FORMATION OF SiC GRAINS IN PULSATION-ENHANCED DUST-DRIVEN WIND AROUND CARBON-RICH ASYMPTOTIC GIANT BRANCH STARS

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ABSTRACT

We investigate the formation of silicon carbide (SiC) grains in the framework of dust-driven wind around pulsating carbon-rich asymptotic giant branch (C-rich AGB) stars to reveal not only the amount but also the size distribution. Two cases are considered for the nucleation process: one is the local thermal equilibrium (LTE) case where the vibration temperature of SiC clusters $T_v$ is equal to the gas temperature as usual, and another is the non-LTE case in which $T_v$ is assumed to be the same as the temperature of small SiC grains. The results of the hydrodynamical calculations for a model with stellar parameters of mass $M_\ast = 1.0 M_\odot$, luminosity $L_\ast = 10^4 L_\odot$, effective temperature $T_{\text{eff}} = 2600$ K, C/O ratio = 1.4, and pulsation period $P = 650$ days show the following: in the LTE case, SiC grains condense in accelerated outflowing gas after the formation of carbon grains, and the resulting averaged mass ratio of SiC to carbon grains of $\sim 10^{-8}$ is too small to reproduce the value of $0.01–0.3$, which is inferred from the radiative transfer models. On the other hand, in the non-LTE case, the formation region of the SiC grains is more internal and/or almost identical to that of the carbon grains due to the so-called inverse greenhouse effect. The mass ratio of SiC to carbon grains averaged at the outer boundary ranges from 0.098 to 0.23 for the sticking probability $\alpha_s = 0.1–1.0$. The size distributions with the peak at $\sim 0.2–0.3 \, \mu m$ in radius cover the range of size derived from the analysis of the presolar SiC grains. Thus, the difference between the temperatures of the small cluster and gas plays a crucial role in the formation process of SiC grains around C-rich AGB stars, and this aspect should be explored for the formation process of dust grains in astrophysical environments.

Key words: circumstellar matter – dust, extinction – stars: AGB and post-AGB – stars: winds, outflows

1. INTRODUCTION

Presolar silicon carbide (SiC) is the abundant and well-studied dust species among presolar grains extracted from meteorites. Based on the isotopic compositions of C, N, Si, and Al, presolar SiC grains are classified into six categories named “mainstream,” A, B, X, Y, and Z grains (e.g., see, Ott 2010 for a review). Among them, the mainstream grains populating about 90% of the presolar SiC grains have been considered to have originated in carbon-rich asymptotic giant branch (C-rich AGB) stars from the isotopic compositions of C, N, and Si (Zinner et al. 1987; Hoppe et al. 1994) and the s-process signatures in the noble gases as well as in the heavy elements (Hoppe & Ott 1997). Amari et al. (1994) have reported that SiC grains extracted from the Murchison meteorite have a log-normal size distribution with the peak at $\sim 0.4 \, \mu m$ in diameter, and 70% of them by number have diameters ranging from 0.3 to 0.7 $\mu m$ (Daulton et al. 2003). Although it was reported that SiC grains are more fine grained in other meteorites than in the Murchison (see Russell et al. 1997), a significant fraction of presolar SiC grains are larger than 0.3 $\mu m$ in diameter (see Hoppe & Zinner 2000). Thus, submicron-sized SiC grains are expected to form around C-rich AGB stars. The presence of SiC grains in C-rich AGB stars was confirmed from the emission feature around 11.3 $\mu m$ (Hackwell 1972; Treffers & Cohen 1974; Goebel et al. 1980), which was prior to the discovery of presolar SiC grains (Bernatowicz et al. 1987). Also, the absorption feature attributed to the SiC grains was observed in several extreme carbon stars (Jones et al. 1978; Speck et al. 1997, 2009). The radiative transfer models fitting the observed spectral energy distributions (SEDs), including the spectral feature attributed to the SiC grains, have estimated the mass ratio of SiC to carbon grains to be in the range of $0.01–0.3$ (Lorenz-Martins & Lefèvre 1993, 1994; Blanco et al. 1994, 1998; Groenewegen 1995; Groenewegen et al. 1998). The variation of the mass ratio of SiC to carbon grains derived from the radiative transfer models arises from the grain models used, and the value could be also influenced by the optical constants of SiC used in the radiative transfer models (see the discussion in Section 6).

Although the isotopic signatures of presolar SiC grains and the observed spectral feature around 11.3 $\mu m$ support the formation of SiC grains in the circumstellar envelopes of C-rich AGB stars, the formation process as well as the formation conditions remain unknown and debatable: thermodynamic equilibrium calculations have been applied to investigate the formation condition of dust grains in C-rich AGB stars (e.g., Lodders & Fegley 1995), and the calculations have claimed that a high gas pressure $(0.3–300 \, \text{dyne cm}^{-2})$ and low C/O ratio $(1.0 < \text{C/O} < 1.1)$ is necessary for reproducing the condensation sequence of presolar TiC, graphite, and SiC grains in this order, which is inferred from the presence of graphitic spherules containing a TiC core (Sharp & Wasserburg 1995; Daulton et al. 2003). On the other hand, McCabe (1982) suggested that the SiC grains form earlier than carbon grains, considering the inverse greenhouse effect that the temperature of the SiC grains, which is transparent in the optical to near-infrared (NIR) region (Spitzer et al. 1959; Hofmeister et al. 2009), is lower than the temperature of the carbon grains in circumstellar envelopes of C-rich AGB stars. In addition, the interferometric observation of IRC+10216 at 11 $\mu m$ has suggested the presence of dust species more transparent than carbon grains in the inner circumstellar envelope close to the photosphere (Danchi et al. 1990). Although thermodynamic equilibrium calculations can tell us the physical conditions in
which a condensate stably exists, the calculations as well as the astronomical observations do not provide direct information on the number and size of the grains that are essential to clarify the physical conditions prevailing in the formation sites of grains and the physical and chemical processes suffered in the interstellar space. Also, it should be pointed out here that the C/O ratio in C-rich AGB stars is not restricted to less than 1.1, and it tends to increase when the effective temperature \( T_{\text{eff}} \) decreases; the low C/O ratio observed in stars with \( T_{\text{eff}} \lesssim 2500 \) K is considered to be caused by neglecting dust present in the model atmosphere (Bergeat et al. 2002; Bergeat & Chevallier 2005).

So far, the dust formation around C-rich AGB stars has been investigated in the framework of pulsation-enhanced dust-driven wind models since the study done by Fleischer et al. (1992), and it has been believed that the hydrodynamical models, including the formation of only carbon grains, reproduce well the observed dynamical behavior of C-rich AGB stars whose mass-loss rates exceed \( 10^{-6} \) \( \dot{M}_\odot \) yr\(^{-1}\) (e.g., Winters et al. 1994, 1997; Nowotny et al. 2005). However, the formation of SiC grains has not yet been pursued in the hydrodynamical models. On the other hand, the formation of a variety of dust species, including SiC grains, has been studied in the steady state dust-driven wind models around AGB stars to investigate the evolution of dust in the interstellar space (see Ferrarotti and Gail 2006; Zhukovska et al. 2008). However, in the models, the number of seed nuclei is assumed in the formation process. Although the models may predict the mass of dust species supplied from AGB stars, no information is available for the size distribution. Taking into account the nucleation process and including the so-called inverse greenhouse effect, Kozasa et al. (1996) have investigated the formation of SiC grains in an outflowing gas with a constant velocity around C-rich AGB stars, and they have shown that SiC grains condense prior to carbon grains for the mass-loss rate smaller than \( \sim 1.5 \times 10^{-3} \) \( \dot{M}_\odot \) yr\(^{-1}\); otherwise, composite grains consisting of carbon and SiC form. The calculated radius of \( \sim 0.01 \) \( \mu \)m is too small to reproduce the size of presolar SiC grains, and the proposed grains consisting of an SiC core and a carbon mantle have not been discovered, except for one in the presolar grains (Croat et al. 2010). Thus, the investigation of the formation of SiC grains in a more realistic hydrodynamical model remains an important subject that, once explored, will reveal the formation process and condition around C-rich AGB stars. The knowledge of the amount and the size distribution of dust grains is crucial for investigating the role of dust in the universe as shown by Yamasawa et al. (2011). Also, the size distribution of SiC grains formed around C-rich AGB stars is vital to obtain insight into the evolution and processings that the presolar SiC grains suffered during the journey from the formation sites to their incorporation into meteorites.

