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Toward understanding the 3.4 μm and 9.7 μm extinction feature variations from the local diffuse interstellar medium to the Galactic center

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Observationally, both the 3.4 μm aliphatic hydrocarbon C–H stretching absorption feature and the 9.7 μm amorphous silicate Si–O stretching absorption feature show considerable variations from the local diffuse interstellar medium (ISM) to Galactic center (GC): both the ratio of the visual extinction (A_V) to the 9.7 μm Si–O optical depth ($\Delta\tau_{9.7\,\mu\mathrm{m}}$) and the ratio of A_V to the 3.4 μm C–H optical depth ($\Delta\tau_{3.4\,\mu\mathrm{m}}$) of the solar neighborhood local diffuse ISM are about twice as much as that of the GC. In this work, we try to explain these variations in terms of a porous dust model consisting of a mixture of amorphous silicate, carbonaceous organic refractory dust (as well as water ice for the GC dust).

Key words: Interstellar extinction, dust, silicate, aliphatic hydrocarbon, infrared astronomy

1. Introduction

The interstellar extinction law is one of the primary sources of information about the interstellar grain population, and one often obtains direct information on the composition of interstellar dust from spectral features in extinction (Draine 2003). These spectral features also provide strong constraints on interstellar grain models. With the advent of ground-based and space borne infrared (IR) telescope facilities, the IR extinction continuum and absorption features have been receiving increasing attention and play an essential role in recovering the intrinsic energy distribution of celestial objects and inferring the characteristics of interstellar dust.

In the interstellar extinction curve, the 2175 Å bump is outstanding in the ultraviolet (UV), while in the IR, there are a number of prominent absorption features as well: (1) the ubiquitous 9.7 μm and 18 μm features respectively due to the Si–O stretching and O–Si–O bending modes of amorphous silicates; (2) the 3.4 μm feature due to the C–H stretching mode of aliphatic hydrocarbon dust, as ubiquitously present in the ISM of the Milky Way and external galaxies as the 9.7 μm and 18 μm silicate bands, except this feature is not seen in dense molecular clouds (see Pendleton 2004 for a review); (3) the 3.3 μm and 6.2 μm weak features seen in both local sources and GC sources (Schutte et al. 1998; Chiar et al. 2000), respectively due to the C–H stretching and C–C stretching modes of polycyclic aromatic hydrocarbon (PAH) molecules; and (4) in dense clouds the 3.1 μm feature due to the O–H stretching mode of water ice as well as a number of weaker features at 4.68 μm (CO), 7.68 μm (CH_4), 4.28 μm, 15.2 μm (CO_2), 3.54 μm, 9.75 μm (CH_3OH).

The 9.7 μm silicate extinction profile varies among different sightlines; in particular, its optical depth $\Delta\tau_{9.7\,\mu\mathrm{m}}$ (relative to the visual extinction A_V) shows considerable variations from the local diffuse ISM (LDISM) to the Galactic center (GC): $A_V/\Delta\tau_{9.7\,\mu\mathrm{m}} \approx 18.2$ for LDISM differs from that of the GC ($A_V/\Delta\tau_{9.7\,\mu\mathrm{m}} \approx 8.4$) by a factor of ~ 2.2 (see Table 1; also see Draine 2003).[1] Roche & Aitken (1985) argued that $A_V/\Delta\tau_{9.7\,\mu\mathrm{m}}$ varies because there are fewer carbon stars in the central regions of the Galaxy and the production of carbon-rich dust may be substantially reduced compared with the outer Galactic disk. However, as shown in Table 1, the 3.4 μm C–H feature of aliphatic hydrocarbon dust also exhibits a similar behavior: $A_V/\Delta\tau_{3.4\,\mu\mathrm{m}} \approx 274$ for LDISM is higher than that of the GC ($A_V/\Delta\tau_{3.4\,\mu\mathrm{m}} \approx 146$) by a factor of ~ 1.9 (see Table 1). If the argument of Roche & Aitken (1985) was valid, one would expect a much smaller $A_V/\Delta\tau_{3.4\,\mu\mathrm{m}}$ ratio in the LDISM than that of the GC. Sandford et al. (1995) tried to quantitatively explain this phenomena by assuming that the abundance of the C–H carrier (relative to other dust components) gradually increases from the

