Astron. Astrophys. 328, 634–640 (1997)

ASTRONOMY AND ASTROPHYSICS

Extinction by porous silicate and graphite grains

D.B. Vaidya[1] **and Ranjan Gupta**[2]

[1] Department of Physics, Gujarat College, Ahmedabad 380006, India
[2] IUCAA, Post Bag 4, Ganeshkhind, Pune 411007, India

Received 5 December 1996 / Accepted 5 August 1997

Abstract. Discrete dipole approximation (DDA) is used to calculate extinction efficiencies of porous silicate and graphite grains. We apply DDA first to the spheroidal solid grains assumed to be made of a large number of small scattering elements (dipoles). Then we systematically reduce the number of dipoles to model the porous grains. The extinction is studied as a function of wavelength, grain size and porosity for both silicate and graphite grains. Finally the extinction efficiencies of the porous silicate and graphite grains are used to evaluate the interstellar extinction curve which is found to fit well with the average observed extinction curve.

Key words: dust, extinction – scattering

1. Introduction

Recent studies of interplanetary, cometary and interstellar dust indicate that cosmic dust grains are porous and fluffy(Greenberg 1990,Hage and Greenberg 1990,Wolff et al 1994). Hence, there is a need for formulating models of electromagnetic scattering by porous and fluffy grains. Mie theory provides an exact series solution to Maxwell's equations to calculate absorption, scattering and extinction of electromagnetic waves by homogeneous spheres (Van de Hulst 1981). Exact solutions to Maxwell's equations are also known for spheroids (Asano and Yamamoto,1975) and infinite cylinders (Greenberg 1960). However, in order to calculate the scattering, absorption and extinction of irregularly shaped and inhomogeneous (e.g. 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 certain large number of dipoles. Then we systematically reduce the number of dipoles (i.e. we reduce the packing density) to model the porous grains. Recently, Lumme and 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 grains and they have studied the extinction properties of astronomical silicate grains. They 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 EMT mixing rules (for discussion on EMT see e.g. Bohren and 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. The Generalised Semi Analytical (GSA) method developed by Rouleau and Martin (1993) and Volume Integration Equation Function (VIEF) method (Hage and Greenberg, 1990) can also be used to study the scattering properties of the porous and fluffy grains. The GSA method may be superior to DDA for the grain sizes smaller than the wavelength and for large dielectric constants (Draine and Flatau 1994, Wolff etal 1994). Draine and Goodman (1993) have shown that the VIEF method has the same intrinsic abilities and limitations as does the DDA. 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 and Stognienko (1993) have used DDA to study the polarization by porous silicate grains. Vaidya and Desai (1996) have used the porous grain model and ddscat.4b.1 program (Draine and 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 we first show how the porous particles are generated. Then we calculate the extinction efficiencies of the porous silicate and graphite grains at several wavelengths between 0.20μm and 0.55μm. In Sect. 2 we describe the DDA, the validity criteria for DDA and the porous models. We present the results in Sect. 3 and show how