In this paper, we aim to explore the formation process of SiC grains and investigate the amount and the size distribution in the framework of the pulsation-enhanced dust-driven wind from C-rich AGB stars. We develop a hydrodynamical model that includes the formation of carbon and SiC grains as well as a non-gray radiative transfer. The formulation by Gauger et al. (1990) is applied for the nucleation and growth processes of carbon grains.\(^3\) We assert that SiC grains nucleate and grow homogeneously starting from the SiC molecule because all of the presolar SiC grains whose internal structure has thus far been analyzed do not contain any seed nuclei at their centers (Stroud & Bernatowicz 2005). Furthermore, there is no evidence in presolar graphite grains for an SiC seed nuclei, except for one grain (Croat et al. 2010). The two cases are considered in the formation process of the SiC grains: one is the local thermal equilibrium (LTE) case where the vibration temperature \( T_v \) of a SiC cluster is the same as the gas temperature. Another is the non-LTE case, taking into account the inverse greenhouse effect on the formation, in which \( T_v \) is assumed to be the same as the temperature of the small SiC grains. We will show that the mass ratio of SiC to carbon grains and the radius of the SiC grains are at most \( 10^{-6} \) and 0.1 \( \mu \)m, respectively, in the LTE case, while the mass ratio ranges from 0.098 to 0.23 and the typical radius ranges from 0.2 to 0.6 \( \mu \)m for the sticking probability \( \alpha_s \) of 0.1–1.0 in the non-LTE case.

This paper is organized as follows: the chemical reactions and gas species relevant to the formation of SiC grains are examined and the formation process of SiC grains is formulated in Section 2. The numerical scheme for calculating the grain formation is presented in Section 3, including the method for tracing the size distribution. Section 4 describes the hydrodynamical model and the modeling procedure for the pulsation-enhanced dust-driven wind model, including dust formation and radiative transfer. The results of the calculations are presented in Section 5 and are discussed in Section 6. The summary is presented in Section 7.

2. FORMATION PROCESS OF SiC GRAINS

In the hydrodynamical models of pulsation-enhanced dust-driven wind from C-rich AGB stars already developed since the work of Fleischer et al. (1992), the formation of carbon grains has been processed according to the recipe developed by Gauger et al. (1990); the abundances of gas species responsible for the nucleation and growth of carbon grains are assumed to be in chemical equilibrium in the gas whose elemental abundance is solar, except for carbon. In the recipe based on Gail & Sedlmayr (1988), the formation of clusters with numbers of constituent molecules (size) up to \( n_{\text{out}} = 1000 \) is evaluated from the steady state nucleation rate, and the growth and the evaporation of grains with sizes \( n \geq n_{\text{out}} \) are treated as macroscopic grains. The formation of carbon grains is considered to proceed through the two-body reactions of \( \text{C}_2 \text{H}_2 \) and \( \text{C}_2 \text{H} \) molecules with carbon clusters, starting from the atomic carbon or diatomic carbon molecule.

In this section, we shall explore the formation process of SiC grains around C-rich AGB stars, following the formulation for the formation of carbon grains (Gail & Sedlmayr 1988; Gauger et al. 1990). First, we examine the gas species responsible for the nucleation and the growth processes of SiC grains from chemical equilibrium calculations. In the same way as the formation of carbon grains, we consider that the nucleation process proceeds through the two-body reactions of the cluster with the gas species, starting from the molecules whose stoichiometric composition is the same as SiC grains. On the other hand, we allow three or more body reactions on the surface for the growth process. Then, the basic equations describing the nucleation and growth processes of SiC grains are presented.

2.1. Si-bearing Gas Species in the Dust Formation Region

Figure 1 shows the temperature dependence of relative abundances of Si-bearing molecules (left) and C-bearing

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\(^3\) In the formulation, it is assumed that carbon grains nucleate and grow homogeneously. The recent analysis of presolar graphite (Croat et al. 2005) revealed that about 40% of the carbide-containing graphites have a carbide core. This implies that at least more than 60% of presolar graphite grains nucleate and grow homogeneously.
molecules (right) in chemical equilibrium in the gas with the density $\rho = 10^{-13}$ g cm$^{-3}$ and C/O ratio = 1.4.

As the starting molecules for the formation of SiC grains, we can see that SiC is most abundant in the region whose gas temperature is higher than 1350 K, while the Si$_2$C$_2$ molecule is abundant in the lower temperature region. Among Si-bearing molecules that are considered to be candidate reactants in the growth process of SiC grains, Si, SiC$_2$, and SiS molecules are abundant in the overall range of gas temperature presented in Figure 1, and Si$_2$C is also abundant in the low temperature region of $T < 1100$ K. As shown in the right panel of Figure 1, hydrocarbon molecules, such as C$_2$H$_2$ or C$_2$H, are expected to be reactants that participate in the growth process on the surface of SiC grains unless these molecules are heavily depleted by the formation of carbon grains.

### 2.2. Nucleation Process of SiC Grains

Including the starting molecules SiC and Si$_2$C$_2$ for the nucleation process, the candidate reactants for the two-body reaction in the nucleation process are confined to 12 Si-bearing molecules: SiC, SiC$_2$, SiC$_3$, SiC$_4$, SiC$_5$, Si$_2$C$_2$, Si$_2$C$_3$, Si$_2$C$_4$, Si$_3$C$_2$, Si$_3$C$_3$, Si$_3$C$_4$, Si$_4$C$_2$, Si$_5$C, and Si$_6$C. We shall exclude the gas species with which the reaction for the formation of SiC clusters is endothermic. Table 1 presents the reaction enthalpies $\Delta H^\circ$ of the 12 candidates for the formation of SiC clusters with $n = 2-3$ calculated by using the thermodynamic data of $\beta$-SiC$^4$ are listed in Table 2. The molecules SiC$_2$ and Si$_3$C are excluded because of

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
Reaction & $\Delta H^\circ$ (kJ mol$^{-1}$) & 1000 K & 1500 K \\
\hline
SiC + SiC $\rightarrow$ Si$_2$C$_2$ & $-$751.5 & $-$751.0 \\
SiC + Si$_2$C$_2$ $\rightarrow$ Si$_3$C & $-$518.8 & $-$514.5 \\
SiC$_2$ + SiC $\rightarrow$ Si$_2$C$_2$ + C & 76.98 & 78.12 \\
SiC$_2$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + C & 309.6 & 314.7 \\
SiC$_3$ + SiC $\rightarrow$ Si$_2$C$_2$ + C & $-$54.88 & $-$58.76 \\
SiC$_3$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + C & 177.8 & 177.8 \\
SiC$_4$ + SiC $\rightarrow$ Si$_2$C$_2$ + Si & $-$110.8 & $-$109.8 \\
SiC$_4$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + Si & 121.9 & 126.7 \\
SiC$_2$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + SiC & 232.7 & 236.5 \\
SiC$_2$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + SiC & $-$199.5 & $-$202.6 \\
SiC$_3$ + SiC $\rightarrow$ Si$_2$C$_2$ + SiC & 110.1 & 112.1 \\
SiC$_3$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + SiC & 33.14 & 33.97 \\
SiC$_4$ + SiC $\rightarrow$ Si$_2$C$_2$ + SiC & $-$53.73 & $-$52.46 \\
SiC$_4$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + SiC & 178.9 & 184.1 \\
SiC$_2$ + SiC $\rightarrow$ Si$_2$C$_2$ + Si & $-$122.4 & $-$119.9 \\
SiC$_2$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + Si & $-$122.6 & $-$124.9 \\
SiC$_3$ + SiC $\rightarrow$ Si$_2$C$_2$ + Si & 110.1 & 111.6 \\
SiC$_3$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + Si & $-$195.5 & $-$199.5 \\
SiC$_4$ + SiC $\rightarrow$ Si$_2$C$_2$ + SiC & $-$16.53 & $-$15.41 \\
SiC$_4$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + SiC & 37.19 & 37.04 \\
SiC$_5$ + SiC $\rightarrow$ Si$_2$C$_2$ + Si & 352.2 & 347.9 \\
SiC$_5$ + Si$_2$C$_2$ $\rightarrow$ Si$_3$C$_3$ + Si & 584.8 & 584.5 \\
\hline
\end{tabular}
\caption{Reaction Enthalpies $\Delta H^\circ$ for the Growth Reactions of the SiC Cluster with Size $n = 2-3$}
\end{table}

$^4$ The presolar SiC grains analyzed thus far show only two polytypic forms (Daulton et al. 2003): $\beta$-SiC (79.4% by number), $\alpha$-SiC (2.7%), and the intergrowths of these two forms (17.1%). Note that the difference of the thermodynamic data between $\alpha$-SiC and $\beta$-SiC does not affect the results of the calculations presented in this paper.
the endothermic reactions. Among the remaining candidates, we adopt SiC and Si$_2$C$_2$ as the reactants in the nucleation process of SiC grains since these molecules are much more abundant than the others in the temperature region of interest (Figure 1 (left)).

We discard the nucleation process starting from the two-body reaction between the Si$_2$C$_2$ molecules since Si$_2$C$_2$ is relatively stable; without the thermodynamic data of Si$_2$C$_2$, it is difficult to judge whether the reaction for the formation of Si$_4$C$_4$ proceeds or not. Thus, we consider the following two reactions in the nucleation process of SiC grains:

\[(\text{SiC})_n + \text{SiC} \rightarrow (\text{SiC})_{n+1}, \quad (1)\]

\[(\text{SiC})_{2n-1} + (\text{SiC})_2 \rightarrow (\text{SiC})_{2n+1}, \quad (2)\]

where $n \geq 1$. Note that we consider SiC as the starting molecule for the nucleation process of SiC grains. We shall discuss the effect of the nucleation process beginning with the two-body reaction of the Si$_2$C$_2$ molecules in Section 6.