[1]Cohen et al. (1989) argued that the observed 9.7 μm dip on which $\Delta\tau_{9.7\,\mu\mathrm{m}}$ was measured may be partly contributed by PAHs (i.e. the red tails of the PAH 7.7 μm and 8.6 μm bands and the blue tail of the 11.3 μm band could form an "artificial" 10 μm dip). But this would result in a smaller $\Delta\tau_{9.7\,\mu\mathrm{m}}$ for the GC and a larger $\Delta\tau_{9.7\,\mu\mathrm{m}}$ for the LDISM (since the PAH emission is more likely to present in the LDISM while toward the GC PAHs are seen in absorption), quite on the opposite.

Table 1. Observational values of $A_V/\Delta\tau_{3.4\,\mu\mathrm{m}}$ and $A_V/\Delta\tau_{9.7\,\mu\mathrm{m}}$

	$A_V/\Delta\tau_{3.4\,\mu\mathrm{m}}$	$A_V/\Delta\tau_{9.7\,\mu\mathrm{m}}$	References
Local diffuse ISM	240±40		Sandford et al. 1991
	250±40		Pendleton et al. 1994
	333	16.7	Adamson et al. 1990
		18.5	Roche & Aitken 1984
		18.5±2	Draine 2003
		19.2±0.6	Bowey et al. 2004
mean for local ISM	274	18.2	
Galactic Center	150±20		Pendleton et al. 1994
	143	8.31	McFadzean et al. 1989
		8±3	Becklin et al. 1978
		9	Roche & Aitken 1985
mean for GC	146	8.4	

local ISM toward the GC.[2] However, this requires that amorphous silicate dust and aliphatic hydrocarbon dust should not be solely responsible for the visual extinction. If one has to invoke an additional dust component (most likely a population of carbon dust which does not show the characteristic 3.4 μm feature, say, graphite) making an appreciable contribution to A_V, one would encounter a severe carbon budget problem (see Snow & Witt 1996).

Along the lines of sight toward the GC, there are dense molecular clouds.[3] In cold, dense molecular clouds, interstellar dust is expected to grow through coagulation (as well as accreting an ice mantle) and the dust is likely to be porous (Jura 1980). In this work, we demonstrate that the observed variations of $A_V/\Delta\tau_{9.7\,\mu\mathrm{m}}$ and $A_V/\Delta\tau_{3.4\,\mu\mathrm{m}}$ from the LDISM to the GC could be explained in terms of composite porous dust.

2. Model

We consider a composite porous dust model consisting of amorphous silicate, carbon, and vacuum (in dense clouds silicate dust and carbon dust are coated with water ice). We take the optical constants of Draine & Lee (1984) for amorphous silicate, of Li & Greenberg (1997) for carbonaceous organic refractory (to represent the carbon dust component), of Li & Greenberg (1998) for water ice. The mass densities of silicate dust, organic refractory dust and ice are taken to be $\rho_{\rm sil} \approx 3.5\,{\rm g\,cm^{-3}}$, $\rho_{\rm carb} \approx 1.8\,{\rm g\,cm^{-3}}$ and $\rho_{\rm ice} \approx 1.2\,{\rm g\,cm^{-3}}$, respectively. We take the mass ratio of organic refractory dust to silicate dust to be $m_{\rm carb}/m_{\rm sil} = 0.7$ and the mass ratio of water ice to organic refractory dust and silicate dust to be $m_{\rm ice}/\left(m_{\rm carb}+m_{\rm sil}\right) = 0.8$, as inferred from the cosmic abundance constraints (see Appendix A of Li & Lunine 2003a).

