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PROBING THE PHYSICAL CONDITIONS OF SUPERNOVA EJECTA WITH THE MEASURED SIZES OF PRESOLAR Al_2O_3 GRAINS

Takaya Nozawa[1], Shigeru Wakita[2], Yasuhiro Hasegawa[1,4], and Takashi Kozasa[3]
[1] Division of Theoretical Astronomy, National Astronomical Observatory of Japan, Mitaka, Tokyo 181-8588, Japan; takaya.nozawa@nao.ac.jp
[2] Center for Computational Astrophysics, National Astronomical Observatory of Japan, Mitaka, Tokyo 181-8588, Japan
[3] Department of Cosmosciences, Graduate School of Science, Hokkaido University, Sapporo 060-0810, Japan
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ABSTRACT

A few particles of presolar Al_2O_3 grains with sizes above 0.5 μm are believed to have been produced in the ejecta of core-collapse supernovae (SNe). In order to clarify the formation condition of such large Al_2O_3 grains, we investigate the condensation of Al_2O_3 grains for wide ranges of the gas density and cooling rate. We first show that the average radius and condensation efficiency of newly formed Al_2O_3 grains are successfully described by a non-dimensional quantity Λ_{on}, defined as the ratio of the timescale with which the supersaturation ratio increases to the collision timescale of reactant gas species at dust formation. Then we find that the formation of submicron-sized Al_2O_3 grains requires at least 10 times higher gas densities than those presented by one-dimensional SN models. This indicates that presolar Al_2O_3 grains identified as having their origin in SNe might be formed in dense gas clumps, allowing us to propose that the measured sizes of presolar grains can be a powerful tool for constraining the physical conditions in which they formed. We also briefly discuss the survival of newly formed Al_2O_3 grains against destruction in the shocked gas within SN remnants.

Key words: dust, extinction – Galaxy: evolution – ISM: supernova remnants – meteorites, meteors, meteoroids – stars: massive – supernovae: general

1. INTRODUCTION

The role of core-collapse supernovae (SNe) as dust producers is a fundamental issue for understanding the evolution history of dust in the universe. Recent far-infrared observations of young supernova remnants (SNRs) revealed that 0.1–1 $M_\odot$ of dust had formed in the metal-rich inner ejecta (Barlow et al. 2010; Sibthorpe et al. 2010; Matsuura et al. 2011, 2015; Gomez et al. 2012; Indebetouw et al. 2014). However, it remains to be clarified what fraction of these newly formed grains can survive destruction in the shock-heated gas within SNRs and be injected into the interstellar medium (ISM). The destruction efficiency of dust grains depends on their chemical compositions and size distributions (e.g., Nozawa et al. 2007), which are determined by the density and temperature evolution of the gas out of which they form (Nozawa & Kozasa 2013) as well as the degree of mixing and clumpiness of the ejecta (Nozawa et al. 2003; Sarangi & Cherchneff 2015). Therefore, the physical condition and structure of the SN ejecta must be fully appreciated through various approaches to unravel the properties of dust that is formed in the ejecta and is finally ejected into the ISM.

Presolar grains, which are identified in meteorites due to their highly anomalous isotopic compositions, are invaluable fossils that enable us to directly observe the detailed chemical compositions and sizes of stellar dust (Clayton & Nittler 2004 and references therein). Their isotopic signatures give clues about nucleosynthesis in stars and mixing of elements in the SN ejecta. In addition, the measured sizes of presolar grains could offer key information on the physical conditions at their formation sites.

Among the presolar grains that are considered to have originated in SNe, Al_2O_3 grains are of great importance because Al_2O_3 is believed to be one of the major dust components in the Cassiopeia A (Cas A) SNR (Douvion et al. 2001; Rho et al. 2008). Furthermore, most of the dust formation calculations have predicted the formation of Al_2O_3 grains in the ejecta of SNe as the first condensate among oxide grains (Kozasa et al. 1989, 1991; Todini & Ferrara 2001; Nozawa et al. 2003, 2008, 2010; Bianchi & Schneider 2007; Kozasa et al. 2009; Sarangi & Cherchneff 2015). However, the calculated sizes of Al_2O_3 grains are below $\simeq$0.03 μm, which is much smaller than the measured sizes of presolar Al_2O_3 grains with 0.5–1.5 μm in diameter (Choi et al. 1998; Nittler et al. 1998), and such small Al_2O_3 grains are found to be almost completely destroyed in the hot gas within the SNRs before being ejected into the ISM (Nozawa et al. 2007; Silvia et al. 2010, 2012). This seems to contradict the fact that we are observing Al_2O_3 grains of an SN origin on the Earth.