Send offprint requests to: Ranjan Gupta

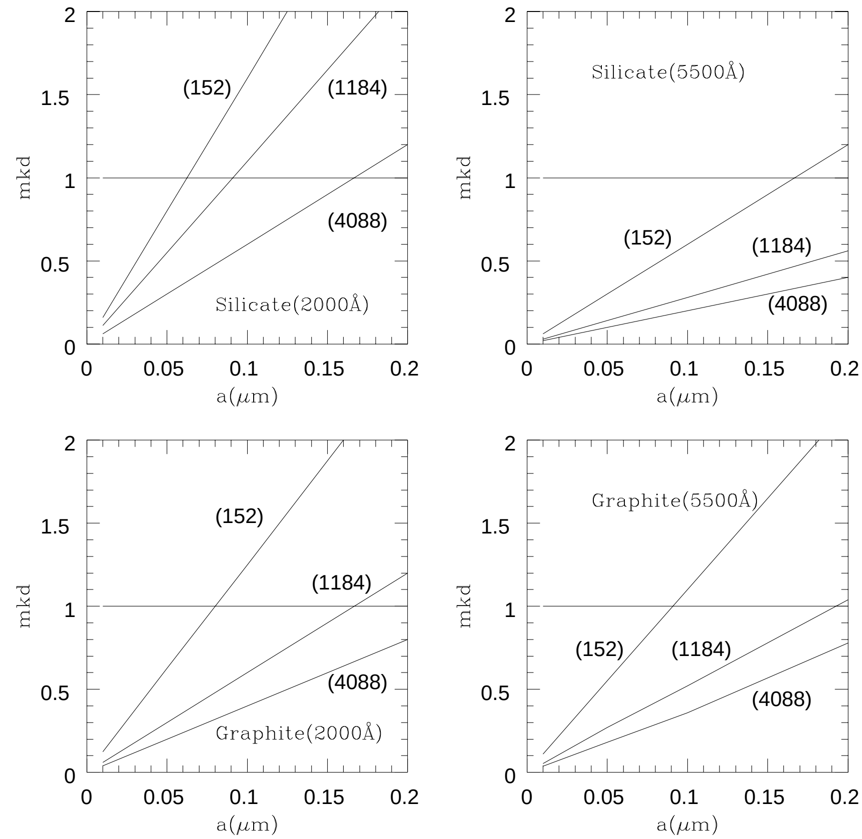

Fig. 1. Lattice dispersion relation mkd as a function of grain size at two wavelengths for the porous silicate and graphite grains.

these results are applied to evaluate the interstellar extinction curve. In Sect. 4 we give the conclusions of the present study.

2. Discrete Dipole Approximation (DDA) and the porous grains

The Discrete Dipole Approximation (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 and Pennypacker (1973) and later developed by Draine (1988). The DDA replaces a solid particle by an array of N point dipoles. We use the DDA program ddscat.4b.1 developed by Draine and Flatau (1994a) to generate porous grains. There are two validity criteria for DDA (Draine and Flatau, 1994b; Wolff et al, 1994); viz. (i) $mkd < 1$, 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 a large number of dipoles Nx, Ny, Nz along the axis x, y, z for the spheroidal target grain . This would result in a certain number of N dipoles in the solid grain; e.g. for Nx=24, Ny=18, Nz=18; we get N=4088 (Draine and Flatau 1994a). Then we reduce Nx, Ny, Nz 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 axis and semi-minor axis of the prolate spheroids are denoted by $x/2$ and $y/2$ respectively then we have $a^3 = (x/2) * (y/2)^2$; 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 Nx=16,Ny=12 and Nz=12, the program ddscat.4b.1 (Draine and Flatau 1994b), will yield $N = 4/3 * \pi * (x/2) * (y/2)^2 = 4/3 * \pi * (8) * (6)^2 = 1184$.

Table 1. No. of dipoles v/s porosity

N	P
4088	0.0
1184	0.3
152	0.7
64	0.8

The porosity P can be defined as $P = 1 - V_{\text{solid}}/V_{\text{total}}$; where V_{solid} is the volume of the solid material inside the grain and V_{total} is the total volume of the grain. Accordingly, depending upon the number of dipoles N in the grain, P varies between $0 < P < 1$ (Greenberg 1990). Table 1 shows the porosity P for various values of N.

Table 2 shows the maximum radius (a) of the grain that satisfies the validity criteria for DDA (viz. $mkd < 1$) at several wavelengths for N = 4088, 1184 and 152.