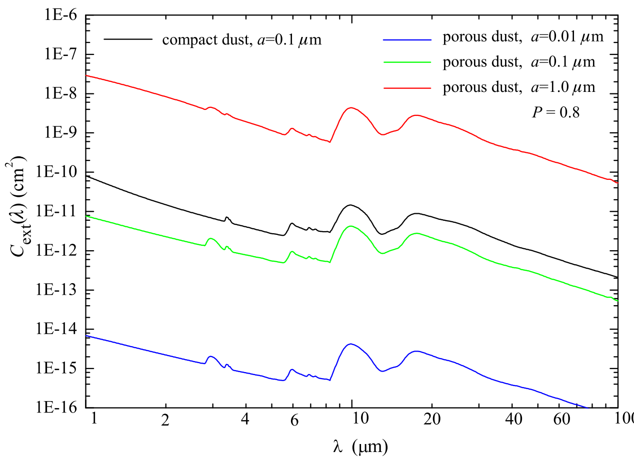

Fig. 1. Extinction cross sections $C_{\rm ext}(\lambda)$ of different types of dust. The 3.1 μm water ice O–H feature shows up in the extinction profiles of porous dust.

For the dust in the local diffuse ISM, we assume the dust to be a solid compact mixture of amorphous silicate and organic refractory materials with $m_{\rm carb}/m_{\rm sil} = 0.7$. We take the dust size to be $a = 0.1\,\mu$m, the typical grain size for the dust in the diffuse ISM (see Draine 1995). For the dust in the dense molecular clouds along the lines of sight toward the GC, we assume that silicate dust and organic refractory dust are equally coated with an ice layer and then form a

[2]They also pointed out that the C–H and Si–O carriers may be coupled, perhaps in the form of silicate-core organic-mantle grains. This idea is challenged by the nondetection of the 3.4 μm feature polarization along sightlines where the 9.7 μm feature polarization is detected (Adamson et al. 1999, Chiar et al. 2006; also see Li & Greenberg 2002). It is possible that the 3.4 μm feature may be not produced by a carrier residing in a mantle on a silicate core but by very small (unaligned) grains (Chiar et al. 2006).

[3]The sightline toward the Galactic center source Sgr A* suffers about $\sim$30 mag of visual extinction (e.g. see McFadzean et al. 1989), to which molecular clouds may contribute as much as $\sim$10 mag (Whittet et al. 1997).