One of the main reasons why only small Al_2O_3 grains are produced in simulations is the low number density of Al atoms in the ejecta, led by the relatively homogeneous ejecta of spherically symmetric SN models (hereafter referred to as 1D SN models). In reality, the SN ejecta should be much more inhomogeneous and complicated, as is suggested from multi-dimensional hydrodynamic simulations (e.g., Kifonidis et al. 2003; Hammer et al. 2010; Joggerst et al. 2010) and various observations of SN 1987A (e.g., Kjær et al. 2010; Larsson et al. 2013). This implies that the formation of dust grains would proceed in the gases with a variety of densities and that large grains could be formed in high-density clumps.

In this Letter, we investigate the formation of Al_2O_3 grains for wide ranges of density and cooling rates of gas to explore the formation condition of presolar Al_2O_3 grains as large as those measured in meteorites. We show that submicron-sized Al_2O_3 grains can be produced only in gas with more than 10 times higher densities than those predicted by 1D SN models, suggestive of the presence of dense gas clumps in the ejecta.

[4] EACOA Fellow.

We also examine the survival of Al_2O_3 grains against the destruction process in SNRs. We propose that the comparison between the calculated sizes and the measured sizes of presolar grains can be a novel and valuable approach that gives insight into the physical conditions and structure of the SN ejecta.

2. MODEL OF DUST FORMATION

The formation of Al_2O_3 grains is calculated by applying the formula of non-steady-state dust formation in Nozawa & Kozasa (2013). In this formula, the formation of small clusters and the growth of grains are self-consistently followed under the consideration that the kinetics of the dust formation process is controlled by collisions of key species, defined as the gas species that have the lowest collisional frequency among reactants. The formula leads us to derive the size distribution and condensation efficiency of newly formed grains, given chemical reactions for the formation of clusters, abundances of the relevant gas species, and time evolutions of gas density and temperature. The detailed prescription of the calculations of non-steady dust formation is given in Nozawa & Kozasa (2013).

In the ejecta of SNe, the most likely formation site of Al_2O_3 grains is the O-rich layer, where Al atoms as well as O atoms abundantly exist. We consider as a chemical reaction at cluster formation $2Al + 3O \rightleftharpoons Al_2O_3$ (Kozasa et al. 1989). The initial number ratio of Al to O atoms is taken as $c_{Al,0}/c_{O,0} = 1/200$, where $c_{Al,0}$ and $c_{O,0}$ are, respectively, the number densities of Al and O atoms at a given initial time $t = t_0$, so that the key species are Al atoms. This abundance ratio approximately corresponds to that in the Al-rich region of solar-metallicity SNe (see, e.g., Kozasa et al. 2009; Nozawa et al. 2010). Note that the results of calculations are little affected by the Al/O ratio as long as $c_{Al,0}/c_{O,0} \ll 1$.

The ejecta of SNe freely expands after ~1 day post-explosion, and the gas density is inversely proportional to the cube of time t. Thus, the number density of a gas species $\tilde{c}_i(t)$ (where i is Al or O), without the depletion of the gas-phase atoms due to the formation of clusters and grains, is given by

$$\tilde{c}_i(t) = c_{i,0}\left(\frac{t}{t_0}\right)^{-3}. \quad (1)$$

As in Nozawa & Kozasa (2013), the gas temperature $T(t)$ is assumed to decrease as

$$T(t) = T_0\left(\frac{t}{t_0}\right)^{-3(\gamma-1)}, \quad (2)$$

where T_0 is the gas temperature at t_0 and γ is a free parameter that prescribes the cooling rate.

As the gas cools down, the formation of dust from gas can be realized in a supersaturated state ($S > 1$); S is the supersaturation ratio defined as $\ln S = -\Delta g/kT$ with k being the Boltzmann constant and Δg the change of the chemical potential per key species for the formation of bulk condensate from the reactants, as is formulated in Equation (30) in Nozawa & Kozasa (2013). Here we take t_0 as a time at which $S = 1$ and determine T_0 for a given $c_{Al,0}$ and $c_{O,0}$ from the equation

$$\ln S = -\frac{\Delta \mathring{g}}{kT_0} + \ln\left(\frac{c_{Al,0}kT_0}{p_s}\right) + \frac{3}{2}\ln\left(\frac{c_{O,0}kT_0}{p_s}\right) = 0, \quad (3)$$

where $\Delta \mathring{g}$ is the change of the chemical potential at the standard pressure p_s and is approximated as $\Delta \mathring{g}/kT = -A/T + B$ with the numerical values A and B taken from Nozawa et al. (2003) (see Table 1).