In the nucleation process, clusters grow through the attachment of the reactants, and the growth rate depends on the number densities and kinetic temperatures of the reactants. On the other hand, clusters decay through the detachment of reactant molecules, and the decay rate depends on the vibration states of the cluster (Gail & Sedlmayr 1988). As pointed out by Kozasa et al. (1996), in the dust formation region around rich AGB stars, the vibration temperature of SiC cluster $T_v$ is not always the same as the kinetic temperature of gas $T$ due to the low gas density and strong radiation field. By applying the principle of detailed balance, the decay rate can be related with the growth rate by considering a hypothetical situation in which the cluster is in an LTE with an ambient gas with a temperature of $T_v$. Then, by assuming that $T_v$ is independent of the size of cluster, the steady state nucleation rate $J_n^i$ for the reaction with (SiC)$_i$ is given by

$$J_n^i = 4\pi a_i^2 n_{\text{SiC}} n_i \frac{k_B T_v}{2\pi m_i} \sqrt{\frac{k_B T_v}{2\pi m_i}} \left[ 1 + \sum_{k=1}^{N_i} \frac{\exp \left\{ 4\pi a_i^2 (ik)^{2/3} \sigma_{ikv} / k_B T_v \right\}}{(ik + 1)^{2/3} S_i(T_v, P_i) \sqrt{T/T_v}} \right]^{-1}, \quad (3)$$

where $i = 1$ (2) denotes the reaction (1) (the reaction (2)) and the quantities related with the reactant SiC (Si$_2$C$_2$) molecule, $a_0$ is the hypothetical radius of a monomer in the bulk phase, and $n_{\text{SiC}}$ is the number density of the starting molecule SiC. The number density, sticking probability, mass, and the partial pressure of the $i$th reactant are represented by $n_i$, $\alpha_i$, $m_i$, and $P_i$, respectively. The Boltzmann constant is $k_B$, $N_i = \left\{ (\sigma_{out} - 2)/i \right\}$ with the floor function $[x]$ and the surface tension of size $n$ is $\sigma_n$. The supersaturation ratio $S_i(T_v, P_i)$ is given by

$$\ln S_i(T_v, P_i) = -\frac{\Delta G_i^0}{k_B T_v} + \frac{P_i}{P_0}, \quad (4)$$

where $P_0$ is the standard pressure. In the above equation, $\Delta G_i^0$ is the Gibbs free energy for the formation of bulk SiC from the $i$th reactant in the standard pressure. The temperature dependence of $\Delta G_i^0/k_B T_v$ is evaluated from the least-squares fitting given by

$$\frac{\Delta G_i^0}{k_B T_v} = a_i + \beta_i \ln T_v + \frac{\gamma_i}{T_v^{1/4}} + \frac{\delta_i}{T_v} + \frac{\eta_i}{T_v^2} + \frac{\epsilon_i}{T_v^3}, \quad (5)$$

whose form is based on a polynomial expression of heat capacity at a constant pressure (Berman & Brown 1985). The coefficients $a_i$, $\beta_i$, $\gamma_i$, $\delta_i$, $\eta_i$, and $\epsilon_i$ are given in Table 3. In the calculations, we adopt $a_0 = 1.71 \times 10^{-8}$ cm, which is evaluated from the bulk density of solid SiC ($\rho = 3.16$ g cm$^{-3}$) taken from the CRC hand book (Lide 2003). The values of the sticking probabilities of SiC and Si$_2$C$_2$ molecules on the SiC cluster are unknown and are assumed to be unity. The surface tension $\sigma_n$ of the SiC cluster with a size $n = 2$ or 3 is directly evaluated from the following definition of surface tension of $n$-mer

$$4\pi a_0^2 (n - 1)^{2/3} \hat{\sigma}_n = \hat{g}(n) - \hat{g}(1) - (n - 1)\hat{g}_s, \quad (6)$$

where $\hat{g}(n)$ and $\hat{g}_s$ are the Gibbs free energies of $n$-mer in the gas phase and the monomer in the bulk phase in the standard state, respectively. On the other hand, we adopt the bulk value of $\sigma = 840$ erg cm$^{-2}$ measured by Allen & Kingery (1959) as the surface tension of SiC clusters with size $n > 3$.

### 2.3. Growth of SiC Grains

We allow three or more body reactions for the growth of SiC grains in addition to the two-body reactions for the nucleation. As shown in Figure 1, the abundant Si- and C-bearing molecules expected to be the reactants for the grain growth are Si, Si$_2$C, Si$_2$C$_2$, C, C$_2$H$_2$, and C$_2$H, except for CO and SiS which are stable against the chemical reactions. Then, we select the following exothermic reactions:

$$\text{(SiC)}_n + \text{SiC} \rightarrow (\text{SiC})_{n+1}, \quad (7)$$

$$\text{(SiC)}_n + \text{Si}_2\text{C}_2 \rightarrow (\text{SiC})_{n+2}, \quad (8)$$

$$\text{(SiC)}_n + 2\text{Si} + \text{C}_2\text{H}_2 \rightarrow (\text{SiC})_{n+2} + \text{H}_2, \quad (9)$$

$$\text{(SiC)}_n + 2\text{Si} + \text{C}_2\text{H} + \text{H} \rightarrow (\text{SiC})_{n+2} + \text{H}_2, \quad (10)$$

$$\text{(SiC)}_n + 2\text{Si}_2\text{C} + \text{C}_2\text{H}_2 \rightarrow (\text{SiC})_{n+4} + \text{H}_2, \quad (11)$$

$$\text{(SiC)}_n + \text{Si} + \text{Si}_2\text{C} \rightarrow (\text{SiC})_{n+2}, \quad (12)$$

$$\text{(SiC)}_n + \text{Si} + \text{C} \rightarrow (\text{SiC})_{n+1}, \quad (13)$$
where \( n > n_{\text{out}} = 1000 \); the reaction enthalpies at 1000 K are 
\(-1265, -1739, -1572, -1206, \) and \(-1240 \text{ kJ mol}^{-1} \) for the chemical reactions from (9) to (13) in this order.

Except for the two-body reactions, it is assumed that each of the chemical reactions proceeds through the attachment of a key species that is defined as the species of the least collision frequencies among the reactants and considered to control the kinetics of the growth process (Kozasa & Hasegawa 1987; Hasegawa & Kozasa 1988). Then, the time evolution of the size of the dust grains with a radius \( a \) is given by

\[
\frac{d}{dt} \left( \frac{a}{a_0} \right) = \frac{1}{3 \tau_{\text{net}}},
\]

where the size-independent net timescale of grain growth \( \tau_{\text{net}} \) (Gauger et al. 1990) is the sum of the net timescales for the reactions from (7) to (13). It is written as follows:

\[
\frac{1}{\tau_{\text{net}}} = \sum_{i=1}^{2} \frac{1}{\tau_{i}^{\text{net}}} + \sum_{n=9}^{13} \frac{1}{\tau_{n}^{\text{net}}}. \tag{15}
\]

In the above equation, \( \tau_{i}^{\text{net}} \) (\( i = 1, 2 \)) is the net timescale of the grain growth by the two-body reaction with \( (\text{SiC}) \) molecule, which is given by

\[
\frac{1}{\tau_{i}^{\text{net}}} = 4 \pi a_i^2 \alpha_i \left( \frac{k_B T}{2 \pi n_i m_i} \right) \left( n_i - \frac{P_{ev}}{k_B \sqrt{T T_i}} \right), \tag{16}
\]

and \( \tau_{n}^{\text{C,n}} \) (\( n = 9–13 \)) is the net timescale of the grain growth for each of the chemical reactions from (9) to (13) and is given in the same form as Equation (16) by replacing \( \alpha_i \), \( m_i \), and \( n_i \) with those for the key species. In Equation (16), \( P_{ev} \) represents the vapor pressure for the key species in the reaction; for example, in the reactions (9) and (10), the vapor pressure of the Si atom is assumed to be the same as that for the reaction: \( (\text{SiC})_h \rightarrow \text{Si} + \text{C} \). In the reaction (11), the vapor pressure of the \( \text{Si}_2\text{C} \) molecule is assumed to be the same as that for the reaction: \( 2(\text{SiC})_h \rightarrow \text{Si}_2\text{C} + \text{C} \). In the calculations, the sticking probability \( \alpha_s \) is assumed to be unity for all reactions.

### 3. NUMERICAL SCHEME FOR GRAIN FORMATION

The number densities of the gas species responsible for the formation process of carbon and \( \text{SiC} \) grains in the pulsation-enhanced dust-driven wind from C-rich AGB stars are evaluated from the chemical equilibrium calculations for a given gas density and temperature coupled with the hydrodynamical calculation. We include four atoms \( (\text{H}, \text{C}, \text{Si}, \text{and S}) \) and 14 molecules \( (\text{H}_2, \text{C}_2, \text{C}_3, \text{C}_2\text{H}, \text{C}_2\text{H}_2, \text{SiH}, \text{SH}, \text{H}_2\text{S}, \text{SiC}, \text{SiC}_2, \text{Si}_2\text{C}, \text{Si}_2\text{C}_2, \text{CS}, \text{and SiS}) \) in the chemical equilibrium calculations, and the abundances of the elements, except for carbon, are taken from the table in Allen (1973). We employ the formulation presented in Section 2 for the formation process of \( \text{SiC} \) grains, while the formulation by Gauger et al. (1990) is applied for the formation of carbon grains. As mentioned before, the sticking probability \( \alpha_s \) for all reactions at the nucleation and growth of \( \text{SiC} \) grains is assumed to be unity in the calculations, whose effect on the results of the calculations is discussed in Section 6.