Fig. 1 shows the plots of the lattice dispersion relation mkd as a function of grain size a at two wavelengths (i.e. 0.20μm and 0.55μm) for the porous silicate and graphite grains. These curves indicate the validity criteria for DDA (viz. $mkd < 1$) at these two wavelengths for the porous (N=152,1184 and 4088)

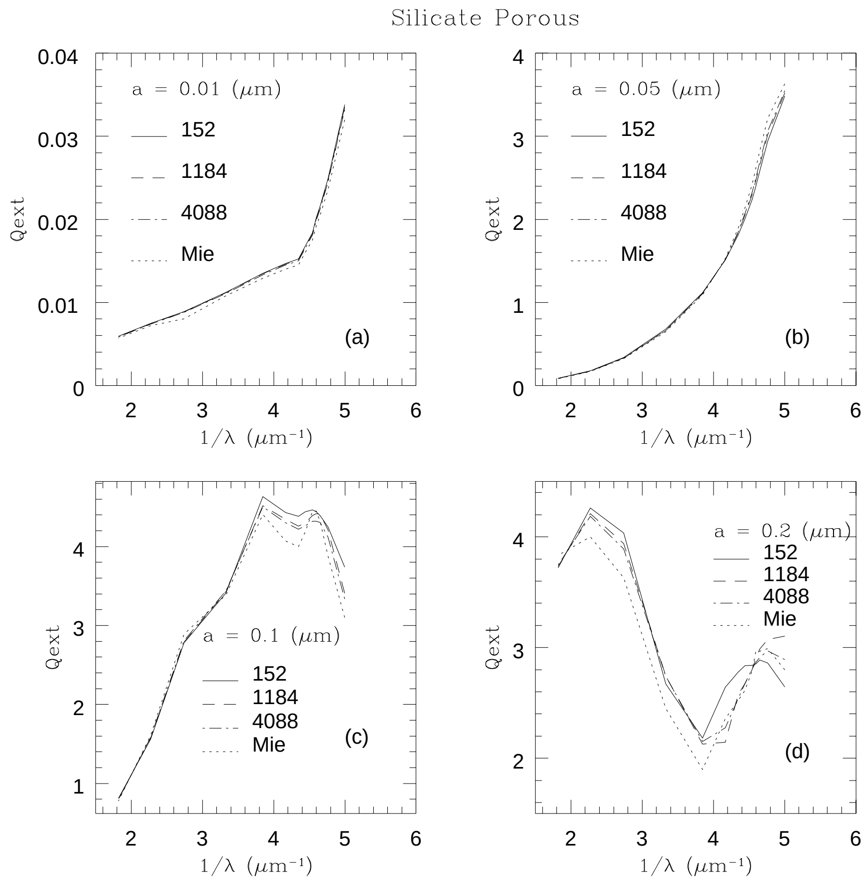

Fig. 2a–d. Extinction efficiencies ($Q_{\rm ext}$) for porous Silicate grains.

Table 2. Validity criteria

Wavelength	Silicate N=152	Silicate N=1184	Silicate N=4088	Graphite N=152	Graphite N=1184	Graphite N=4088
(μm)	$a(\mu)$	$a(\mu)$	$a(\mu)$	$a(\mu)$	$a(\mu)$	$a(\mu)$
0.2000	0.055	0.11	0.17	0.080	0.17	0.25
0.2200	0.062	0.13	0.20	0.066	0.14	0.20
0.2400	0.070	0.14	0.21	0.055	0.11	0.17
0.3000	0.090	0.19	0.25	0.050	0.10	0.15
0.4400	0.134	0.27	0.40	0.078	0.15	0.25
0.5500	0.170	0.35	0.50	0.091	0.19	0.27

silicate and graphite grains ; similar curves at other wavelengths can be drawn from the mkd values obtained using the ddscat.4b.1 program (Draine and Flatau, 1994a).

