Where have all the interstellar silicon carbides gone?

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ABSTRACT
The detection of the 11.3\,$\mu$m emission feature characteristic of the Si–C stretch in carbon-rich evolved stars reveals that silicon carbide (SiC) dust grains are condensed in the outflows of carbon stars. SiC dust could be a significant constituent of interstellar dust since it is generally believed that carbon stars inject a considerable amount of dust into the interstellar medium (ISM). The presence of SiC dust in the ISM is also supported by the identification of presolar SiC grains of stellar origin in primitive meteorites. However, the 11.3\,$\mu$m absorption feature of SiC has never been seen in the ISM and oxidative destruction of SiC is often invoked. In this work we quantitatively explore the destruction of interstellar SiC dust through oxidation based on molecular dynamics simulations and density functional theory calculations. We find that the reaction of an oxygen atom with SiC molecules and clusters is exothermic and could cause CO-loss. Nevertheless, even if this is extrapolable to bulk SiC dust, the destruction rate of SiC dust through oxidation could still be considerably smaller than the (currently believed) injection rate from carbon stars. Therefore, the lack of the 11.3\,$\mu$m absorption feature of SiC dust in the ISM remains a mystery. A possible solution may lie in the currently believed stellar injection rate of SiC (which may have been overestimated) and/or the size of SiC dust (which may actually be considerably smaller than submicron in size).

Key words: stars: carbon; circumstellar matter; dust; stars: AGB and post-AGB; stars: mass-loss;

1 INTRODUCTION
Nearly nine decades ago, Wildt (1933) had already argued that solid silicon carbide (SiC) grains might form in N-type stars. It is now well recognized that SiC solids are a major dust species, second to amorphous carbon grains, condensed in the cool atmospheres of mass-losing, carbon-rich asymptotic giant branch (AGB) stars (e.g., see Nanni et al. 2021). This was originally computationally demonstrated over half a century ago by Friedemann (1969) and Gilman (1969) based on molecular equilibrium calculations, and observationally confirmed later by Treffers & Cohen (1974) who, by the first time, detected in two carbon stars, IRC+10216 and IRC+30219, a broad emission band in between 788 and 973 cm\textsuperscript{-1} attributed to SiC dust. Subsequent spectroscopic observations have revealed the widespread presence of SiC grains in carbon stars through the prominent 11.3\,$\mu$m emission feature characteristic of the Si–C stretch of SiC solids (Speck et al. 1997, Mutschke et al. 1999). In addition, presolar SiC grains of stellar origin have also been identified in primitive meteorites based on isotope anomalies (e.g., see Bernatowicz et al. 1987).

Although the exact mass fraction of the condensates in carbon stars which are in the form of SiC is not precisely known and it depends on stellar mass and metallicity (Nanni et al. 2021), radiative transfer modeling of the observed infrared emission of carbon stars has shown that the

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mass ratio of SiC to amorphous carbon could be as much as \( \sim 25\% \) for the Milky Way (e.g., see Groenewegen et al. 1998) and \( \sim 43\% \) for the Large Magellanic Cloud and \( \sim 11\% \) for the Small Magellanic Cloud (Groenewegen et al. 2009, Nanni et al. 2019). Theoretical dust-yield calculations have predicted that the mass fraction of SiC over the total dust (i.e., SiC plus amorphous carbon) produced in carbon stars of an initial mass of 3 \( M_\odot \) around solar metallicity is \( \sim 25\% \) (Nanni et al. 2013; also see Zhukovska & Henning 2013), although different AGB models produce different yields at varying metallicity because of the uncertainties in modelling the mass-loss and third-dredge up processes (e.g., see Nanni et al. 2013, 2014, 2019; Ventura et al. 2012, 2014, 2018).