The number density and the size of grains as well as the fraction of the condensible molecules locked into the grains are evaluated by taking the \( j \)th moment of the size distribution of grains per H-element \( \hat{K}_j \) defined as

\[
\hat{K}_j = \sum_{n=n_{\text{out}}}^{\infty} N^\frac{j}{2} \frac{f(n, t)}{n_{\text{HI}}}, \tag{17}
\]

where \( f(n, t) \) is the number density of the grains with the size \( n \) at time \( t \) and \( n_{\text{HI}} = n_{\text{H}} + 2n_{\text{H}_2} \). Normally, the moments are calculated by reducing to the simultaneous differential equations (Gail & Sedlmayr 1988). The time variation of gas (gas) temperature is not always monotonic, and it can be rather complicated in the pulsation-enhanced dust-driven winds. In case the formed grains are lost by the destruction due to the evaporation at time \( t \), the extinction term is included in the differential equations by using the number density of the grains with the minimum size \( f(n_{\text{out}}, t) \), which has to be derived by tracing the size distribution. Therefore, solving the differential equations must be compensated with the evaluation of the size distribution of the grains with a limited number of size bins in the hydrodynamical simulations (Fleischer 1994).

Thus, in this paper, we calculate the moments by employing the finite and adaptive size grids rather than solving a set of the simultaneous differential equations. Each of the size bins is co-moved in the size space (Krüger et al. 1995; Woitke & Niccolini 2005). The \( i \)th size bin is characterized by the number of grains per H-element \( \hat{w}(I) \) in the size interval with a lower limit \( a_{i_{\text{min}}} \) and an upper limit \( a_{i_{\text{max}}} \). The lower and upper limits are calculated by integrating Equation (14). When the net timescale \( \tau_{\text{net}} \) is positive, the number of grains per H-element in the lowest size bin \( \hat{w}(I) \), where \( I \) is the total number of size bins, is given by integrating the equation

\[
\frac{d \hat{w}(I)}{dt} = \frac{J_S}{n_{\text{HI}}}. \tag{18}
\]

When the net timescale \( \tau_{\text{net}} \) is negative, the destruction rate of the grains \( J_{\text{des}} \) is estimated by

\[
J_{\text{des}} = \frac{d a}{dt} \alpha_{i_{\text{max}}} - a_{\text{lowest}}, \tag{19}
\]

where \( a_{\text{lowest}} = a_{i_{\text{out}}} \) and \( \hat{w}(I) \) is derived by integrating the equation

\[
\frac{d \hat{w}(I)}{dt} = - \frac{J_{\text{des}}}{n_{\text{HI}}}. \tag{20}
\]

### Table 3

| \( i \) | \( \alpha_i \) | \( \beta_i \) | \( \gamma_i \) | \( \delta_i \) | \( \eta_i \) | \( \epsilon_i \) |
|---|---|---|---|---|---|---|
| 1 | 3.16656 \times 10^1 | -1.12418 \times 10^0 | 1.71784 \times 10^2 | -1.01082 \times 10^5 | 1.01432 \times 10^6 | -8.78548 \times 10^7 |
| 2 | -2.96847 \times 10^3 | 2.79219 \times 10^2 | 5.55156 \times 10^4 | -8.91964 \times 10^7 | 1.15759 \times 10^8 | -1.28618 \times 10^10 |
According to Woitke & Niccolini (2005), the discrete moment $K_{j}^{\text{discr}}$ is evaluated by

$$
K_{j}^{\text{discr}} = \frac{1}{(j+1)a_{0}^{3}} \left\{ \sum_{i=1}^{I} \hat{w}(i) \sum_{k=0}^{l-1} a_{i,\min}^{k} a_{i,\max}^{j-k} + \hat{w}(I) \sum_{k=0}^{l} a_{\text{lowest}}^{k} a_{i,\max}^{j-k} \right\},
$$

(21)

for $j = 0$–3. The 0th moment $K_{0}^{\text{discr}}$ and the third moment $K_{3}^{\text{discr}}$ give the number of grains per H-element and the number of condensable molecules incorporated into the grains per H-element, respectively. The volume equivalent radius of grains $\langle a \rangle$ at a time is defined by $\langle a \rangle = a_{0} K_{j}^{\text{discr}} / K_{0}^{\text{discr}})^{1/3}$.

4. THE MODEL

4.1. Hydrodynamics

The basic equations for the time-dependent, spherically symmetric hydrodynamical model are written in the standard finite difference form and solved by explicit integration along the lines of the difference scheme given by Richtmyer & Morton (1967). This modeling method has been adopted by the Berlin group (e.g., Fleischer et al. 1992; Winters et al. 2000; Helling et al. 2000; Dreyer et al. 2011). Actually, this method is time consuming since the time steps are restricted by the Courant–Friedrichs–Levy stability condition (see Höflner et al. 1996). However, since the advection term drops from the equation of motion in the Lagrangian coordinate, we can easily trace the size distribution of the grains, which is one of the main subjects of this study.

The continuity equation representing the conservation of mass is replaced with the definition of gas velocity $v$, given by

$$
\frac{\partial r}{\partial t} = v,
$$

(22)

where $r$ is the radial position of the Lagrangian mass element at a time $t$. Under the assumption of the position coupling between the gas and grains, the equation of motion is described as

$$
\frac{\partial v}{\partial t} = -\frac{1}{\rho} \frac{\partial p}{\partial r} - \frac{G M(r)}{r^{2}} (1 - \alpha),
$$

(23)

where $p$ is the thermal gas pressure, $\rho$ is the gas density, $G$ is the gravitational constant, and $M(r)$ is the mass inside a radius $r$. In the above equation, $\alpha$ is the ratio of radiation pressure force to gravity and is expressed as

$$
\alpha = \frac{\kappa_{\text{pr}} L_{*}}{4 \pi c G M(r)},
$$

(24)

where $\kappa_{\text{pr}}$ is the sum of the flux-weighted mean of mass radiation pressure coefficient for gas $\kappa_{\text{pr}}^{\text{gas}}$ and that for dust $\kappa_{\text{pr}}^{\text{dust}}$, $L_{*}$ is the luminosity, and $c$ is the speed of light. The mass inside a radius $r$ in the above equations is replaced with the stellar mass $M_{*}$ because the mass contained in the circumstellar envelope is small compared with the stellar mass during the calculations presented in this paper. In the calculations, we adopt the constant gas opacity of $\kappa_{g} = 2 \times 10^{-4} \text{ cm}^{2} \text{ g}^{-1}$ (Bowen 1988). Following the previous works for hydrodynamic models of dust-driven wind solved with frequency-dependent radiative transfer calculations (Höfner et al. 2003; Woitke 2006; Mattsson et al. 2010), we evaluate the dust opacity $\kappa_{d}^{\text{dust}}$ at a wavelength $\lambda$ in the Rayleigh approximation. The optical constants of the carbon and SiC grains used in the calculation are taken from Draine (1985) and Choyke & Palik (1985), respectively. The radiation field in the circumstellar envelope is derived from the frequency-dependent radiative transfer calculation using the variable Eddington factor method under the assumption of radiative equilibrium. Then, the gas temperature $T_{\text{gas}}$ is given by

$$
\int_{0}^{\infty} \kappa_{\lambda,\text{abs}}^{\text{gas}} J_{\lambda} d\lambda = \int_{0}^{\infty} \kappa_{\lambda,\text{abs}}^{\text{gas}} B_{\lambda}(T_{\text{gas}}) d\lambda,
$$

(25)

where the subscript “abs” refers to absorption. $J_{\lambda}$ is the mean intensity, and $B_{\lambda}(T_{\text{gas}})$ is the Planck function. The temperature of $i$th grain species $T_{\text{dust},i}$ is given by

$$
\int_{0}^{\infty} \kappa_{\lambda,\text{abs}}^{\text{dust},i} J_{\lambda} d\lambda = \int_{0}^{\infty} \kappa_{\lambda,\text{abs}}^{\text{dust},i} B_{\lambda}(T_{\text{dust},i}) d\lambda.
$$

(26)