3. Results and discussion

As mentioned earlier, recent studies of interplanetary and interstellar dust provide evidence that cosmic dust grains are porous and fluffy in structure. The optical properties of these porous irregular particles should be quite different from those of solid homogeneous particles such as spheres, cylinders and ellipsoids. The main objective of the paper, therefore, is to study the effect of porosity on the extinction of the silicate and graphite grains. These materials have been the ingredients of the earlier grain models (Mathis,Rumpl & Nordsieck 1977; Hong and Greenberg 1980, Mathis and Whiffen 1989, Wolff et al 1993). Using ddscat.4b.1 program (Draine and Flatau 1994a) we have obtained extinction efficiency factor $Q_{\rm ext}$, the ratio of the cross section of the extinction to the geometrical cross section for the silicate and graphite porous grains (i.e. with N=152,1184 and 4088). In the present study we assume the prolate spheroids are randomly oriented. The geometric cross section of a randomly oriented prolate spheroid is given by $\pi * (y/2)^2$. We present the results for grain sizes: 0.01μ,0.05μ, 0.10μ and 0.2μ at several wavelengths between 0.2000μm and 0.5500μm, i.e. between 1.8μm^{-1} and 5.0μm^{-1} (total 13 wavelengths). For the solid grains the extinction efficiency factors $Q_{\rm ext}$ are obtained using Mie theory. The optical constants (i.e. refractive indices) for silicate and graphite are taken from Draine (1985,1987).

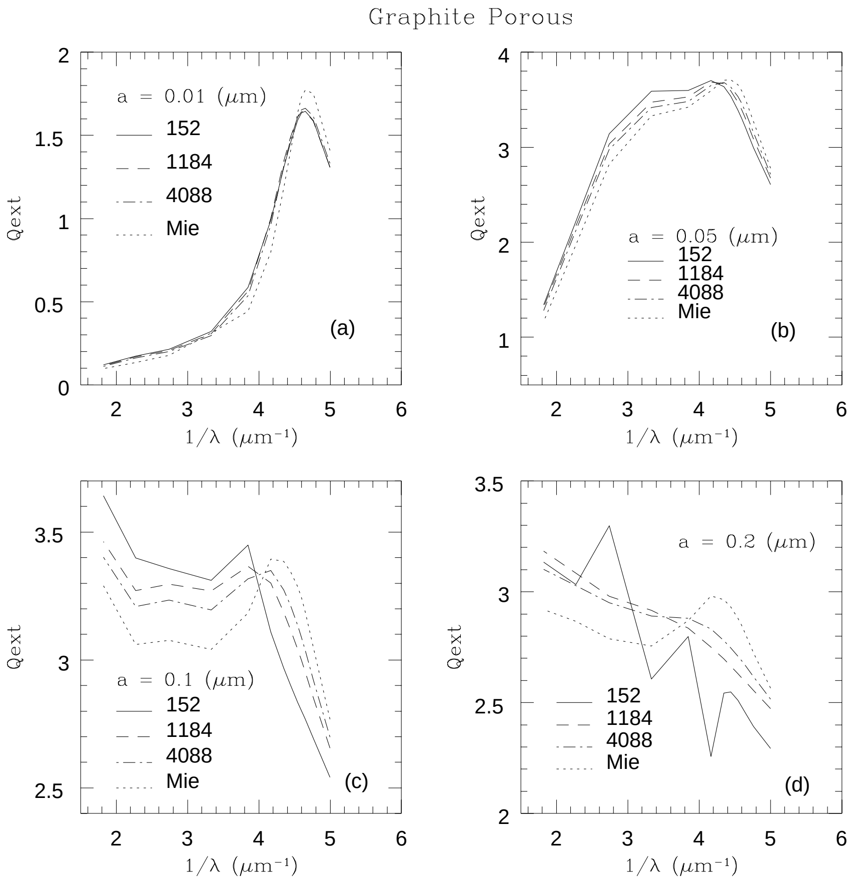

Fig. 3a–d. Extinction efficiencies (Q_{ext}) for porous Graphite grains

Silicates

Fig. 2 shows the extinction efficiency curves for the porous silicate grains.