Solid grains—SiC and amorphous carbon condensed in carbon stars as well as silicates and oxides condensed in oxygen-rich stars will be driven out of the stellar atmospheres and injected into the interstellar medium (ISM) by radiation pressure. If the contribution of carbon stars to the Galactic dust budget is about comparable to that of oxygen-rich stars as generally believed (e.g., see Gehrz 1989), then SiC should be a significant constituent of interstellar dust. However, the nondetection of the characteristic 11.3 \( \mu m \) feature of SiC in the ISM puts this at odds (Whittet et al. 1990). In this work we explore the physical and chemical processes subjected by SiC in the ISM, with special attention paid to the destruction of SiC by oxidation. We apply the Born-Oppenheimer molecular dynamics (BOMD; Helgaker et al. 1990, Uggerud & Helgaker 1992) and density functional theory (DFT; Lee et al. 1988, Becke 1992) to investigate the oxidation reaction pathway related to SiC grains in the ISM. The DFT technique is among the most popular and versatile methods for computational quantum-mechanical modelling of molecules and clusters. In comparison with other quantum chemical methods, DFT simplifies the \( N \)-body problem to a tractable 3\( N \) non-interacting system, which makes DFT more efficient and scalable for large systems. In BOMD simulations, the energies and forces are computed from DFT at quantum levels. Therefore, the BOMD method is more accurate than classical molecular dynamics in which the energies and forces are calculated from empirical formulae or force fields.

2 COMPUTATIONAL METHODS

A typical, submicron-sized SiC grain contains hundreds of millions of atoms (e.g., there are \( \sim 4 \times 10^{10} \) atoms in a spherical SiC grain of radius \( a = 0.1 \mu m \)). Even for SiC nanoparticles, it is extremely expensive to study such systems with \textit{ab initio} methods like BOMD and DFT, requiring tremendous computational power and time. Nevertheless, it is generally believed that SiC grains are built up via bottom-up processes, starting with small gas-phase molecules and successive growth to clusters by molecular additions. Thus, SiC clusters are indispensable for the formation of SiC grains—they are the initial states of SiC grains (e.g., see Gobrecht et al. 2017). Therefore, SiC molecules and clusters could be reasonable candidates or alternatives of SiC grains for molecular dynamics modeling. To this end, we consider the most favourable structures of \( \text{Si}_3\text{C}_3 \) and \( \text{Si}_{12}\text{C}_{12} \) with the former representing a triangle structure (see Figure 4a of Gobrecht et al. 2017, also see Müller et al. 1993) with a high surface-to-volume ratio and the latter exhibiting a spherical structure (see Figure 16a of Gobrecht et al. 2017, also see Watkins et al. 2009) and possessing a low surface-to-volume ratio. \( \text{Si}_3\text{C}_3 \) is selected because it is the smallest cluster with a 3D structure (see Gobrecht et al. 2017) and thus allows us to investigate the reactions for the low-end cluster. \( \text{Si}_{12}\text{C}_{12} \) is selected because of its bumpy-like symmetrical structure which minimizes the considerations of the incident directions of oxygen atoms. \( \text{Si}_{16}\text{C}_{16} \) is also symmetrical in structure but it is computationally more expensive (see Gobrecht et al. 2017).

To evaluate the stability or reactivity of the studied molecule or cluster, we calculate the binding and dissociation energies and transition barriers for each target system, using DFT as implemented in the Gaussian16 package (Frisch et al. 2016). All structures are optimized to their ground states using the 6-311++G(2d,p) basis set. Here the Slater-type atomic orbitals (AOs) are described by “basis functions” and each basis function is described by a sum of several Gaussian functions. To take the intermolecular forces into account, the D3 version of Grimme’s dispersion with Becke-Johnson damping (Grimme et al. 2011) is included in the calculations. Here, “D3” denotes a function of interatomic distances, which contains adjustable parameters that are fitted to the conformational and interaction energies computed using high-level methods.