4.2. Vibration Temperature of the SiC Cluster

According to the hydrodynamical models that have already been developed for dust-driven wind from C-rich AGB stars (Fleischer et al. 1992; Höfner et al. 1995), the vibration temperature of the carbon cluster is, as usual, equal to the gas temperature. On the other hand, to investigate the influence of the inverse greenhouse effect suggested by McCabe (1982) for the formation of the SiC grains, we consider two cases for the vibration temperature of the SiC cluster: one is a case, in which the vibration temperature of the SiC cluster is the same as the gas temperature, referred to as the “LTE case” hereafter. The other is a non-LTE case where the vibration temperature is assumed to be the same as the temperature of the small SiC grains (Kozasa et al. 1996). Assuming that the gas species mainly consisting of H, H$_{2}$, and He can accommodate the grains completely upon colliding, and placing a small SiC grain hypothetically at a position in the gas flow, we derive the vibration temperature of the SiC cluster $T_{v}$ by balancing the heating with the cooling through the interaction with radiation and gas as follows:

$$
\int_{0}^{\infty} \pi Q_{\lambda,\text{abs}}^{\text{SiC}}(a_{cl})[J_{\lambda} - B_{\lambda}(T_{v})] d\lambda = \sum_{j} n_{\text{gas},j} \left( \frac{k_{B} T_{v}}{2 \pi m_{j}} \right)^{3/2}
$$

$$
\times \left( C_{V,j} + \frac{1}{2} k_{B} \right) \left( T_{v} - T_{\text{gas}} \sqrt{\frac{T_{\text{gas}}}{T_{v}}} \right),
$$

(27)

where $Q_{\lambda,\text{abs}}^{\text{SiC}}(a_{cl})$ is the absorption efficiency factor of the SiC grain with a radius $a_{cl}$, whose value is set to be $10^{-3} \mu \text{m}$, and $n_{\text{gas},j}$, $m_{j}$, and $C_{V,j}$ are the number density, the mass, and the specific heat at a constant volume of the $j$th gas species, respectively.

4.3. Modeling Procedure

The models of pulsation-enhanced dust-driven wind are specified by six parameters: the stellar mass $M_{*}$, the stellar
luminosity $L_\ast$, the effective temperature $T_{\text{eff}}$, the C/O ratio, the period of the pulsation $P$, and the velocity amplitude of the pulsation $\Delta u_\rho$. As the first step of the hydrodynamical simulation, a dust-free static model atmosphere is constructed as follows: the initial stellar radius $R_\ast$ is given by the Stefan–Boltzmann law $L_\ast = 4\pi R_\ast^2 \sigma T_{\text{eff}}^4$, where $\sigma$ is the Stefan–Boltzmann constant. Given a guess value for gas density at $R_\ast$, the radial profiles of the density and temperature are calculated by solving the equation

$$\frac{1}{\rho} \frac{d \rho}{dr} = -\frac{GM_\ast}{r^2}$$

(28)
coupled with the radiative transfer calculation with sufficiently fine grids. The procedure is iterated until the geometrically diluted optical depth at $R_\ast$ converges to 2/3.

The dynamical model calculations, including the formation of grains, are carried out by placing the piston at $R_{\text{init}}$ whose position is two times the pressure scale height around $R_\ast$ below from the photosphere of the static model atmosphere. It is defined as the inner boundary of the dynamical model at $t=0$. Then, the radius $R_{\text{in dyna}}$ of the inner boundary is varied sinusoidally with time as

$$R_{\text{in dyna}} = R_{\text{in0}} + \Delta u_\rho \frac{P}{2\pi} \sin \left(\frac{2\pi}{P} t\right),$$

(29)

and the velocity $u_{\text{in dyna}}$ at the inner boundary is given by

$$u_{\text{in dyna}} = \Delta u_\rho \cos \left(\frac{2\pi}{P} t\right).$$

(30)

In the simulation, a mass flow is not assumed through the inner boundary. The radiative flux is assumed to be constant over time and to be equal to $\pi B(T_{\text{eff}}) = \pi \int_0^\infty B_\nu(T_{\text{eff}})d\nu$ at the photosphere of the dynamical model $R_{\text{phot}}$ where the diluted optical depth of gas is 2/3; thus, the stellar luminosity $L_\ast = 4\pi R_{\text{phot1}}^2 \sigma T_{\text{eff1}}^4$ varies with time. The piston velocity amplitude $\Delta u_\rho$ is increased slowly from 1 cm s$^{-1}$ to the specified value to prevent the first outwardly moving subsonic wave from growing into an enormous transient shock, following Bowen (1988).

After the onset of dust formation, the dust-driven wind takes place. As the gas expands, the spacing between radial grids in the acceleration region becomes wider and the rezoning procedure that is necessary for resolving the density structures of the circumstellar envelope is introduced by adopting the method proposed in Fleischer et al. (1992). After the outermost zone passes through the outer boundary of the dynamical model, which is placed at 25 $R_\ast$ in the simulation, the outermost Lagrangian grid is eliminated. Then, at the outer boundary, we trace the time variations of the mass-loss rate, gas outflowing velocity, dust-to-gas mass ratio, and condensation efficiency $f_C$ ($f_S$), which is defined as the fraction of carbon (silicon) atoms in C-bearing molecules except for the CO (Si-bearing molecules) locked into carbon (SiC) grains. In the case where all Si atoms in Si-bearing molecules are locked into SiC grains, note that the maximum value of $f_C$ is ~0.9 in the model with C/O = 1.4.

5. RESULTS

We adopt the following model parameters in the calculation: $T_{\text{eff}} = 2600$ K, $L_\ast = 10^4 L_\odot$, $M_\ast = 1.0 M_\odot$, C/O = 1.4, $P = 650$ days, and $\Delta u_\rho = 2.0$ km s$^{-1}$, which are typical values adopted in the previous studies (e.g., Fleischer 1994; Winters et al. 2000). The values are almost the same as those employed in the models of C-rich AGB stars that reasonably reproduce the observed dynamical behaviors (Winters et al. 1994, 1997; Nowotny et al. 2005). The number of radial grids used in the hydrodynamical calculations depends on the density structure, and it is between 800 and 1200 throughout the calculations. The wavelength region covered in the radiative transfer calculation ranges from 0.35 to 120 $\mu$m, and the number of wavelength grids is 100. The simulations have been performed for 180 cycles (stellar pulsation periods). In this paper, we neglect the radiation pressure force acting on the SiC grains because of the transparency in the optical to infrared region (up to ~9 $\mu$m) (Choyke & Palik 1985; Pitman et al. 2008; Hofmeister et al. 2009).

The formation of SiC grains in the pulsation-enhanced dust-driven wind is closely related to the formation of the carbon dust shell that stems from the rapid formation of carbon grains in the high-density gas induced by the stellar pulsation and the resulting acceleration of the dense region caused by the radiation pressure force acting on the carbon grains. The carbon dust shell is characterized by the inversions of density distributions of gas and carbon grains and plays a crucial role in the time evolution of the gas temperature and density through the backwarming caused by the thermal emission from the carbon grains. First, we outline the formation of carbon dust shells in this model, and then we show how SiC grains form in the LTE and non-LTE cases.

5.1. Formation of Carbon Dust Shells

The carbon dust shell (CDS) appears in the present model quasi-periodically once a stellar pulsation period and is classified into two types by the peak value of $f_C$ in the shell. Here, we shall overview the formation of each type of the carbon dust shells and its dynamics, referring to Figure 2, which displays the radial structure of the quantities related to the gas dynamics and the formation of carbon and SiC grains in the LTE case throughout the period from $t = 166.7$ to 168.8 $P$.

The first type of carbon dust shell (hereafter referred to as the 1st type CDS) is defined as the high-density region with the peak value of $f_C \gtrsim 0.9$, and it is located around 4 $R_\ast$ at $t = 167.9$ $P$ (see the bottom row in Figure 2). The formation of this 1st type CDS actually starts at $t \sim 166.7$ $P$, and the behavior of the formation process is almost the same as that of the 1st type CDS whose formation starts at $t \sim 168.8$ $P$; the nucleation of carbon grains takes place in the dust-free region ranging from 1.8 to 3.0 $R_\ast$ where gas temperature decreases to 1300 K (see the radial variation of the nucleation rate of carbon grains at $t = 168.8$ $P$ and the time variation of the distribution of the number of carbon grains in this region from $t = 168.5$ to 168.8 $P$ in Figure 2). Then, the backwarming by thermal emission from the carbon grains subsequently formed in the outer part of this region not only raises up the gas temperature but it also evaporates the carbon grains in the inner part (see the third rows at $t = 167.0$ $P$ and $t = 167.3$ $P$ in Figure 2). However, in the outer part, the nucleation and growth of the carbon grains still proceed and the ratio of radiation pressure force to gravity $\alpha$ around 2.5 $R_\ast$ exceeds unity at $t = 167.0$ $P$ with increasing the volume equivalent radius ($\mu_C$) and the condensation efficiency $f_C$ of carbon grains up to ~0.1 $\mu$m and ~0.3 (see the third and bottom rows of Figure 2). As a result, this part is accelerated outward. On the other hand, the gas density in the outer region compared with the accelerated region is insufficient to produce enough abundant carbon grains to accelerate this region efficiently despite the ongoing nucleation.
Figure 2. Radial structure in the LTE case for $t = 166.7$ to $167.6\,P$ (top panel) and for $t = 167.9$ to $168.8\,P$ (bottom panel). Top row: the gas velocity $v$ (blue) and the gas temperature $T_{\text{gas}}$ (black). Second row: the gas density $\rho$ (blue) and the ratio of radiation pressure force to gravity $\alpha$ (black). Third row: the nucleation rates per H-element $J_{\text{C}}/n_{\text{H}}$ of carbon (black solid) and SiC (red) grains, the destruction rate per H-element $J_{\text{des}}/n_{\text{H}}$ of carbon grains (black dashed), and the numbers per H-element $K_{\text{discr}}$ of carbon (gray) and SiC (green) grains. Bottom row: the condensation efficiencies $f_{\text{C}}$ (black) and $f_{\text{Si}}$ (red), and the volume equivalent radii $\langle a \rangle$ of carbon (gray) and SiC (green) grains.