In Fig. 2a for the grain size a = 0.01μ the enhancement in the extinction for the porous (for N=152,1184 and 4088) silicate grains is indicated (i.e. the extinction for the porous grains is more than that is obtained for the solid grains using Mie theory) in the entire wavelength range considered here i.e. between 0.55μm and 0.20μm. However, since the grain size is small (0.01μ) there does not seem to be any variation in the extinction with the porosity. For the grain size a = 0.05μ (Fig. 2b), no appreciable deviation in the extinction is indicated in the wavelength range 0.55μm and 0.25μm however, between 0.25μm and 0.20μm the extinction for the porous grains seems to be lower than that is obtained for the solid grains (Mie curve). For the grain size a = 0.1μ (Fig. 2c) the effect of porosity on the extinction is clearly seen between 4.0μm^{-1} and 5.0μm^{-1}(i.e. between the wavelength range 0.25μm and 0.20μm). The extinction for the grains with N=152 is more than that is obtained for N=1184, N=4088 and solid grains(Mie curve).This means that the extinction is enhanced as the particle becomes more porous (i.e. as the number of dipoles decreases). For the larger grains with a = 0.2μ (Fig. 2d) the extinction for the porous grains is enhanced in the wavelength range 0.55μm - 0.25μm. Beyond 0.25μm 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 (check Table 2, Fig. 1) for the grain size a = 0.2μ in the wavelength range 0.25μm-0.20μm.

These results on silicates indicate the enhancement in extinction for small (a = 0.01μ and 0.05μ) porous grains in the entire wavelength range of 0.55μm and 0.20μm, while for the grains with a = 0.1μ the enhancement in the extinction is seen between the wavelength range of 0.25μm and 0.20μm and for the grains with a = 0.2μ the enhancement is indicated between 0.55μm and 0.25μm. Earlier, Jones(1988) had shown porous silicate grains to produce enhanced infrared, ultraviolet and far ultraviolet extinction. Using DDA, Wolff et. al. (1994) have found enhancement in the extinction for the astronomical porous silicate grains and they have compared their results with those obtained using the effective medium theory (EMT). Perrin and Lamy (1990) have shown the limitations of the effective medium theory for the inhomogeneous dust particles.

Graphites

Figs. 3a-3d show extinction efficiency curves for the porous graphite grains. In Fig. 3a, for the grain size a = 0.01μ, the effect of porosity on the extinction is clearly seen. The extinction for the porous grains is enhanced in the wavelength range 0.55μm-0.23μm (i.e between 1.8μm^{-1} - 4.4μm^{-1}),whereas in the absorption band between 0.23μm-0.20μm the extinction for the porous grains is lower than that is obtained for the solid grains (Mie curve). For the grain size a = 0.05μ and a = 0.1μ

(Figs. 3b and 3c) the enhancement in the extinction is much more between $1.8\mu m^{-1}$ - $4.4\mu m^{-1}$. The wavelength of peak extinction seems to be shifting (Fig. 3c) as the porosity increases. The extinction peak seems to shift from $4.4\mu m^{-1}$ for the solid grain (Mie curve) to $3.8\mu m^{-1}$ for the porous grains with N=152. In Fig. 3d for the grain size a = 0.2μ the extinction for the porous grains with N=1184 and N=4088 is enhanced as expected but for N=152 it is very erratic as the number of dipoles N is not large enough to describe the shape of the particle (check Table 2, Fig. 1). The extinction peak has become broader but the shift in the peak is indicated with the increasing porosity. Perrin and Sivan (1990) have studied the effect of porosity and impurities on extinction by graphite grains in the spectral range between 1600Å and 3000Å. They have found that the width of the extinction bump is modified by porosity and impurities (inclusions of amorphous carbon) both, while the central wavelength is significantly shifted only by impurities.

Interstellar extinction

Our results clearly indicate that porosity significantly affects the extinction cross sections of the silicate and graphite grains. It would be interesting therefore to see how these porous grain models fit the observed interstellar extinction in the spectral region we have considered in the present study i.e. between 2000Å and 5500Å (total 13 wavelengths). Using the power law grain size distribution (Mathis,Rumpl & Nordsieck 1977) and the extinction efficiencies of the porous silicate and graphite grains we have evaluated the interstellar extinction curve in this spectral region. The average observed interstellar extinction curve (Savage and Mathis, 1979; Seaton, 1979) is then compared with the model curve formed from a χ^2 minimized and best fit linear combination of porous silicate and graphite grains in the following way:

The two model interstellar extinction curves for silicate and graphite porous grains are linearly combined as p times silicate and q times graphite to render a net curve for comparison with the observed curve. By varying p and q individually from 0.1 to 1.0 in steps of 0.1, a set of 20 curves are generated and the comparison with the observed curve gives a set of reduced $\tilde{\chi^2}_j$ values. The combination of p and q which gives a minimum $\tilde{\chi^2}_j$ value in this set is chosen and such combinations and corresponding minimum $\tilde{\chi^2}_j$ values are shown in the Table 3.