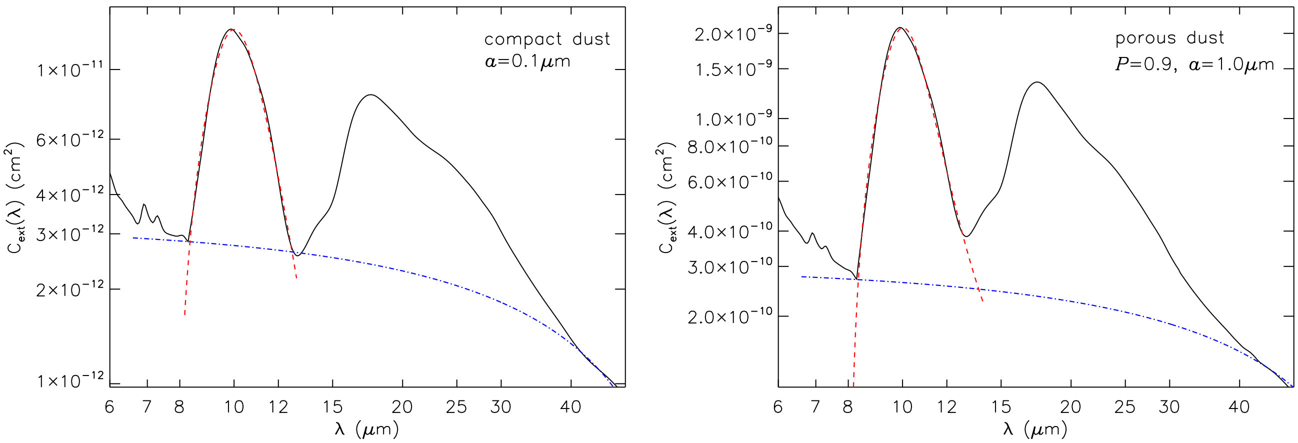

Fig. 2. Schematic illustration of obtaining $\Delta C_{\rm ext}(9.7\,\mu{\rm m})$, the excess 9.7 μm extinction cross section above the continuum. It is obtained by (1) fitting the 9.7 μm model profile with a Drude function and subtracting the continuum which is fitted with a six-order polynomial, (2) integrating the continuum-subtracted extinction profile (which is approximated by a Drude function) over wavelength, and finally (3) dividing the integrated value with the width of the interstellar 9.7 μm silicate absorption feature.

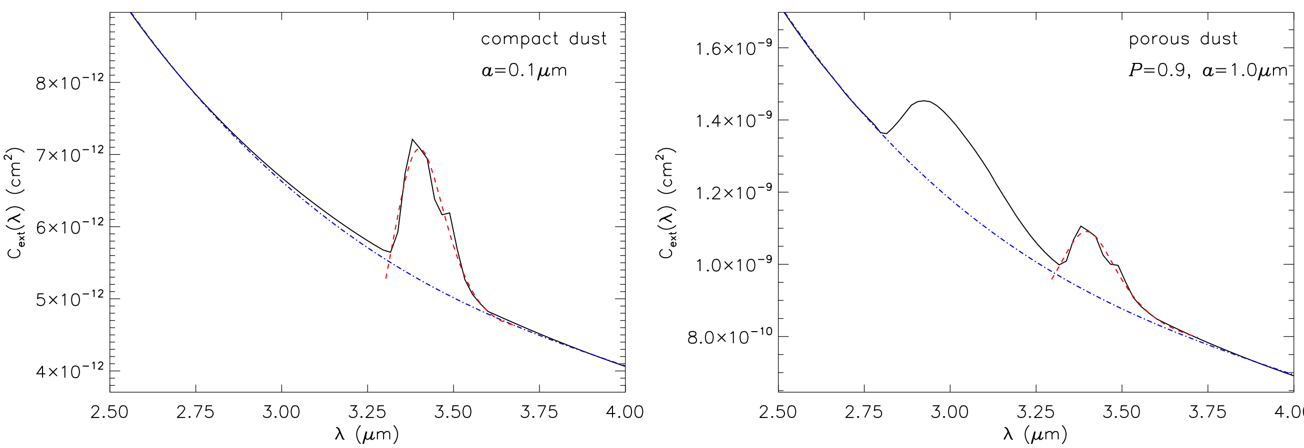

Fig. 3. Same as Figure 2 but for the 3.4 μm feature. In the right panel, the 3.1 μm water ice O–H feature shows up in the extinction profile of porous dust.

porous aggregate (see Li & Lunine 2003b). For porous dust, a key parameter is the porosity P (or fluffiness; the fractional volume of vacuum in a grain). We will consider a range of porosities. We assume all grains are spherical in shape; the porous grain size a is defined as the radius of the sphere encompassing the entire porous aggregate. In order to find suitable porosity P and dust size a for the dust in the dense molecular clouds to reproduce the observed $A_V/\Delta\tau_{9.7\,\mu{\rm m}}$ and $A_V/\Delta\tau_{3.4\,\mu{\rm m}}$ ratios toward the GC, we leave both P and a adjustable.

We use Mie theory in combination with the Maxwell-Garnett and Bruggeman effective medium theories (Bohren & Huffman 1983; see eqs.7–9 of Li & Lunine [2003b] and Kimura et al. 2008b) to calculate the optical properties of composite porous grains. This approach is valid for computing the integral scattering characteristics (e.g. extinction, scattering, absorption cross sections, albedo and asymmetry parameter; see Hage & Greenberg 1990, Wolff et al. 1994).