Thus, the radial compression due to the velocity difference causes the outer part of the accelerated region to increase more through the increased nucleation and growth rates of the carbon grains, resulting in the shell structure. Note that the shell structure is not associated with the pulsation shock, but instead is induced by the formation of carbon grains. The shell structure becomes prominent by decreasing the gas density in the inner region compared with the accelerated region due to the radial expansion (see the second rows from $t = 167.3$ to $167.6\,P$ in Figure 2). The formation of the 1st type CDS completes at $t \sim 167.9\,P$.

The formation of the second type of carbon dust shell (hereafter referred to as the 2nd type CDS), defined as the high-density region with the peak value of $0.3 < f_{\text{C}} < 0.7$ onsets
around 2.2 $R_*$ at $t = 168.2$ $P$, is triggered by the merging of the two consecutive shocks induced by the stellar pulsations, which can be seen from the time variations of the gas velocity and $\alpha$ in this region from $t = 167.9$ to 168.2 $P$; the carbon grains in front of the precedent shock, which nucleated at $t \sim 166.7$ $P$ and survived the evaporation process that was associated with the evolution of the 1st type CDS starting at $t \sim 167.0$ $P$, grow up from $(\alpha_c) = 0.05$ to 0.1 $\mu$m in the region further compressed by merging with the following shock (see the bottom rows from $t = 167.6$ to 168.2 $P$ in Figure 2). After then, the nucleation and growth of carbon grains in the compressed outer part of this region develops the shell structure with increasing $\alpha$, while the rapid decrease of the gas density caused by the outward velocity already exceeding 10 km s$^{-1}$ suppresses the growth rate of carbon grains and the increase of $f_c$. The evolution of this carbon dust shell ends up as the 2nd type CDS with the peak value of $f_c \sim 0.7$ at $t \sim 169.0$ $P$. The density profile as well as the peak value of $f_c$ of the 2nd type CDS varies from cycle to cycle (e.g., see the 2nd type CDS located around 4.5 $R_*$ at $t = 167.0$ $P$). The alternating formation of the 1st and 2nd type CDSs is sometimes disturbed, in which case the 2nd type CDS fails to grow up without increasing the peak value of $f_c$ up to 0.3. The appearance and periodicity of the carbon dust shell depend on the stellar parameters in a complicated manner as investigated by Fleischer et al. (1995), Höfner et al. (1995), and Dreyer et al. (2009, 2011). For example, in our model with $C/O = 1.8$, only the 1st type CDS forms every stellar pulsation period.

5.2. Formation of SiC Grains in LTE Case

The values of mass-loss rate, gas terminal velocity, and dust-to-gas mass ratio averaged over the last 60 pulsation periods at the outer boundary are $1.24 \times 10^{-5} \, M_\odot$ yr$^{-1}$, 20.4 km s$^{-1}$, and $1.64 \times 10^{-3}$, respectively, in the hydrodynamical model with the LTE case for the formation of SiC grains. As can be seen from Figure 2, the nucleation of SiC grains begins when the gas cools down to 1100 K after the formation of carbon grains, and is activated in the temperature range of 800–1000 K. The corresponding formation region is located around 3.5–5.5 $R_*$, unless the gas temperature is increased to higher than 1100 K by the backwarming from the precedent 1st or 2nd type CDS. In the formation region, the $\text{Si}_2\text{C}_2$ molecule is more abundant than the SiC molecule and the nucleation proceeds through reaction (2) rather than reaction (1). In particular, the formation of SiC grains is most efficient in the region around the outer boundary of the 1st type CDS because of the lower temperature and higher gas density, and the nucleation rate per H-element reaches the maximum value of $\sim 10^{-25}$ s$^{-1}$ at $t = 167.9$ $P$. However, the subsequent decrease of the gas density caused by the accelerated radial expansion depresses the nucleation and growth processes of SiC grains; the number of SiC grains per H-element is limited to smaller than $10^{-11}$ (see the third row at $t = 168.8$ $P$ in Figure 2), and the volume-equivalent radius of the SiC grains ($a_{\text{SiC}}$) is typically $(3–6) \times 10^{-2}$ $\mu$m. In the other regions, the number and size of the SiC grains are much smaller. Thus, the depletion of Si-bearing molecules does not take place substantially in the LTE case (see the radial variation of $f_{\text{Si}}$ in the bottom row throughout the time in Figure 2), and almost all of the SiC grains form around the outer boundary of the carbon dust shell.

Figure 3 represents the radial distribution of the gas and grains in the region of $r < 25 \, R_*$ at $t = 166.8$ $P$. The radial distribution of $f_c$ (the second row of Figure 3) clearly shows that the different types of carbon dust shell form by turn as addressed in Section 5.1. The carbon dust shells broaden by moving outward from the formation sites because the outer part with more abundant carbon grains is accelerated more efficiently than the inner part, and the broadening in the outer circumstellar envelope of $r > 10 \, R_*$ is caused by the pressure gradient. In addition, the slower-moving 2nd type CDS seems to be caught up by the faster-moving 1st type CDS around 21 $R_*$. Note that the shell (shock) structure seen in the radial distribution of the gas density precedes the corresponding carbon dust shell in the outer circumstellar envelope (see the top row of Figure 3). The distributions of $\rho_{\text{SiC}}$ and $f_{\text{SiC}}$ (the top and second row, respectively, in Figure 3) demonstrate that the SiC grains reside in a thin shell around the outer boundary of the carbon dust shell, reflecting the formation site. The value of $f_{\text{SiC}}$ ($\rho_{\text{SiC}}/\rho_{\text{gas}}$) and the mass ratio of SiC to carbon grains Si/C are, at most, $10^{-6}$ ($10^{-5}$) and $10^{-6}$, respectively (see the lower three rows in Figure 3). The value of $f_c$ ($\rho_{\text{C}}/\rho_{\text{gas}}$) averaged over the last 60 pulsation periods at the outer boundary is 0.707 (1.64 $\times 10^{-3}$), while the averaged value of $f_{\text{SiC}}$ ($\rho_{\text{SiC}}/\rho_{\text{gas}}$) is on the order of magnitude of $10^{-8}$ ($10^{-11}$). The resulting averaged value of Si/C is 4.93 $\times 10^{-8}$, which is much smaller than the value inferred from the radiative transfer models (0.01–0.3).

Figure 4 shows the size distribution of the SiC grains by mass averaged over the last 60 pulsation periods at the outer boundary. The distribution is characterized by the single-peaked profile with the peak around $\alpha = 6.0 \times 10^{-2}$ $\mu$m, and the radius of the SiC grains is limited to be less than 0.1 $\mu$m. The modal size is almost a factor of four smaller than the size of the presolar SiC grains extracted from the Murchison meteorite (Amari et al. 1994). The LTE case with the lower C/O ratio that results in a
lower gas outflow velocity makes the formation of SiC grains with radii of 0.2–0.3 μm possible as long as the gas outflow exhibits a layered structure with the CDSs. On the other hand, regardless of the C/O ratio, the amount of SiC grains formed in the LTE case is too small to reproduce the amount of SiC grains inferred from the astronomical observations.

5.3. Formation of SiC Grains in the Non-LTE Case

Figure 5 displays the radial structure of the quantities related to the gas dynamics and the formation of grains in the non-LTE case throughout the period from \( t = 166.7 \) to 168.8 \( P \). The vibration temperature of the SiC cluster defined in Section 4.2 and depicted in the top row (solid red) of Figure 5 is evaluated by hypothetically placing the small SiC grain with \( a_{\text{Si}} = 10^{-3} \) μm in the dynamic calculations. The difference between the gas temperature \( T_{\text{gas}} \) and the vibration temperature \( T_v \) is negligible in the high-density region of \( \rho > 10^{-12} \) g cm\(^{-3} \) where the collision with gas dominates the energy balance and controls \( T_v \). As the gas density decreases and the collision with the gas becomes less effective than the interaction with the radiation in the energy balance, \( T_v \) deviates from and is lower than \( T_{\text{gas}} \) because the small SiC grain is almost transparent from the visible to the infrared region (up to \( \sim 9 \) μm) (Choyke & Palik 1985; Pitman et al. 2008; Hofmeister et al. 2009). Also, it should be noted that \( T_v \) is not affected so much by the backwarming due to the thermal emission from the outer carbon dust shell compared with the gas temperature. Thus, the temperature difference \( \Delta T = T_{\text{gas}} - T_v \) is magnified in the less-dense inner region compared with the opaque carbon dust shell (e.g., see around 2.5 \( R_s \) at \( t = 167.3 \) \( P \)).