Table 1
Numerical Constants Used for Dust Formation Calculations

$A/10^4$ K	B	a_0[a] (Å)	σ[b] (erg cm^{-2})
18.4788	45.3542	1.718	690

Notes.
[a] Hypothetical radius of the condensate per key molecule.
[b] Surface tension of bulk condensate (Overbury et al. 1975).

In this study, we regard the clusters containing more than 100 Al atoms as grains. This corresponds to the minimum grain radius of $a_* = 8.0$ Å (Al_2O_3 grains are assumed to be spherical). The sticking probability of gas species is assumed to be unity for any sizes of clusters and grains. In the calculations, we take $t_0 = 300$ days, so the free parameters are $c_{Al,0}$ and γ, for which we consider the ranges of $c_{Al,0} = 10^4$–10^{11} cm^{-3} and $\gamma = 1.1$–1.7. The calculations are performed until the gas density becomes so low that grain growth is negligible. In what follows, we mainly examine the resultant behavior of the final average radius $a_{ave,\infty}$ and condensation efficiency $f_{con,\infty}$ which are obtained at the end of the calculations. The condensation efficiency is defined as the fraction of Al atoms locked up in Al_2O_3 grains.

3. RESULTS OF DUST FORMATION CALCULATIONS

Figure 1 shows the size distributions of newly formed Al_2O_3 grains calculated for $\gamma = 1.25$, adopting $c_{Al,0} = 10^7$, 10^8, and 10^9 cm^{-3}. For these cases, all Al atoms are finally locked up in Al_2O_3 grains (that is, $f_{con,\infty} = 1$). As seen from the figure, the size distribution is lognormal-like for any of $c_{Al,0}$ considered here, with a narrower width for a higher $c_{Al,0}$. More importantly, the average radius increases with increasing $c_{Al,0}$: $a_{ave,\infty} = 0.0067$, 0.047, and 0.36 μm for $c_{Al,0} = 10^7$, 10^8, and 10^9 cm^{-3}, respectively. This is because a higher gas density leads to more efficient growth of grains. The results in Figure 1 point out that, for $\gamma = 1.25$, the number density of Al atoms at dust formation must be higher than $\sim 5 \times 10^8$ cm^{-3} in order for Al_2O_3 grains with radii larger than 0.25 μm ($\gtrsim 0.5$ μm in diameter) to form.

Nozawa & Kozasa (2013) demonstrated that the formation process of dust grains is described in terms of the timescales of two physical quantities: the timescale with which the supersaturation ratio S increases τ_{sat} and the collision timescale of key species τ_{coll}. They found that, for C and $MgSiO_3$ grains, the average radius and condensation efficiency are universally scaled by one non-dimensional quantity $\Lambda_{on} \equiv \tau_{sat}(t_{on})/\tau_{coll}(t_{on})$, where t_{on} is the onset time of dust formation ($t_{on} \gtrsim t_0$) and is taken as a time at which the condensation

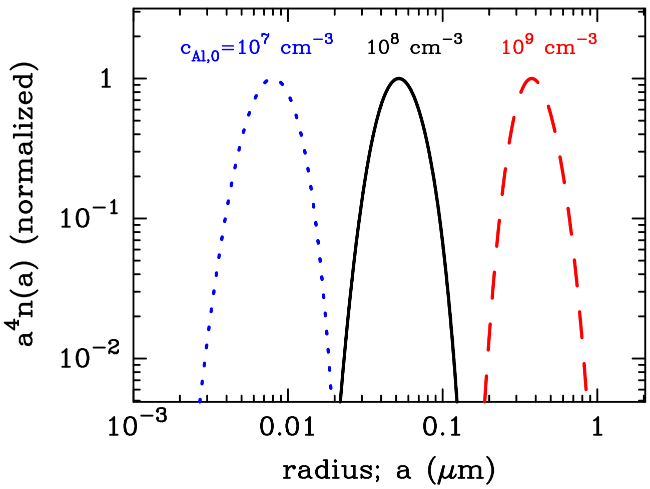

Figure 1. Final size distribution spectrum of newly formed Al_2O_3 grains calculated for $\gamma = 1.25$ and $t_0 = 300$ days. The size distributions are plotted as $a^4\ n(a)$ so as to represent the mass distribution per logarithmic grain radius, where $n(a)$ is the arbitrarily normalized number density of grains with radii between a and $a + da$. Three cases are considered for the number density of Al atoms at $t = t_0$; $c_{\rm Al,0} = 10^7$ (dotted), 10^8 (solid), and 10^9 cm^{-3} (dashed).