For illustration, we plot in Figure 1 the 1–100 μm extinction cross sections $C_{\rm ext}(\lambda)$ of compact dust (for the local diffuse ISM) and porous dust (for dense clouds toward the GC). For a given dust size, both A_V and $\Delta\tau_{3.4\,\mu{\rm m}}$, $\Delta\tau_{9.7\,\mu{\rm m}}$ decrease with the porosity P, although the degree of decrease is somewhat less significant for $\Delta\tau_{3.4\,\mu{\rm m}}$ and $\Delta\tau_{9.7\,\mu{\rm m}}$ than for A_V (thus $A_V/\Delta\tau_{3.4\,\mu{\rm m}}$ and $A_V/\Delta\tau_{9.7\,\mu{\rm m}}$ decrease moderately with the increase of P; see Table 2). This is because with the same size, a porous grain contains less dust material than its solid counterpart. The effective dielectric functions of porous dust are reduced. In the IR the extinction for dust of $\sim 0.1\,\mu$m is dominated by absorption (i.e. in the Rayleigh regime) and is roughly proportional to the imaginary parts of the dielectric functions (see Li 2008). Therefore porous dust produces smaller $\Delta\tau_{3.4\,\mu\rm m}$ and $\Delta\tau_{9.7\,\mu\rm m}$ than its solid counterpart of the same size. In the optical, both absorption and scattering are important. The introduction of vaccum leads to a reduction of the dielectric functions of the dust which will decrease both the absorption and scattering.

For models consisting of single-sized dust, the ratio of A_V to the optical depth of the 9.7 μm silicate feature is simply $A_V/\Delta\tau_{9.7\,\mu\rm m} \approx 1.086\,C_{\rm ext}(V)/\Delta C_{\rm ext}(9.7\,\mu\rm m)$, where $C_{\rm ext}(V)$ is the extinction cross section at V band ($\lambda = 5500\,\rm Å$), $\Delta C_{\rm ext}(9.7\,\mu\rm m)$ is the *excess* extinction cross section of the 9.7 μm feature above the continuum, and the factor "1.086" arises from the conversion of extinction (in magnitude) to optical depth. We obtain $\Delta C_{\rm ext}(9.7\,\mu\rm m)$ by integrating the 9.7 μm model extinction profile (with the continuum subtracted) over wavelength (see Fig. 2 for illustration) and then dividing the integrated value with the width of the interstellar 9.7 μm silicate absorption feature. The same procedure is applied to the 3.4 μm feature to calculate $\Delta C_{\rm ext}(3.4\,\mu\rm m)$ so as to obtain $A_V/\Delta\tau_{3.4\,\mu\rm m}$ (see Fig. 3 for illustration).

3. Results and Discussion

We calculate $A_V/\Delta\tau_{3.4\,\mu\rm m}$ and $A_V/\Delta\tau_{9.7\,\mu\rm m}$ for various dust models with a range of porosities and dust sizes. The results are tabulated in Table 2. For a given dust size $a = 0.1\,\mu\rm m$, porous dust results in smaller $A_V/\Delta\tau_{3.4\,\mu\rm m}$ and $A_V/\Delta\tau_{9.7\,\mu\rm m}$ values than compact dust (see §2). This is encouraging that porous dust which is likely present in the dense molecular clouds along the sightlines toward the GC indeed is on the right track to account for the observed $A_V/\Delta\tau_{3.4\,\mu\rm m}$ and $A_V/\Delta\tau_{9.7\,\mu\rm m}$ variations from the local diffuse ISM to the GC. More specifically, from Table 2 we see that the dust with $P \sim 0.8 - 0.9$ and $a \sim 0.5 - 1\,\mu\rm m$ can approximately explain the observed variations of $A_V/\Delta\tau_{3.4\,\mu\rm m}$ and $A_V/\Delta\tau_{9.7\,\mu\rm m}$ (by a factor of ~ 2) from the local diffuse ISM to the GC. Both high porosities ($P \sim 0.8 - 09$) and large sizes ($a \geq 0.5\,\mu\rm m$) are required for the GC dust to account for the lower $A_V/\Delta\tau_{3.4\,\mu\rm m}$ and $A_V/\Delta\tau_{9.7\,\mu\rm m}$ ratios.