As the gas density decreases, the supersaturation ratio of SiC grains quickly exceeds unity with increasing \( \Delta T \) as well as decreasing \( T_v \). The nucleation process of SiC grains can be activated in the region with \( \rho < 10^{-12} \) g cm\(^{-3} \) as long as \( T_v \lesssim 1200 \) K and \( \Delta T \gtrsim 200 \) K, even in the region with \( T_{\text{gas}} \gtrsim 1400 \) K where the nucleation process of carbon grains is nearly depressed. On the other hand, if \( T_v \) is higher than 1200 K, the nucleation process of SiC grains is not activated regardless of the gas temperature since the abundances of the molecules responsible for the formation of SiC grains are not sufficient to make the supersaturation ratio large enough to begin nucleation.

The active nucleation and growth of SiC grains takes place in the infalling gas around 1.8–2.2 \( R_s \) at \( t = 166.7 \) \( P \) when the gas density drops down to a few times \( 10^{-13} \) g cm\(^{-3} \), \( T_v \) decreases down below 1200 K, and \( \Delta T \) increases by larger than \( \sim 200 \) K, almost concurrently with the onset of the formation of the 1st type CDS as explained in Section 5.1. Then, the backwarming from the evolving 1st type CDS raises up \( T_v \) and \( T_{\text{gas}} \) high enough so as to evaporate the SiC grains in the inner dense region with \( \rho \gtrsim 10^{-11} \) g cm\(^{-3} \) at \( t = 167.0 \) \( P \). However, in the less-dense, outer region, the SiC grains grow up to \( \sim 0.3 \) μm thanks to the increase of \( \Delta T \), and the condensation efficiency \( f_{\text{Si}} \) reaches 0.1. In the region around 2.5 \( R_s \), the nucleation of the SiC grains proceeds, and at \( t = 167.3 \) \( P \) the increase of \( f_{\text{Si}} \) is distinguishable while carbon grains evaporate due to the backwarming, which continues up to \( t \sim 167.5 \) \( P \) (see the third and bottom rows of Figure 5). On the other hand, in the region around 2 \( R_s \), the evaporation of the SiC grains ceases and growth starts at \( t = 167.3 \) \( P \) by weakening the backwarming as the 1st type CDS moves outward. Then, the increase of gas density up to \( 10^{-11} \) g cm\(^{-3} \), which was caused by the pulsation shock, leads to the efficient nucleation and growth of the SiC grains, and \( f_{\text{Si}} \) increases to \( \sim 0.7 \) quickly until \( t = 167.6 \) \( P \). Then, the efficient growth of the SiC grains in the region compressed by the merging of the consecutive shocks (starting from \( t \sim 167.9 \) \( P \)) results in the complete consumption of the Si-bearing molecules (\( f_{\text{Si}} = 1.0 \)) around \( t \sim 168.1 \) \( P \), and (\( \Delta a_{\text{Si}} \)) in this region is typically larger than \( \sim 0.2 \) μm, which is in contrast with the LTE-case. Hereafter, the region with the condensation efficiency \( f_{\text{Si}} \sim 1.0 \) is referred to as the Si-depletion region. Concurrently, the 2nd type CDS formed and developed in this region outwardly stretches the Si-depletion region (see the radial distribution of \( f_{\text{Si}} \) in the bottom row from \( t = 168.2 \) to 168.8 \( P \) in Figure 5), while the backwarming from the 2nd type CDS makes \( T_v \) higher than 1200 K and depresses the nucleation of SiC grains in the inner region compared with the Si-depletion region (see \( T_v \) in the top row at \( t = 168.5 \) \( P \) in Figure 5). It should be noted that the 2nd type CDS moves outward more slowly than the 1st type CDS as mentioned in Section 5.2. Thus, the Si-depletion region with a slower outward velocity is finally caught up and pushed by the 1st type CDS, which can be seen from the time evolution of the Si-depletion region spreading across 3.5 to 5.5 \( R_s \) at \( t = 167.6 \) \( P \) that formed two cycles before.

As mentioned above, the formation of the Si-depletion region begins with the infalling gas in front of the coming pulsation shock, and the region moves outward with the formation of the 2nd type CDS that is triggered by merging with the next pulsation shock. Thus, the Si-depletion region forms once every two pulsation periods. Also, even in the other regions, the resulting value of \( f_{\text{Si}} \) often exceeds 0.1. Thus, in contrast to the very small value of, at most, \( 10^{-6} \) in the LTE case, a large amount of SiC grains can condense thanks to the inverse greenhouse effect in the non-LTE case.

Figure 6 presents the radial variations of the gas and grains at \( t = 176.3 \) \( P \). It seems that the SiC grains are concentrated around the outer boundaries of the 1st type CDSs in the density distribution (see the top row in Figure 6) because the shock associated with the formation of the carbon dust shell sweeps up the gas. Reflecting the variation of the gas density, the radial distribution of \( p_{\text{SiC}} \) does not always correspond to the Si-depletion region, which is shown in the second row of Figure 6. It should be noted that the extended Si-depletion region does not develop without the 2nd type CDS. This can be demonstrated from an example of the failure of the
alternating formation of both types of carbon dust shells located at 18 \( R_\star \), where the Si-depletion region, which is restricted in a narrow region, resides just ahead of the 1st type CDS that was formed about one cycle after the formation of the Si-depletion region (see the second row in Figure 6). Apart from the 1st type CDS located at 18 \( R_\star \), the extended SiC dust shell corresponding to the Si-depletion region between the 1st and 2nd type CDSs can be clearly recognized in the radial distribution of \( \rho_{\text{SiC}}/\rho_{\text{gas}} \) (see the second and third rows in Figure 6). The radial distribution of \( f_{\text{Si}} \) shows that the Si-depletion region stretched over by the slower-moving 2nd type CDS narrows with outward movements and is compressed by the faster-moving 1st type CDS. Thus, in the outer circumstellar envelope, the radial width tends to be on the order of the stellar radius (see \( f_{\text{Si}} \) around 24 \( R_\star \) where the 2nd type CDS almost merges with the 1st type CDS), and the narrower Si-depletion region...
region seems to reside around the outer boundary of the 1st type CDS.

The radial distribution of the mass ratio SiC/C has a sharp peak in the region just ahead of the outer boundary of the 1st type CDS, and the mass ratio decreases by 0.1 (10^{-4}) toward the outer boundary of the precedent 2nd (1st) type CDS (see the bottom row in Figure 6). The peak value exceeds 10 in the inner circumstellar envelope, and it decreases with increasing r because of the subsequent growth of carbon grains. However, the value of SiC/C in the Si-depletion region still remains larger than 0.2 with the peak value exceeding unity.

The resulting values of the mass-loss rate, terminal velocity, and dust-to-gas mass ratio averaged over the last 60 stellar pulsation periods are 1.10 \times 10^{-3} M_\odot yr^{-1}, 19.5 km s^{-1}, and 1.85 \times 10^{-3}, respectively, for the non-LTE case. The reduction of the terminal velocity compared with the LTE case reflects the weakened acceleration resulting from the reduced amount of carbon grains due to the incorporation of C-bearing gas species into the SiC grains. Averaged over the condensible C-bearing molecules is incorporated into the SiC grains. The averaged value of \rho_C/\rho_{\text{gas}} (f_C) is 1.51 \times 10^{-3} (0.652), while the value of \rho_{\text{SiC}}/\rho_{\text{gas}} (f_{\text{SiC}}) is 3.41 \times 10^{-4} (0.403). The resulting averaged value of SiC/C is 0.226 and is close to the upper value derived from the radiative transfer models. The size distribution of the SiC grains by mass averaged over the last 60 stellar pulsation periods at the outer boundary is depicted in Figure 7. The size distribution shows the broad profile with the mean radius of 0.3 \mu m, which is in contrast to the sharp and single-peaked size distribution of the LTE case presented in Figure 4. In the size range of 0.03 to 4.0 \mu m, 80% of the SiC grains by mass populate in the radii between 0.2 and 1.0 \mu m: the distribution covers the size range of the presolar SiC grains found in the Murchison meteorite well. Thus, the hydrodynamical model of the non-LTE case for the formation of the SiC grains reasonably reproduces the amount of SiC grains inferred from the astronomical observations and the size of the presolar SiC grains extracted from the Murchison meteorite.

6. DISCUSSION

In the calculations of the hydrodynamical models presented in Section 5, we assume that SiC is the starting molecule for the nucleation process of the SiC grains, excluding the process starting from the two-body reaction of the Si2C2 molecules. This may underestimate the amount of the SiC grains in the LTE case since the Si2C2 molecule is more abundant in the lower temperature region than the SiC molecule as shown in Figure 1 (left). In the LTE case where carbon grains condense in prior to SiC grains, the nucleation process, beginning with the two-body reaction of the Si2C2 molecules, dominates the nucleation rate in the region around 6–8 R_*, whose gas temperature ranges from 600 to 800 K. However, the gas density in the region of \rho \sim 10^{-12} g cm^{-3} is too low to increase the amount of SiC grains; even if this process is included in the calculation, the resulting values of both f_{\text{Si}} and SiC/C are limited to 10^{-4}, even though the nucleation rate is much larger than that starting from the SiC molecule. In addition, this nucleation process produces the population of grains whose radii are much smaller than 6.0 \times 10^{-2} \mu m, making the modal radius smaller than 3.0 \times 10^{-2} \mu m. Thus, the nucleation process that begins with the two-body reaction of the Si2C2 molecules does not change the conclusion that the hydrodynamical models with the LTE-case cannot reproduce the amount of SiC grains around the C-rich AGB stars inferred from the astronomical observation and the size range derived from the analysis of the presolar grains.

