

On the crystallinity of silicate dust in the interstellar medium

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ABSTRACT

An accurate knowledge of the mineralogy (chemical composition and crystal structure) of the silicate dust in the interstellar medium (ISM) is crucial for understanding its origin in evolved stars, the physical and chemical processing in the ISM, and its subsequent incorporation into protostellar nebulae, protoplanetary discs and cometary nuclei where it is subjected to further processing. While an appreciable fraction of silicate dust in evolved stars, in protoplanetary discs around pre-main-sequence stars, in debris discs around main-sequence stars and in cometary nuclei is found to be in crystalline form, very recent infrared spectroscopic studies of the dust along the sightline toward the Galactic Centre source Sgr A* placed an upper limit of ~ 1.1 per cent on the silicate crystalline fraction, well below the previous estimates of ~ 5 or ~ 60 per cent derived from the observed $10\text{-}\mu\text{m}$ absorption profile for the local ISM toward Cyg OB2 No. 12. Since the sightline toward Sgr A* contains molecular cloud materials as revealed by the detection of the 3.1- and $6.0\text{-}\mu\text{m}$ water ice absorption features, we argue that by taking into account the presence of ice mantles on silicate cores, the upper limit on the degree of silicate crystallinity in the ISM is increased to $\sim 3\text{--}5$ per cent.

Key words: ISM: clouds – dust, extinction – ISM: lines and bands – Galaxy: centre – infrared: ISM.

1 INTRODUCTION

The mineralogical composition of dust contains important information about its origin and evolution, and may reveal the physical, chemical and evolutionary properties of the astrophysical regions where the dust is found. Silicate, one of the major components of cosmic dust species, is ubiquitously seen in various astrophysical environments, ranging from the Galactic diffuse interstellar medium (ISM), H II regions and the dust torus around active galactic nuclei to dust envelopes around evolved stars, protoplanetary discs around pre-main-sequence stars, debris discs around main-sequence stars, cometary comae and interplanetary space. The chemical composition and crystal structure of silicate grains vary with local environments.

Interstellar spectroscopy provides the most diagnostic information on dust composition. In the infrared (IR), the strongest interstellar spectral features are the 9.7- and $18\text{-}\mu\text{m}$ absorption (or emission) bands which are generally attributed to the Si–O stretching and O–Si–O bending modes, respectively. While the absorption profiles measured in the laboratory for crystalline olivine and pyroxene show many sharp features, in the diffuse ISM, the observed 9.7- and $18\text{-}\mu\text{m}$ silicate features are broad and relatively featureless, suggesting that interstellar silicates are mainly amorphous rather than crys-

talline. Since the crystallinity of silicate dust is intimately connected to the energetic processing occurring in the evolutionary life cycle of dust and depends on the environmental properties, of particular interest to silicate astromineralogy is the abundance of crystalline silicates in different astrophysical environments, especially in the diffuse ISM.

Recently, a number of studies have been made to determine the crystallinity degree of silicates in the diffuse ISM. From the observed $9.7\text{-}\mu\text{m}$ absorption profile for dust in the local ISM toward Cyg OB2 No. 12, Li & Draine (2001) estimated the fraction of Si in crystalline silicates to be ≤ 5 per cent. Demyk et al. (1999) derived an upper limit of $\sim 1\text{--}2$ per cent of crystalline silicates in mass toward two massive protostars. However, Bowey & Adamson (2002) argued that a complex mixture of crystalline silicates (60 per cent by mass) and amorphous silicates (40 per cent by mass) could explain the observed smooth silicate absorption profile at $9.7\text{ }\mu\text{m}$ toward Cyg OB2 No. 12. More recently, Kemper, Vriend & Tielens (2004) placed a more strict constraint of ≤ 1.1 per cent on the crystallinity of interstellar silicates, based on a detailed analysis of the $9.7\text{-}\mu\text{m}$ feature obtained with the Short Wavelength Spectrometer (SWS) on board the *Infrared Space Observatory* (ISO). This upper limit, ~ 1.1 per cent, of crystalline silicates was derived from a direct comparison of the Sgr A* spectrum with theoretical spectra for pure silicates.