The vibrational frequencies are calculated under the harmonic oscillator approximation for the optimized geometries. The transition states are estimated based on our molecular dynamics simulations followed by relaxed scanning (with geometry optimization at each point) on the potential energy surface (PES). The transition barrier is calculated as the energy difference between the ground states of the reactant and the transition state. For reactions without transition state, the dissociation energy is computed as the energy difference between the ground states of the reactant and the product. The intermolecular forces are taken into account in all the calculations. The dynamical processes are simulated using BOMD (Helgaker et al. 1990, Uggerud & Helgaker 1992) as implemented in the Gaussian16 package (Frisch et al. 2016). The B3LYP hybrid functional in combination with the 6-31G(d,p) basis set is utilized for the BOMD simulations. For all these simulations, again, the D3 version of Grimme’s dispersion with Becke-Johnson damping (Grimme et al. 2011) is also included.

3 RESULTS

Over 30 years ago, Whittet et al. (1990) searched for the 11.3 \( \mu m \) absorption band of SiC in the diffuse ISM along the line of sight toward the Galactic center. The lack of any spectral evidence for solid SiC led Whittet et al. (1990) to place an upper limit on the abundance of silicon relative to hydrogen (i.e., Si/H) in SiC dust to be at most \( \sim 5\% \) of that \( ^2 \text{Si}_3\text{C}_3 \) has many isomers and the number of structural isomers for \( \text{Si}_{12}\text{C}_{12} \) gets literally astronomical. Here we are confined to the isomers with the lowest energy.
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in silicate dust. They speculated that SiC grains could be destroyed in the ISM by oxidation. Motivated by this, we first model the interaction between a Si3C2 molecule and an incident oxygen atom. This applies to the diffuse ISM where atomic oxygen is the dominant form of gaseous oxygen. The oxidation of SiC solids by O2 has been extensively studied experimentally (e.g., see Ervin 1958) and is not relevant since there is little O2 in the ISM (e.g., see Larsson et al. 2007). In dense molecular clouds where oxygen is mostly locked up in water ice, SiC dust, if present, is expected to be coated by a layer of water ice and oxidation is unlikely since the reaction of SiC with water to produce SiO2 and methane only takes place at a temperature of above 1300°C (e.g., see Park et al. 2014).

As the oxygen atom is much smaller than a SiC cluster or grain, the incident oxygen atom would only influence a few atoms in the target SiC cluster or grain, i.e., the reaction would only take place in an area near the incident atom and depends on the incident direction. Figure 1 shows the BOMD simulations for collisions between a Si3C2 molecule and an incident oxygen atom arriving from three different directions. The simulations demonstrate that, due to the impact of an oxygen atom, CO and SiO molecules can be released rapidly from the molecule within 1 ps. The fragmentation products are highly dependent on the incoming direction of the oxygen atom: if the oxygen atom first collides with a carbon atom, then a CO molecule is formed and ejected, while a SiO-loss would be triggered if the incident oxygen atom first hits a silicon atom.

To better understand the reaction mechanism, DFT calculations for the three reaction scenarios as illustrated in Figure 1 are performed and shown in Figure 2. The corresponding binding energies for O + Si3C2 and dissociation energies for Si3C2–O – CO or Si3C2–O – SiO are illustrated in Figure 2 as well. Most prominently, the reactions for absorbing an oxygen atom to a Si3C2 molecule are exothermic, which release ~7.9 eV energy, depending on the incoming direction of the incident oxygen atom. This is not surprising since association reactions of the form A + B → AB are usually exothermic, as the number of bonds is increased in the product. The energy generated from these reactions will traverse through all of the vibrational modes of the molecule, and the chemical bonds with lower binding energies will be dissociated. Moreover, for the Si3C2O system SiO-loss is also an exothermic reaction, which releases ~1 eV energy. In contrast, CO has a binding energy of ~0.6 eV and therefore it requires ~0.6 eV to eject CO from the Si3C2O system. However, with the much larger amount of energy (~7–9 eV) gained from the first step, such a low binding energy can be easily crossed, leading to a rapid CO-loss.