The set of reduced $\tilde{\chi^2}_j$ values is defined as (Bevington 1969):

$$\tilde{\chi^2}_j = \frac{\sum_{i=1}^{n} (S_i^j - T_i^k)^2}{pp} \quad (1)$$

where pp is the degrees of freedom, $S_i^j(\lambda_i)$ is the j^{th} model curve for the corresponding p and q linear combination of silicate and graphite porous grains and $T_i^k(\lambda_i)$ is for the observed curve, λ_i are the wavelength points with $i = 1, n$ for $n = 13$ points of the extinction curves.

The interstellar extinction curves for the lowest $\tilde{\chi^2}_j$ values taken from Table 3 in the three categories of number of dipoles

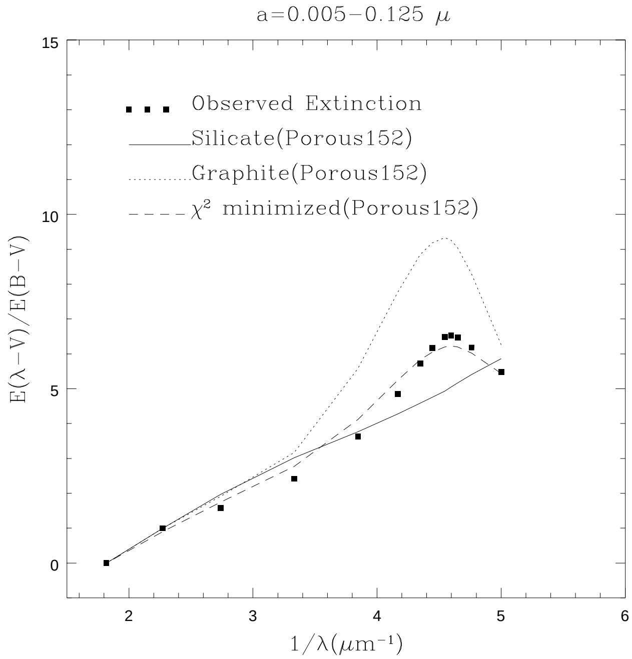

Fig. 4. Comparison of the observed interstellar extinction curve with the best fit model combination curve of porous silicate and graphite grains with the number of dipoles n =152.

Table 3. Best fit values of p, q and minimized χ^2 for porous grains of sizes $0.005-0.250\mu$, $0.005-0.125\mu$ and $0.005-0.100\mu$ and number of dipoles 152, 1184 and 4088

Parameters	0.005-0.250	0.005-0.125	0.005-0.100
No. of dipoles 152			
p	0.4	0.5	0.3
q	0.5	0.4	0.5
χ^2	0.0835	0.0784	0.0818
No. of dipoles 1184			
p	0.5	0.3	0.4
q	0.4	0.5	0.4
χ^2	0.0570	0.0802	0.0905
No. of dipoles 4088			
p	0.5	0.3	0.4
q	0.4	0.5	0.4
χ^2	0.0458	0.0741	0.0477

in the porous grains i. e. 152,1184,4088 are shown along with the observed curve in Figs. 4, 5 and 6.