However, it is evident from the detection of the 3.1- and $6.0\text{-}\mu\text{m}$ water ice features respectively attributed to the O–H stretching and bending modes that there are molecular cloud materials along the

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line of sight toward Sgr A* (McFadzean et al. 1989; Tielens et al. 1996; Chiar et al. 2000). This is further confirmed by the detection of solid CO₂ absorption toward Sgr A* (Lutz et al. 1996; de Graauw et al. 1996). In order to infer the precise mineralogical composition of dust, we have to take the grain ice mantles into account when interpreting the observed silicate features. Indeed, in this Letter we show that ignoring the ice mantles coating the silicate cores can result in an underestimation of the crystalline degree of silicate dust, by as much as ~3–5 per cent.

The purpose of this work is to address the question of how the ice mantles affect the determination of dust mineralogical composition (i.e. whether and to what degree the inclusion of ice mantles will hide the sharp features of crystalline silicates and lead to an underestimation of the silicate crystallinity), not to model any specific astronomical objects. Therefore, neither the specific choice of silicate dielectric functions nor the precise constituents of the ice mantles would affect our conclusion.

2 VOLUME FRACTION OF WATER ICE

The sightline toward the Galactic Centre source Sgr A* suffers about ~30 mag of visual extinction (e.g. see McFadzean et al. 1989), to which molecular clouds may contribute as much as ~10 mag (Whittet et al. 1997). Except for H₂O features, there are many additional molecular absorption features, attributed to CO₂, NH₃, CO, CH₃OH, CH₄ and other species. These icy molecules might accrete on to the pre-existing silicate core inside dense molecular clouds and form an ice mantle. As for further evolution, the accreted icy grain mantles could be photoprocessed and converted into organic refractory residues (Greenberg et al. 1995).

Assuming that the 3.1- μ m water ice absorption results from the water ice mantles uniformly coating silicate grains which produce the 9.7- μ m absorption, we estimate the volume ratio of the ice mantles to the silicate cores from the observed optical depths $-\tau_{3.1}$ for the 3.1- μ m O–H feature, and $\tau_{9.7}$ for the 9.7- μ m Si–O feature. Let V_{sil} and V_{ice} respectively be the volumes of the silicate cores and the ice mantles. Let $A_{\text{ice}}^{3.1}$ and $A_{\text{sil}}^{9.7}$ be the integrated band strengths for the 3.1- μ m O–H feature and the 9.7- μ m Si–O feature, respectively. For spherical silicate core–ice mantle grains, we use Mie theory (Bohren & Huffman 1983) to obtain $A_{\text{ice}}^{3.1} = \int_{3.1 \mu\text{m}} (C_{\text{ice}}^{3.1}/V) d\lambda$ and $A_{\text{sil}}^{9.7} = \int_{9.7 \mu\text{m}} (C_{\text{sil}}^{9.7}/V) d\lambda$, where $C_{\text{ice}}^{3.1}$ ($C_{\text{sil}}^{9.7}$) is the continuum-subtracted absorption cross-section of the 3.1- μ m (9.7- μ m) ice (silicate) feature, and V is the volume of a spherical grain with radius a . For the Sgr A* sightline, $\tau_{3.1} \approx 0.50$ and $\tau_{9.7} \approx 3.52$ (Chiar et al. 2000). We therefore obtain $V_{\text{ice}}/V_{\text{sil}} = (\tau_{3.1}/\tau_{9.7}) (A_{\text{sil}}^{9.7}/A_{\text{ice}}^{3.1}) \approx 0.55$, assuming that all silicate grains are coated by a layer of ice mantle.¹