The collisions between an oxygen atom with larger molecules, e.g., Si12C12, demonstrate a rather different scenario. Figure 3 shows the BOMD simulations for collisions between an oxygen atom and a Si12C12 molecule. No fragmentation is found, instead, the oxygen atom is captured by the Si12C12 molecule. The symmetry of the molecule is broken due to the incoming oxygen atom, which forms two new covalent bonds, one connected with a carbon atom and the other one connected with a silicon atom. The DFT calculations show that, as illustrated in Figure 3 the absorption of an oxygen atom is still an exothermic reaction, which releases ~7.5 eV energy. However, the dissociation of CO and SiO requires ~2.6 eV and ~4.0 eV, respectively. Due to its larger size, Si12C12 could redistribute the excess energy across its degrees of freedom to avoid fragmentation.

Nevertheless, in the diffuse ISM oxygen atoms are far more abundant than SiC grains. It is therefore highly probable that a SiC grain would be hit by multiple oxygen atoms. Figure 4 shows the collisions of Si12C12O with another oxygen atom. The Si12C12O molecule is adopted from the simulation illustrated in Figure 3 but is set to its vibrationally ground state. Two opposite incident directions are simulated for the incoming oxygen atom. In both cases, we see CO loss within 1 ps. This is because, the presence of oxygen atoms (aka O-substituted molecules) decreases the transition energy barriers in the region where the oxygen atom is located, which makes CO-losses highly favorable in comparison to other channels.

4 DISCUSSION

We have shown in §3 that the reaction between an oxygen atom and a SiC molecule is exothermic and would result in CO-loss almost instantly for small SiC molecules, or after the absorption of one or several oxygen atoms for large SiC molecules. Therefore, the destruction rate of SiC in the ISM is essentially determined by the collision rate of oxygen atoms with SiC grains. Let nO be the number density of oxygen atoms in the diffuse ISM, vO be the mean thermal velocity of oxygen atoms, and τcoll be the collision time scale of an oxygen atom with a SiC grain of radius a. The collision rate (in s⁻¹) is τ⁻¹ coll = nO vO πa², where nO ≈ [O/H]gas nH, vO = √(3kBTgas/mO), nH is the hydrogen number density, kB is the Boltzman constant, Tgas is the gas temperature, and nO is the mass of an oxygen atom. If we adopt an interstellar gas-phase oxygen abundance of [O/H]gas = 320 ppm (Meyer et al. 1998), nH = 1 cm⁻³ and Tgas = 100 K for the diffuse ISM, we obtain τcoll ≈ 2.52 × 10⁸ × (0.1 μm/a)² s ≈ 7.99 × (0.1 μm/a)² yr.

Let [Si/H]SiC be the abundance of silicon (relative to hydrogen) tied up in SiC dust in the ISM, ρSiC = 40 be the molecular weight of SiC, ρSiC ≈ 3.2 g cm⁻³ be the mass density of SiC dust, mSiC = (4/3) πa³ρSiC be the mass of a spherical SiC grain of radius a, and M_H be the total interstellar hydrogen gas mass in the Milky Way. The total number of SiC grains would be N_SiC ≈ M_H [Si/H]SiC ρSiC/mSiC ≤ 1.44 × 10⁻³ (0.1 μm/a)³, if we adopt M_H = 4.9 × 10¹⁰ Mʘ (Draine 2011), [Si/H]SiC ≤ 5 ppm (Whittet et al. 1990), and assume that all SiC grains have the same size a. If each collision of an oxygen atom with a SiC grain results in an ejection of CO, we would expect a total SiC dust mass

3 If we take a gas-phase abundance of [O/H]gas = 320 ppm for atomic oxygen in the diffuse ISM (Meyer et al. 1998), and assume that all SiC grains have the same size of a = 0.1 μm and consume an upper limit of 5 ppm of Si/H (Whittet et al. 1990), the number density of oxygen atoms exceeds that of SiC grains by a factor of ∼1.3×10¹⁰.