It is seen from these figures that the porous grain models with N=152 and 1184 do not fit well with the observed curve, whereas the model with N=4088 and the grain size distribution of $0.005\mu - 0.250\mu$ fits reasonably well. It is to be noted however that the present study is limited to the spectral region between 2000Å and 5500Å. In our forthcoming paper (Vaidya and Gupta 1997) we have extended the calculations in the infrared region upto 3.4μm, which would help put more constraints on the grain models. Also, the extinction calculations for the porous grains in the uv region ($< 0.20\mu$m) are required to explain the variation

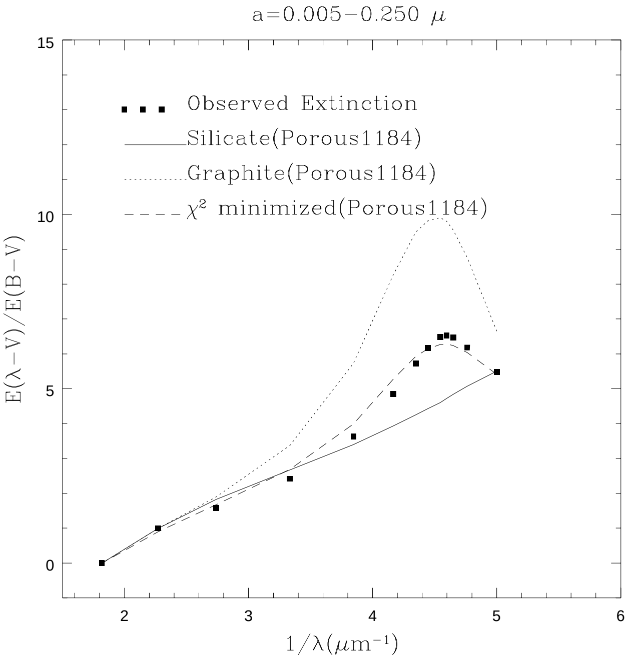

Fig. 5. Comparison of the observed interstellar extinction curve with the best fit model combination curve of porous silicate and graphite grains with n =1184.

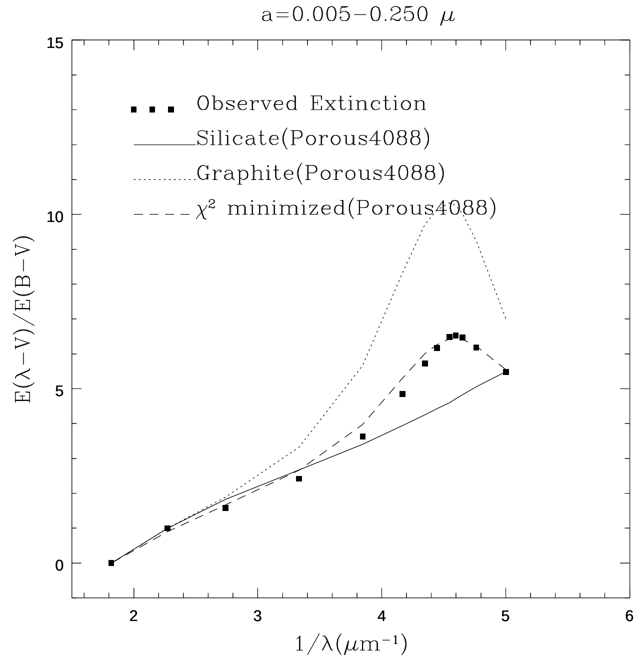

Fig. 6. Comparison of the observed interstellar extinction curve with the best fit model combination curve of porous silicate and graphite grains with n = 4088.

in the width of the 'bump' region and the shift in the central peak wavelength in the extinction curves of graphite grains (Perrin and Sivan, 1990).

4. Conclusions

The main conclusions from the present study are:

Using the discrete dipole approximation and the ddscat.4b.1 (Draine and Flatau 1994a) program we have obtained the extinction efficiencies for the porous silicate and graphite grains. For the small silicate porous grains (a = 0.01μ and 0.05μ) the enhancement in the extinction is indicated in the entire wavelength range of consideration of this paper i.e. 0.55μm to 0.20μm. For the grains with a = 0.1μ the enhancement in the extinction is indicated between 0.25μm and 0.20μm. For the large grains with a = 0.2μ the enhancement in the extinction is indicated in the wavelength range 0.55μm-0.25μm but beyond 0.25μm the effect of porosity on the extinction is not clear. For the graphite grains the effect of porosity on the extinction is clearly seen for all the sizes considered here (viz. a = 0.01, 0.05, 0.1, 0.2μ). The extinction in the wavelength range 0.55μm-0.23μm is enhanced with porosity whereas in the absorption band in the wavelength range of 0.23μm-0.20μm the extinction for the porous grains is lower than that is obtained for the solid grains. The wavelength of the peak extinction in graphite seems to be shifting with the porosity. In the present study, we have restricted the maximum number of dipoles to (N=4088), as it was sufficient to satisfy the validity criteria for DDA for all the grain sizes and the wavelengths considered in this study except perhaps for the large silicate grains (a = 0.20μ) at wavelengths between 0.25μm and 0.20μm. As an application of these porous grain models we use the extinction efficiencies of the porous silicate and graphite grains to evaluate the interstellar extinction curve and find it to fit well with the average observed extinction curve. Though these models are not unique, we only wish to illustrate how the porous grains can reproduce the average observed interstellar extinction curve. Further calculations in the infrared as well as in the uv region are required to help put more constraints on the grain models.

Acknowledgements. We thank Prof.B.T.Draine for providing the DDSCAT.4b.1 program. We also take this opportunity to convey our thanks to the referee Prof. J. M. Perrin for giving us extremely useful suggestions/comments. Finally the first author (DBV) thanks Physical Research Laboratory, Ahmedabad for providing the computational and other facilities.

References

Asano S. and Yamamoto G.,(1975), Appl. Optics, 14, 29
Bevington, P. R., (1969), Data Reduction and Error Analysis for the Physical Sciences (New York: McGraw-Hill), Chapter 1-4
Bohren C.F. and Huffman D.R.,(1983),Absorption and Scattering of Light by Small Particles, John Wiley, New York.
Draine B.T., (1985), A & A (supp), 57, 587
Draine B.T., (1987), Princeton Observatory Preprint No. 213
Draine B.T., (1988), Ap. J., 333, 848
Draine B.T. and Flatau P.J., (1994a), User Notes for DDSCAT.4b.1
Draine B.T. and Flatau P.J., (1994b), J. O. S. A., 11, 1491
Draine B.T. and Goodman J.,(1993), ApJ, 405, 685
Greenberg J.M., (1960), J. Appl. Phys., 31, 82
Greenberg J.M., (1990), in Comet Halley, Vol.2, Ed. Mason J., 105

Hage J.I. and Greenberg J.M., (1990), ApJ, 361, 251
Henning Th. and Stognienko R., (1993), A & A, 280, 609
Hong S.S. and Greenberg J.M., (1980), A & A, 88, 194
Jones A.P., (1988), MNRAS, 234, 209
Lumme K. and Rahola J., (1994), ApJ, 415, 653
Mathis J.S., Rumpl W. and Nordsieck K.H., (1977), ApJ, 217, 425
Mathis J.S. and Whiffen G., (1989), ApJ, 341, 808
Perrin J.M. and Lamy P.L., (1990), ApJ, 364, 146
Perrin J.M. and Sivan J.P., (1990), A & A, 228, 238
Purcell E.M. and Pennypacker C.R., (1973), ApJ, 186, 705
Rouleau F. and Martin P.G.,(1993), ApJ, 414, 803
Savage and Mathis., (1979), Ann. Rev. A & A, 17, 73
Seaton M.J., (1979), MNRAS, 187, 73
Vaidya D.B. and Desai J.N., (1996), A.S.P. Conf. Series, 1996, 104,433
Vaidya D.B. and Gupta R., (1997), in preparation
Van de Hulst H.C., (1981), in Light Scattering by Small Particles, Dover, N.Y.
Wolff M.J.,Clayton G.C. and Meade M.R., (1993), ApJ, 403, 722
Wolff M.J.,Clayton G.C.,Martin P.G. and Sculte-Ladback R.E., (1994), ApJ, 423, 412

This article was processed by the author using Springer-Verlag LaTeX A&A style file *L-AA* version 3.