3 SPHERICAL GRAINS

We consider three types of dust materials: amorphous olivine, crystalline olivine and pure water ice. We adopt the dielectric functions of Dorschner et al. (1995) for amorphous olivine, of Li & Draine

¹ In reality, a thicker ice mantle would be expected for the silicate dust in the molecular cloud component which contributes about 10 mag to the total ~30 mag of visual extinction toward Sgr A*. An ice mantle as thick as $V_{\text{ice}}/V_{\text{sil}} \approx 7.6$ was implied for the dust in the dense molecular cloud toward the field star Taurus Elias 16 (Bowey, Adamson & Whittet 1998). A thicker ice mantle would hide a larger fraction of crystalline silicates.

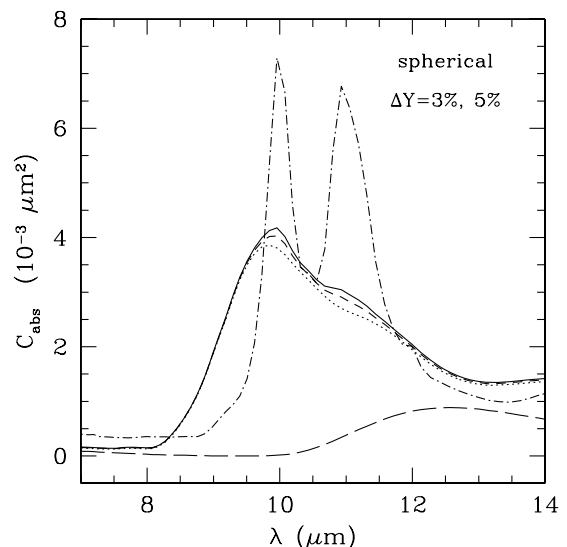


Figure 1. Absorption cross-sections of spherical grains for $V_{\text{ice}}/V_{\text{sil}} = 0.55$. Dotted: amorphous silicate core–ice mantle grains ($C_{\text{abs}}^{\text{am}}$); dot–dashed: crystalline olivine silicate core–ice mantle grains ($C_{\text{abs}}^{\text{cryst}}$); long–dashed: equal-volume ice spheres for the ice mantles; solid: $C_{\text{abs}} = C_{\text{abs}}^{\text{am}} + \Delta Y C_{\text{abs}}^{\text{cryst}}$ where $\Delta Y = 5$ per cent is the crystalline olivine silicate fraction; short–dashed: $C_{\text{abs}} = C_{\text{abs}}^{\text{am}} + \Delta Y C_{\text{abs}}^{\text{cryst}}$ with $\Delta Y = 3$ per cent. Note that water ice produces a shoulder at $\lambda > 11 \mu\text{m}$. This should not be interpreted as a crystalline silicate feature.

(2001) for crystalline olivine, and of Hudgins et al. (1993) for water ice.

We first consider spherical silicate core–water ice mantle grains. We take the silicate core size to be $a_{\text{sil}} = 0.1 \mu\text{m}$, a typical size for interstellar dust. We should note that the choice of an exact grain size is not critical, since in the wavelength range considered here submicron-sized interstellar grains are in the Rayleigh regime. Also because of this, we do not need to consider dust size distributions.

In Fig. 1 we plot the absorption cross-sections for amorphous olivine silicate core–H₂O ice mantle grains and for crystalline olivine silicate core–H₂O ice mantle grains. As shown in Fig. 1, the absence of narrow features near 10.0 and 11.1 μm in the absorption spectrum suggests that the inclusion of water ice mantles would hide up to ~3–5 per cent crystalline mass fraction without being noticed. Note that water ice has a broad absorption band at ~12.2 μm (see Fig. 1; Léger et al. 1983; Hudgins et al. 1993). The inclusion of an ice mantle on silicate dust (no matter whether it is amorphous silicate or crystalline silicate) results in a weak shoulder at $\lambda > 11 \mu\text{m}$. This is noticeable even in the model spectrum of ice-coated pure amorphous silicate dust (see Fig. 1). One should caution that this should not be interpreted as a crystalline silicate feature.