4 We note that such a mass density is applicable for bulk, macroscopic SiC dust. For small SiC clusters, this would underestimate the actual “size” since small SiC clusters are hollow and not compactly packed (e.g., such a mass density would imply a radius of a ≈ 3.90 Å for a spherical Si12C12 cluster).
Figure 1. Snapshots from molecular dynamics simulations for collisions between an oxygen atom (red ball) and a Si$_3$C$_3$ molecule (in which gray balls represent carbon atoms and yellow balls correspond to silicon atoms), with the oxygen atom arriving from three different directions. The actual time in the simulation is shown beneath each molecular structure. SiO-loss (upper and middle panels) and CO-loss (bottom panel) can be seen on the rightmost panels.

Figure 2. Calculated binding and dissociation energies for reactions between a Si$_3$C$_3$ molecule and an incident oxygen atom arriving at three different positions.

Figure 3. Snapshots from molecular dynamics simulations for collisions between an oxygen atom (red ball) and a Si$_{12}$C$_{12}$ molecule. Due to the high symmetry of Si$_{12}$C$_{12}$, only one incident direction is simulated for the oxygen atom.
The destruction rate of \((dM/dt)_{\text{SiC}}\) from carbon stars, i.e., \((dM/dt)_{\text{SiC}}\) for the destruction rate to exceed the current injection rate of \(\text{SiC}\) grains seen in the Murchison meteorite is in the fraction of \(\sim 10^{-4} \, M_\odot \, \text{yr}^{-1}\). However, the destruction rates of \(\text{SiC}\) dust derived above do not rely on the exact oxidation rates of \(\text{SiC}\) clusters. Therefore, the nondetection of the 11.3 \(\mu\)m absorption feature of \(\text{SiC}\) grains only constitutes a small fraction of the \(\text{SiC}\) dust condensed in AGB stars and then ejected into the ISM. Cristallo et al. (2020) examined the evolution of the AGB stars that polluted the solar system at 4.57 Gyr ago and found that the submicron-sized presolar \(\text{SiC}\) grains predominantly originated from AGB stars with solar metallicity and an initial mass of \(\sim 2 \, M_\odot\). Theoretical calculations have shown that the typical grain size of \(\text{SiC}\) condensed in AGB stars can be dependent on the stellar metallicity and can be smaller than presolar \(\text{SiC}\) grains for stars with metallicities lower than solar (e.g., see Figures 11 and 12 in Nanni et al. 2013, Sect. 5.3 in Ventura et al. 2014, Section 5.3). If the majority of the interstellar \(\text{SiC}\) grains originated from AGB stars are smaller than 0.02 \(\mu\)m or even nano-sized, they will be destroyed more rapidly than the currently believed stellar injection rate since the \(\text{SiC}\) destruction rate increases as the \(\text{SiC}\) dust size decreases. 

\[ (dM/dt)_{\text{SiC}} \propto 1/\alpha. \]

In the diffuse ISM, nano-sized \(\text{SiC}\) grains will be stochastically heated by single, individual stellar photons (Draine & Li 2001) and will emit at the Si–C stretch, presumably at 11.3 \(\mu\)m. Admittedly, the average mass loss rates and total numbers for carbon stars in the Galaxy are not accurately known. The dust production rates of carbon stars depend on the star formation history and metallicity of the galaxy under consideration. The \(\text{SiC}\) mass fraction depends on the metallicity as well. Nanni et al. (2019) found that the \(\text{SiC}\) mass fraction could be up to 43\% of the total dust mass produced by the carbon stars in the Large Magellanic Cloud and 11\% for the Small Magellanic Cloud. However, these are upper limits reached by the dustiest carbon stars, and the spreads in the \(\text{SiC}\) mass fractions are large (see Figure 9 of Nanni et al. 2019). As a consequence, the injection rate of \(\text{SiC}\) dust into the ISM may be much smaller. In Groenewegen et al. (1998) where the spectral energy distribution fitting had been performed for carbon stars in the Galaxy, the \(\text{SiC}\) mass fractions are smaller than 10\% for most (37/44) of their stars. Therefore, the nondetection of the 11.3 \(\mu\)m absorption feature of \(\text{SiC}\) dust could merely be due to a lower injection rate of carbon dust and/or a lower \(\text{SiC}\) mass fraction than that adopted here.