In Figure 4, we show $A_V/\Delta\tau_{3.4\,\mu\rm m}$ and $A_V/\Delta\tau_{9.7\,\mu\rm m}$ as a function of dust size for $P = 0.8,\,0.9,\,0.95$. It is clearly seen that for a given porosity, the variation of $A_V/\Delta\tau_{3.4\,\mu\rm m}$ with dust size exhibits a tendency similar to that of $A_V/\Delta\tau_{9.7\,\mu\rm m}$. This suggests that with a dust size distribution taken into account, we would still maintain the variation tendency. For small, highly porous grains ($a < 0.05\,\mu\rm m$), $A_V/\Delta\tau_{3.4\,\mu\rm m}$ and $A_V/\Delta\tau_{9.7\,\mu\rm m}$ are nearly independent of size since they are more or less in the Rayleigh regime in the optical-IR and therefore $A_V/V_{\rm dust}$, $\Delta\tau_{3.4\,\mu\rm m}/V_{\rm dust}$ and $\Delta\tau_{9.7\,\mu\rm m}/V_{\rm dust}$ are independent of grain size (where $V_{\rm dust}$ is the dust volume). The visual extinction A_V reaches its maximum at $a \sim \lambda/\left[2\pi\,a\,(n-1)\right]$ (where n is the real part of the refractive index of the porous dust at wavelength λ; see Li 2008). At even large sizes, while A_V reaches a constant (i.e. in the geometric optics regime) $\Delta\tau_{3.4\,\mu\rm m}$ and $\Delta\tau_{9.7\,\mu\rm m}$ increase

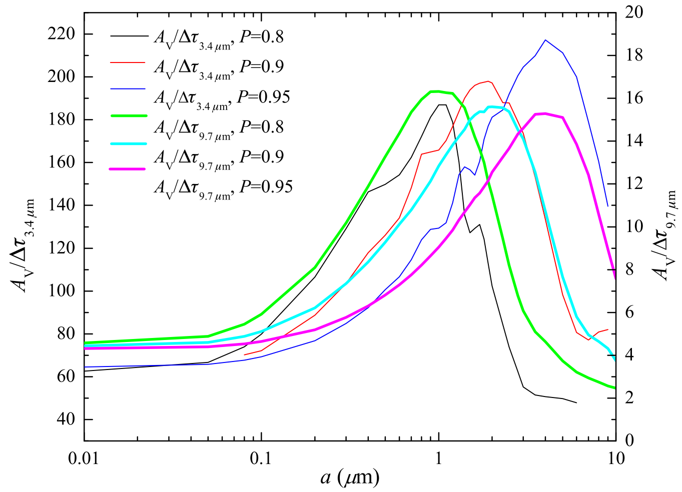

Fig. 4. Variations of $A_V/\Delta\tau_{3.4\,\mu\rm m}$ and $A_V/\Delta\tau_{9.7\,\mu\rm m}$ with dust size.

with a (till they reach their respective peak values). This explains why $A_V/\Delta\tau_{3.4\,\mu\rm m}$ and $A_V/\Delta\tau_{9.7\,\mu\rm m}$ decrease with a after they reach their peak values.

For $A_V/\Delta\tau_{3.4\,\mu\rm m}$, our model with $m_{\rm carb}/m_{\rm sil} = 0.7$ (and $P = 0.8$, $a = 0.5 - 1.5\,\mu\rm m$) is consistent with the observed factor-of-two variations in the local ISM and toward the GC (see Tables 1,2). However, the model values of $A_V/\Delta\tau_{9.7\,\mu\rm m}$ for both the diffuse ISM dust ($A_V/\Delta\tau_{9.7\,\mu\rm m} \approx 38.2$) and the GC dust ($A_V/\Delta\tau_{9.7\,\mu\rm m} \approx 16.3$) are higher by a factor of $\sim$1.5–2 than that observed in the local diffuse ISM ($A_V/\Delta\tau_{9.7\,\mu\rm m} \approx 18.2$) and the GC ($A_V/\Delta\tau_{9.7\,\mu\rm m} \approx 8.4$). This discrepancy may result from the underestimation of the silicate mass fraction.