We also consider a model in which only the molecular cloud dust is coated with a layer of ice mantle. If we assume that silicate dust and carbon dust equally contribute to the ~10 mag visual extinction, the volume ratio of the ice mantle to the silicate core for the molecular cloud dust would be $V_{\text{ice}}/V_{\text{sil}} \approx 0.83$. The bare diffuse cloud dust is responsible for the remaining ~20 mag of visual extinction. In Fig. 2 we show the model cross-sections obtained by summing one-third of that produced by the molecular cloud dust and two-thirds of that produced by the diffuse cloud dust. Similarly, ~3–5 per cent crystalline silicate would be hidden because of

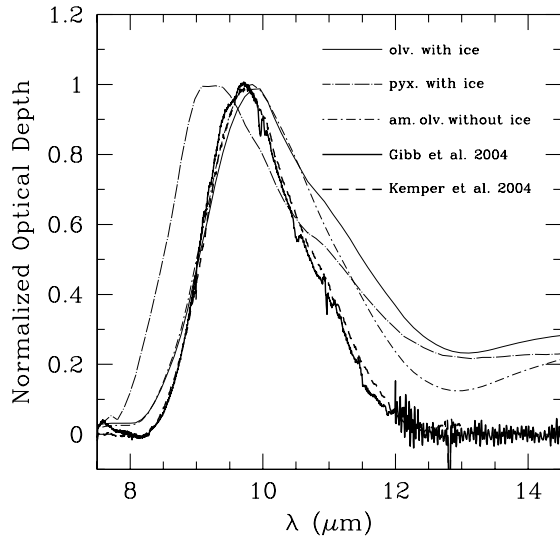


Figure 2. Comparison of the *ISO* spectra of Sgr A* (thick solid: Gibb et al. 2004; thick dashed: Kemper et al. 2004) and the absorption spectra of olivine (thin solid) and pyroxene (dot-long-dashed) spheres with 3 per cent crystallinity, with one-third of the dust coated by a layer of ice mantle ($V_{\text{ice}}/V_{\text{sil}} = 0.83$) and two-thirds of the dust being bare silicates. The $\lambda > 11 \mu\text{m}$ shoulder of the model spectra arises from the ice mantles (also see Fig. 1). Also shown is the absorption spectrum of pure amorphous olivine dust without an ice mantle (dot-short-dashed).

the presence of an ice mantle on the molecular cloud dust toward Sgr A*.²

So far, we have only considered olivine silicate dust. It is possible that there is a considerable amount of pyroxene dust in the ISM (see Bowey & Adamson 2002, and references therein). For illustration, we carry out similar calculations for pyroxene and obtain similar conclusions (see Fig. 2). Again, we should stress that the purpose of this work is not to model any specific astronomical objects, but to investigate the effects of ice mantles on the estimation of silicate crystallinity. We do not expect that either olivine or pyroxene alone could closely reproduce the interstellar silicate absorption feature observed toward Sgr A*. For comparison, we also show in Fig. 2 the *ISO* spectra of Sgr A* obtained by Kemper et al. (2004) and Gibb et al. (2004).³ The fact that, while the 10- μm feature of olivine peaks at relatively longer wavelengths than the observed spectra, pyroxene peaks at wavelengths that are too short, suggests the co-existence of both olivine and pyroxene in the ISM.

² Admittedly, the approach adopted here is simplified. The molecular cloud silicate dust may differ from that of the diffuse cloud [e.g. their 10- μm Si–O features may have different line profiles (particularly line widths) – see Bowey et al. (2001), and references therein]. Their optical properties which are temperature-dependent (Bowey et al. 2001) may also differ from one another since the molecular cloud dust is generally colder than the diffuse cloud dust (e.g. see Greenberg & Li 1996a). Moreover, it is not clear if the molecular cloud silicate dust has the same iron fraction as the diffuse cloud silicate dust [it is well recognized that, as most recently experimentally demonstrated by Bowey et al. (2007), the optical properties of silicate dust are very sensitive to the proportion of iron].