Alternatively, as argued by Draine (1990), interstellar dust is not stardust, i.e., the bulk of the solid material in interstellar grains actually condensed in the ISM rather than in stellar outflows. While carbon stars do eject an appreciable amount of \(\text{SiC}\) dust into the ISM, supernova shock waves destroy \(\text{SiC}\) dust (as well as silicate and carbon dust) at a

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5 While Amari et al. (1994) found that \(\sim 20\%\) of all the presolar \(\text{SiC}\) grains seen in the Murchison meteorite is in the fractions greater than 1 \(\mu\)m and only about 4\% in the fraction less than 0.3 \(\mu\)m, NanoSIMS measurements of the Murchison meteorite with a resolution of \(\sim 50 \, \text{nm}\) revealed that submicron-sized grains are much more abundant than their larger, micron-sized counterparts (see Hoppe et al. 2010).
rate faster than its production (McKee 1989), while grain re-growth in the oxygen-rich ISM unlikely leads to SiC.

Finally, we note that the B3LYP hybrid functional employed here had been shown to outperform for SiC cluster systems (see Byrd et al. 2016). While the triangle isomer of Si$_3$C$_3$ and the spherical isomer Si$_{12}$C$_{12}$ adopted here correspond to their respective global minimum based on DFT calculations made at the M11/cc-pvTZ level of theory (Gobrecht et al. 2017), a different global minimum which is lower than the spherical isomer by $>0.4$ eV was found for Si$_{12}$C$_{12}$ from calculations at the B3LYP/6-311++G(2d,p) level (Byrd et al. 2016). In view of this inaccuracy, we have also calculated the binding energies for the O + Si$_3$C$_3$ system and the O + Si$_{12}$C$_{12}$ system using the M11/cc-pvTZ level of theory applied by Byrd et al. (2016). It is found that the energy difference between M11/cc-pvTZ and B3LYP/6-311++G(2d,p) is at most 0.24 eV for O + Si$_3$C$_3$ and only $\sim 0.01$ eV for O + Si$_{12}$C$_{12}$. Such energy differences will not affect the major results of this work.

5 CONCLUSION

We have utilized molecular dynamics simulations and performed DFT calculations to investigate the oxidation of SiC dust in the ISM. It is found that, although the reaction of an oxygen atom with a SiC molecule is exothermic and could cause CO-loss, the destruction rate of SiC dust through oxidation is considerably smaller than the currently believed stellar injection rate and therefore the nondetection of the 11.3 $\mu$m absorption feature of SiC dust in the diffuse ISM cannot be explained by the destruction of SiC dust through oxidation, unless the currently believed SiC dust injection rate from carbon stars is overestimated and/or interstellar SiC dust is considerably smaller than submicron in size.

ACKNOWLEDGEMENTS

The calculations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC). We thank D. Gobrecht, M.A.T. Groenevagen, P.F. Miceli, A. Nanni, D.J. Singh, X.J. Yang and the anonymous referees for very helpful suggestions. CYX is supported in part by the Talents Recruiting Program of Beijing Normal University and the NSFC Grant No.91952111. A.L. is supported in part by NSF AST-1816411 and NASA 80NSSC19K0572.

DATA AVAILABILITY

The data underlying this article will be shared on reasonable request to the corresponding authors.

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