With an increased silicate mass fraction, say, $m_{\rm carb}/m_{\rm sil} = 0.5$ which is consistent with the *in situ* measurements of comet Halley (Jessberger & Kissel 1991) and widely adopted in cometary dust modeling (Greenberg 1998; Greenberg & Li 1999; Kimura et al. 2006, 2008a; Kolokolova et al. 2004, Kolokolova & Kimura 2008; Mann et al. 2006), we obtain $A_V/\Delta\tau_{3.4\,\mu\rm m} \approx 252$ and $A_V/\Delta\tau_{9.7\,\mu\rm m} \approx 27.1$ for the local ISM (assuming compact dust), and $A_V/\Delta\tau_{3.4\,\mu\rm m} \approx 154$ and $A_V/\Delta\tau_{9.7\,\mu\rm m} \approx 11.3$ for the GC (assuming porous dust). These values are closer to that observed. It is expected that with a smaller $m_{\rm carb}/m_{\rm sil}$ (i.e. a larger silicate mass fraction), one would obtain a smaller $A_V/\Delta\tau_{9.7\,\mu\rm m}$ while $A_V/\Delta\tau_{3.4\,\mu\rm m}$ does not change much. Thus the observed variations of $A_V/\Delta\tau_{3.4\,\mu\rm m}$ and $A_V/\Delta\tau_{9.7\,\mu\rm m}$ from the local ISM to the GC could be explained. It is worth noting that, based on a detailed analysis of the GC 5–8 μm absorption spectra obtained from the Kuiper Airborne Observatory, Tielens et al. (1996) argued that silicate dust may contribute as much as 60% of the interstellar dust volume. This would translate to $m_{\rm carb}/m_{\rm sil} \approx 0.34$ if we assume that the remaining 40% of the interstellar dust volume is all from the 3.4 μm C–H feature carrier (which is indeed a very generous assumption).

Table 2. $A_V/\Delta\tau_{3.4\,\mu m}$ and $A_V/\Delta\tau_{9.7\,\mu m}$ calculated for various dust models

Dust Model	Porosity P	size (μm)	$A_V/\Delta\tau_{3.4\,\mu m}$	FWHM (μm)	$A_V/\Delta\tau_{9.7\,\mu m}$	FWHM (μm)
diffuse ISM Dust[a]	0	0.1	243	0.14	38.2	2.18
	0.1	0.1	216	0.14	32.3	2.19
	0.2	0.1	192	0.14	27.3	2.19
GC Dust	0.8	0.1	80	0.14	5.9	2.18
		0.5	150	0.15	13.3	2.18
		1.0	186	0.17	16.3	2.18
		1.5	127	0.19	14.8	2.21
		2.0	102	0.19	11.5	2.26
		3.0	55	0.20	6.1	2.34
	0.9	0.1	72	0.14	5.1	2.08
		0.5	126	0.14	9.3	2.08
		1.0	165	0.15	12.8	2.09
		1.5	193	0.16	15	2.11
		2.0	198	0.15	15.6	2.11
		3.0	174	0.16	14.1	2.16

[a]

Diffuse ISM dust is taken to be a mixture of amorphous silicate and organic refractory substance.

Admittedly, the proposed explanation is oversimplifed. In the future we will consider more realistic models in which more dust species (e.g. hydrogenated amorphous carbon with a range of C/H ratios), the distribution of dust along the line of sight toward the GC (e.g. see Sandford et al. 1995), a distribution of dust sizes, and the possible porous nature of the diffuse ISM dust (e.g. see Mathis & Whiffen 1989) will be considered.

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