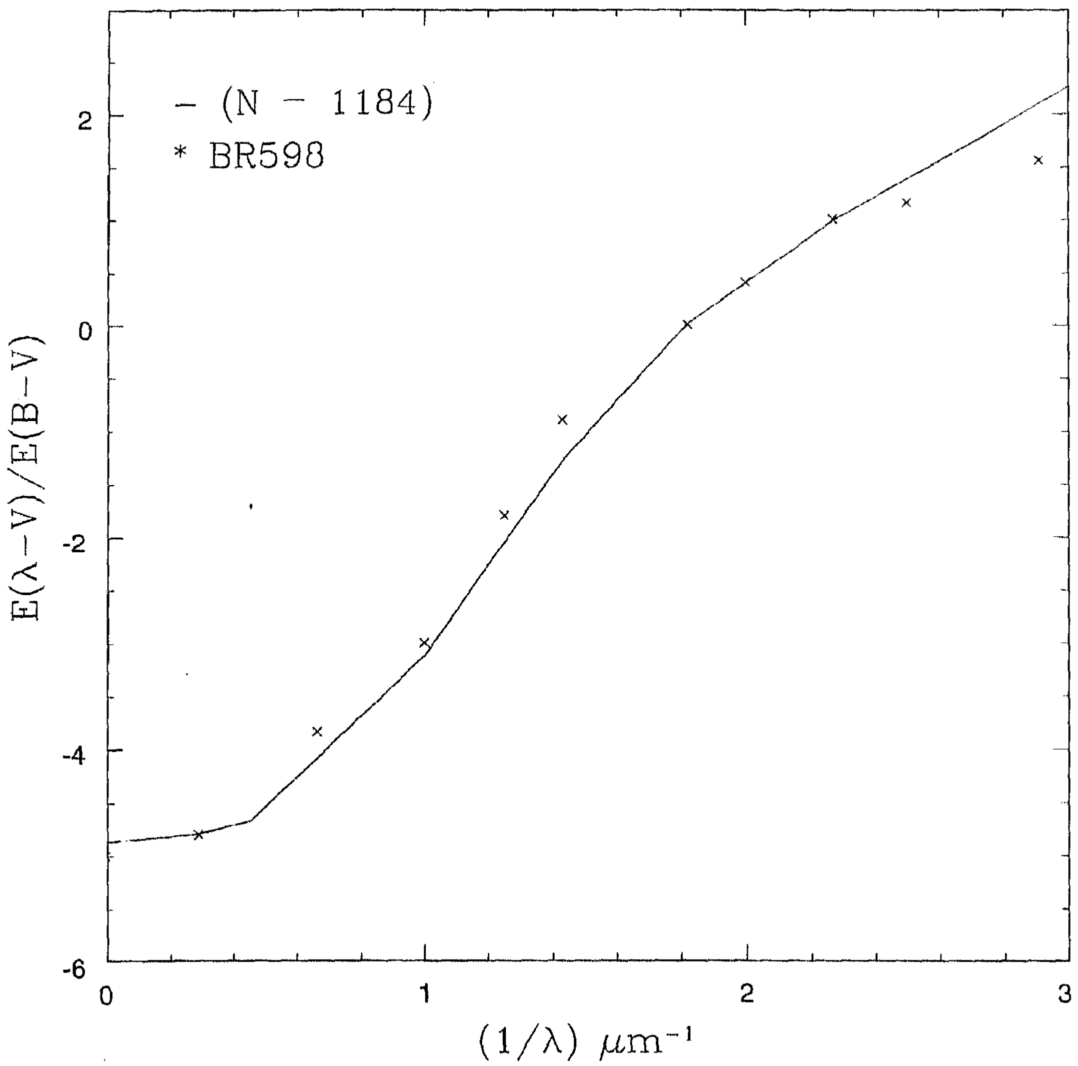

Figure 5. Same as Fig. 4 but with $N = 1184$.

(Mathis 1996; Dwek 1997). In order to quantify the material content from the model one needs to compare it with some spectral feature in the observed curve or one should assume that only one type of grain composition accounts for the infrared flux in the wavelength range considered. Earlier, Leger *et al.* (1983) have reported that large grains (1.2 μm) are required to fit the observed data in molecular clouds and in the high density interstellar medium. Our results indicate that the grains do not grow very large in the regions of anomalous extinction but they are porous. In these regions the grains can attach to each other by collisions in slow motion and coagulate. In case of accretion gas phase atoms and molecules are adsorbed on the surface of a core becoming a core-mantle grain. Further, it is shown (Jura 1980; Whittet 1992) that the time scale for grain-grain collision is

$$t_{\rm col} = \frac{n_d}{\pi a^2 v_d} \tag{1}$$

where n_d and v_d are the density and velocity of the grain and a its size. Jura (1980) finds for $n_d = 10^9\ {\rm m}^{-3}$ and $v_d = 0.1$ km/s, $t_{\rm col} \sim 3$ myr. This shows that the coagulation is possible within the life time of a cloud. Also, from the observations on the Ophiuchi sources Tanaka *et al.* (1990) have shown that stars having large R have moderate visual extinction ($1 \leq A_V \leq 10$) while the ice mantle particles are detected only towards the sources with $A_v \geq 10$. The value of A_v for BR598 is 1.68 (Breger