In the non-LTE case, this nucleation process dominates the formation of SiC grains in the region of r > 4 R_*, and is particularly activated in the outer part of the carbon dust shell. Although the number of SiC grains produced through this process reaches about 10 times that produced through the nucleation beginning with the SiC molecule, the typical radius of SiC grains formed in the region with a low gas density is limited to 3 \times 10^{-3} to 6 \times 10^{-2} \mu m. Thus, the inclusion of this nucleation process does not affect the size distribution of
SiC grains whose radius is larger than 0.1 μm. This is also true for the amount of SiC grains since the averaged $f_{\alpha}$ increases by only a few percent. Thus, we conclude that the inclusion of the nucleation process beginning with the two-body reaction of the Si$_2$C$_2$ molecules does not affect the result of the calculations in the non-LTE case, except for the size distribution in the range of $\alpha_{SC} < 6 \times 10^{-2} \mu m$.

The sticking probability set to be unity for the nucleation and growth processes of SiC grains may overestimate the size and amount of the SiC grains formed in the non-LTE case. Figure 8 shows the time-averaged size distributions by mass of the SiC grains for given values of $\alpha_s$. In the range of $\alpha_s = 0.1$ to 1.0, the mass fraction of the large-sized grains with $a > 1.0 \mu m$ decreases significantly and the profile becomes narrow with decreasing $\alpha_s$, while the reduction of $\alpha_s$ does not affect the mass fraction of small-sized grains with $a \leq 0.1 \mu m$. The modal radii are 0.30 and 0.22 μm for $\alpha_s = 0.5$ and 0.1, respectively. Although the SiC grains with radii larger than 1.0 μm do not form for the case of $\alpha_s = 0.1$, the hydrodynamical models in the non-LTE case reasonably reproduce the size range of the presolar SiC grains extracted from the Murchison meteorite (Amari et al. 1994) as long as $\alpha_s \gtrsim 0.1$. The averaged value of SiC/C decreases with decreasing $\alpha_s$; the values are 0.199 and $9.77 \times 10^{-2}$ for $\alpha_s = 0.5$ and 0.1, respectively, which are within the range of the value inferred from the radiative transfer models. Although the reduction of $\alpha_s$ substantially changes the radial distribution of the SiC grains, we conclude that the hydrodynamical models in the non-LTE case cover the ranges of size derived from the analysis of presolar grains and the amount evaluated from the radiative transfer models unless the sticking probability $\alpha_s \lesssim 0.1$.

The mass ratio of SiC inferred from the radiative transfer models depends on the models used in the calculation; the evaluated values for the C-rich AGB stars with the emission feature of the SiC grains are in the range of 0.01 to 0.29 (Lorenz-Martins & Lefèvre 1994), 0.01–0.15 (Groenewegen 1995; Groenewegen et al. 1998), and 0.1–0.3 (Blanco et al. 1998). The smaller value by Groenewegen (1995) and Groenewegen et al. (1998) is considered to be ascribed to the grain model; the temperature of the composite grain consisting of carbon and SiC used in their model is higher than that of the isolated SiC grains used in the other models as is shown in Blanco et al. (1998), since carbon grains are more absorptive in the visible to the NIR region than SiC grains. Therefore, to reproduce the observed SEDs, if the inner boundary of the dust layer is placed close to the photosphere, the high temperature of the composite grains reduces the value of SiC/C. Also, the smaller value of 0.01–0.06 derived by Lorenz-Martins & Lefèvre (1994) for C-rich AGB stars showing the SiC emission feature with optically thick shells ($r_{\mu m} > 3.0$) would arise from the optical constant of the SiC grains used in the models; the radiative transfer models usually employ the optical constants derived from the SiC powder synthesized in the laboratory (Borghesi et al. 1985; Pégourié 1988). The absorption coefficients in the visible to infrared regions (up to $\sim 9 \mu m$) is much larger than those of the crystalline SiC (Choyke & Palik 1985; Pitman et al. 2008; Hofmeister et al. 2009), which results in the higher temperature of SiC grains and the smaller SiC/C. In addition, the mid-infrared observation of C-rich AGB stars by the Spitzer shows that the 30-μm emission feature attributed to MgS grains becomes prominent with the decrease in the strength of the SiC emission feature in the stars with a mass-loss rate larger than $10^{-6} M_{\odot}$ yr$^{-1}$ (Leisenring et al. 2008). Zhukovska & Gail (2008) demonstrate that the absorption efficiency around 11.3 μm of grains consisting of an SiC core and an MgS mantle decreases by increasing the volume fraction of the MgS mantle. Therefore, if it is true, the radiative transfer model could underestimate the value of SiC/C without including SiC grains coated by the MgS mantle. Thus, the mass ratio of SiC to carbon grains derived from the radiative transfer models depends on the optical constants of SiC as well as the model of grains used in the calculations. The value of SiC/C up to $\sim 0.23$ calculated in the non-LTE case for C-rich AGB stars is not always considered to be in conflict with the values derived from the SED fittings.

7. SUMMARY

The formation of SiC grains around C-rich AGB stars is investigated for the first time in the framework of the hydrodynamical model for the pulsation-enhanced dust-driven wind. We formulate the nucleation and growth processes of SiC grains, considering that SiC grains nucleate and grow homogeneously starting from a SiC molecule. In the calculations, we consider two cases for the nucleation process of the SiC grains: (1) the LTE case in which the vibration temperature $T_v$ of the SiC cluster is equal to the gas temperature, and (2) the non-LTE case in which $T_v$ is assumed to be the same as the temperature of the small SiC grain whose radius is $10^{-3} \mu m$. On the other hand, the vibration temperature of the carbon cluster is considered to be the same as the gas temperature, which is usually assumed in the hydrodynamical models for C-rich AGB stars.

The results of the calculations for the model parameters $M_s = 1.0 M_{\odot}$, $L_s = 10^4 L_{\odot}$, $T_{\text{eff}} = 2600$ K, $C/O$ ratio = 1.4, $P = 650$ days, and $\Delta V_p = 2.0$ km s$^{-1}$ are summarized as follows: in the LTE case, SiC grains form in the accelerated and low-density outflowing gas after the formation of carbon grains. The resulting time-averaged number fraction of Si atoms locked into SiC grains (condensation efficiency $f_{\alpha}$) of at most $10^{-8}$ is too small to reproduce the amount of SiC grains inferred from the astronomical observations, and the radius is limited to less than 0.1 μm. On the other hand, in the non-LTE case, the time-averaged mass ratio of SiC to carbon grains ranges from
0.098 to 0.23 for the sticking probability $\alpha_s = 0.1 - 1.0$, which is not in conflict with the value of 0.01 - 0.3 inferred from the radiative transfer models. The time-averaged size distribution of SiC grains by mass with a peak at the radius of 0.2 - 0.3 $\mu$m covers well the size range of the presolar SiC grains extracted from the Murchison meteorite. Thus, we conclude that the so-called inverse greenhouse effect plays a crucial role in the formation process of SiC grains in the pulsation-enhanced dust-driven winds from C-rich AGB stars, apart from the validity of the underlying assumption made in the non-LTE case. The non-LTE effect should be explored for the formation process of dust grains in astrophysical environments.

The hydrodynamical model provides the two types of carbon dust shells, the 1st (2nd) type CDS with the peak value of $f_c \geq 0.9$ ($0.3 \leq f_c \leq 0.7$). The formation region and the resulting radial distribution of SiC grains in the hydrodynamical model with the non-LTE case is closely related with the formation and dynamics of the carbon dust shell, especially through the density enhancement and the backwarming effect. In the inner circumstellar envelope, the SiC dust shell can be discriminated from the 1st type CDS through the extended Si-depletion region caused by the 2nd type CDS formed in the outer part of the active SiC formation region. However, in the outer circumstellar envelope of $r > 20 R_*$, the SiC dust shell is localized around the outer boundary of the 1st type CDS. Not only the formation region and the radial distribution but also the amount and the size distribution of the SiC grains could heavily depend on the C/O ratio as well as the other model parameters. For instance, in the non-LTE case with $M_\ast = 2.0 M_\odot$, the mass ratio of Si to gas and size of SiC are almost the same as those with $M_\ast = 1.0 M_\odot$ while the mass-loss rate decreases by a factor of five. A more comprehensive study that covers a wide range of model parameters is necessary for revealing the amount and size distribution of SiC grains formed around C-rich AGB stars. Also, the difference between the radial distributions of carbon and SiC grains could greatly influence the appearance of the spectral feature attributed to SiC grains. These aspects will be investigated in forthcoming papers.

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