³ We note that the *ISO* spectrum of Sgr A* appears to have a feature at $\sim 6.9 \mu\text{m}$, attributed to crystalline melilite (Bowey & Hofmeister 2005).

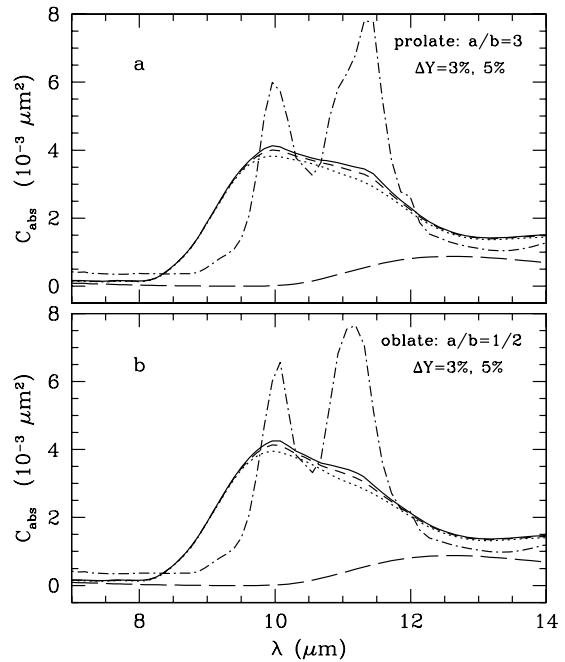


Figure 3. As Fig. 1 but for (a) $a/b = 3$ prolates and (b) $a/b = 1/2$ oblates.

4 SPHEROIDAL GRAINS

The previous analysis assumed spherical grains; however, interstellar grains must be non-spherical, as indicated by interstellar polarization. We now consider a spheroidal shape which can be exactly solved in the Rayleigh limit (see Li, Greenberg & Zhao 2002, and references therein).

We consider confocal silicate core–ice mantle spheroidal grains with a volume-equivalent sphere radius $r_{\text{sil}}^{\text{eq}} = (ab^2)^{1/3} = 0.1 \mu\text{m}$, where a and b are the semi-axes along and perpendicular to the symmetry axis, respectively. Again, we take the volume ratio of the ice mantles to the silicate cores to be $V_{\text{ice}}/V_{\text{sil}} = 0.55$.

We first consider prolate grains with $r_{\text{sil}}^{\text{eq}} = 0.1 \mu\text{m}$ for the silicate cores and $a/b = 3$ for the ice mantles.⁴ In Fig. 3(a) we plot the absorption cross-sections for ice coated–amorphous silicate prolates and ice coated–crystalline prolates. Just like spherical grains, the inclusion of water ice mantles would hide up to ~ 3 per cent crystalline mass fraction without being noticed. Similarly, we perform the same calculations but for oblate grains with $a/b = 1/2$ for ice mantles.⁵ As seen in Fig. 3(b), a crystallinity degree of as much as ~ 3 per cent can be covered by the ice mantles.

5 GRAINS WITH DISTRIBUTIONS OF ELLIPSOIDAL SHAPES

The shape of a spheroidal grain is characterized by its eccentricity e [and the depolarization factors L^{\parallel} and L^{\perp} via equation (4) of Li et al. (2002)]. In Section 4 we considered grains with a single shape. We now consider an average of a distribution of shapes. We assume

⁴ Greenberg & Li (1996b) found that prolates of $a/b = 3$ provide an almost perfect match to the 10- and 18- μm silicate polarization features of the Becklin–Neugebauer (BN) object.

⁵ Lee & Draine (1985) and Hildebrand & Dragovan (1995) found that $a/b = 1/2$ oblates fit well the 3.1- μm ice polarization and the 10- μm silicate polarization of the BN object.