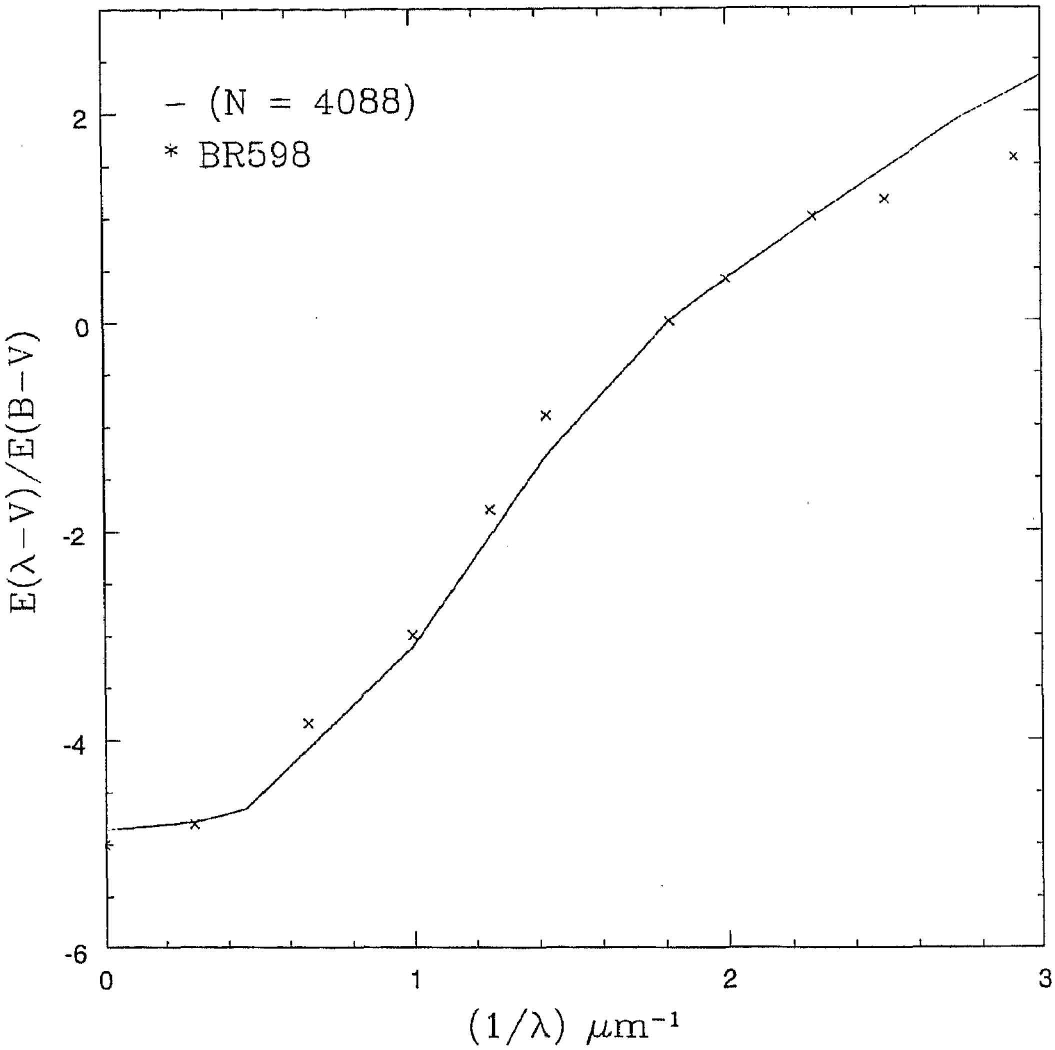

Figure 6. Same as Fig. 5 but with $N = 4088$.

et al. 1981) hence in this region the dust grains are more likely to be porous rather than core-mantle.

4. Conclusions

Using discrete dipole approximation (DDA) we have obtained the extinction efficiencies of the porous astronomical silicate grains at several wavelengths between 0.30 μm and 3.4 μm. Our results show that the porosity affects the extinction efficiency of the particles. These porous grain models reproduce the observations of extinction toward Orion at wavelengths greater than 0.30 μm. These results indicate that grains do not grow very large in the regions of anomalous extinction but they might be porous and fluffy. These models are not unique but we only wish to illustrate how porous grains can reproduce the observations in the regions of anomalous extinction. The laboratory study using microwave analog technique has shown that the scattering properties of porous particles differ considerably from those of spheres (Giese *et al.* 1978; Greenberg & Gustafson 1981; Zerull *et al.* 1993). These laboratory data are used to interpret the observed data on zodiacal light and comets (Giese *et al.* 1978). Similarly, laboratory data on the extinction by porous particles are required to help interpret better the observed data in these regions of anomalous extinction.

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