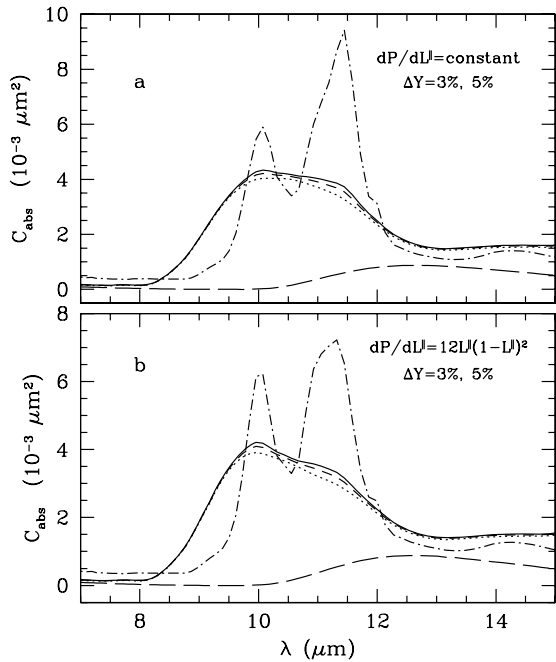


Figure 4. As Fig. 1 but (a) for grains with a uniform distribution of ellipsoidal shapes (i.e. $dP/dL^{\parallel} = \text{constant}$) and (b) for grains with $dP/dL^{\parallel} = 12L^{\parallel} (1 - L^{\parallel})^2$.

two kinds of shape distribution function: (1) $dP/dL^{\parallel} = \text{constant}$, i.e. all shapes are equally probable (Bohren & Huffman 1983); (2) $dP/dL^{\parallel} = 12L^{\parallel} (1 - L^{\parallel})^2$ (Ossenkopf, Henning & Mathis 1992).⁶

Averaging over the shape distribution, we have the resultant absorption cross-section $C_{\text{abs}} = \int_0^1 dL^{\parallel} dP/dL^{\parallel} C_{\text{abs}}(L^{\parallel})$, where $C_{\text{abs}}(L^{\parallel})$ is the absorption cross-section of a particular shape L^{\parallel} [note that L^{\parallel} is for the mantle; the core depolarization factor is derived from equations (4)–(6) of Li et al. (2002)]. Again, we assume confocal geometry for core–mantle grains, with the above dP/dL^{\parallel} (as well as e) applying to the outer surface.

The results are shown in Fig. 4. Similar to spherical grains and grains of a single ellipsoidal shape, with ~ 3 per cent crystalline silicates included, the absorption profiles still do not seem to exhibit the sharp features of crystalline silicates.

6 SUMMARY

We have investigated the effects of ice mantles coating silicate cores of various shapes on the determination of the crystallinity degree of silicates. It is found that for the dust in the line of sight toward the Galactic Centre source Sgr A*, ~ 3 per cent crystalline silicates could be hidden by ice mantles, well exceeding the upper limit of ~ 1.1 per cent of Kemper et al. (2004) derived from the assumption of the absence of dense molecular materials in this line of sight. We take the standard approach by assuming that the silicates are amorphous and then adding in crystalline components. As shown in Kemper et al. (2004), however, the smooth, featureless 10- μm amorphous silicate spectrum allows as much as ~ 2.2 per cent crystalline

silicates (or even higher; see Bowey & Adamson 2002). Therefore the total allowable degree of crystallinity would be ~ 5 per cent, consistent with the earlier estimates of Li & Draine (2001).

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⁶ This distribution peaks at spheres ($L^{\parallel} = L^{\perp} = 1/3$) and is symmetric about spheres with respect to eccentricity e . It drops to zero for the extreme cases: for infinitely thin needles ($a \gg b$) $L^{\parallel} \rightarrow 0$; and for infinitely flattened pancakes ($a \ll b$) $L^{\parallel} \rightarrow 1$.