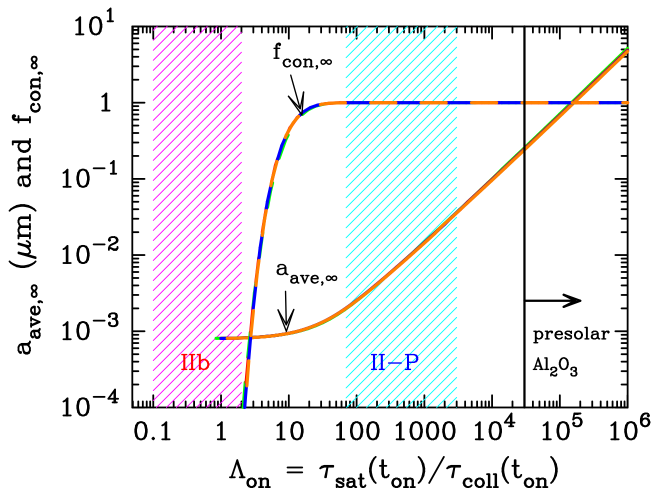

Figure 2. Dependence of the final average radii $a_{\rm ave,\infty}$ and condensation efficiencies $f_{\rm con,\infty}$ of newly formed Al_2O_3 grains on $\Lambda_{\rm on}$. The results for four different γ (γ = 1.1, 1.3, 1.5, and 1.7) are shown in each color but they are plotted as almost the same curve. The hatched regions depict the expected ranges of $\Lambda_{\rm on}$ for the formation of Al_2O_3 grains in the Al-rich region, referring to 1D models of a Type II-P SN (cyan; Kozasa et al. 2009) and a Type IIb SN (Nozawa et al. 2010). The solid vertical line denotes the minimum value of $\Lambda_{\rm on}$ ($=3 \times 10^4$) necessary for explaining the measured sizes (radius of $\geqslant$0.25 μm) of presolar Al_2O_3 grains.

efficiency reaches 10^{-10}. According to their study, it would be interesting to see if such a scaling relation holds for Al_2O_3 grains.

Figure 2 depicts the average grain radii $a_{\rm ave,\infty}$ and condensation efficiencies $f_{\rm con,\infty}$ obtained from the calculations with a variety of $c_{\rm Al,0}$ for each of $\gamma = 1.1$, 1.3, 1.5, and 1.7, as a function of $\Lambda_{\rm on}$. In the present study, $\Lambda_{\rm on}$ is approximately written as (Nozawa & Kozasa 2013)

$$\Lambda_{\rm on} \simeq \frac{1082}{\gamma - 1}\left(\frac{t_{\rm on}}{300\ {\rm days}}\right)\left[\frac{\tilde{c}_{\rm Al}(t_{\rm on})}{10^8\ {\rm cm}^{-3}}\right]\left[\frac{T(t_{\rm on})}{2000\ {\rm K}}\right]^{\frac{3}{2}}. \quad (4)$$

Figure 2 clearly shows that the results for different γ are well overplotted, indicating that both $a_{\rm ave,\infty}$ and $f_{\rm con,\infty}$ are uniquely determined by $\Lambda_{\rm on}$ even for Al_2O_3 grains. As is the case for C and $MgSiO_3$ grains, the formation of Al_2O_3 grains can be realized at $\Lambda_{\rm on} \gtrsim$ 1–2, and $f_{\rm con,\infty} = 1$ at $\Lambda_{\rm on} \geqslant 20$. In addition, $a_{\rm ave,\infty}$ becomes large as $\Lambda_{\rm on}$ increases, which means that the final average radius is larger for a higher gas density and/or a slower gas cooling because $\Lambda_{\rm on}$ is roughly proportional to the product of gas density and cooling timescale that is reflected by $t_{\rm on}$.

In Figure 2, we also plot the ranges of $\Lambda_{\rm on}$ expected in the ejecta of Type II-P and IIb SNe, referring to 1D SN models used in Kozasa et al. (2009) and Nozawa et al. (2010), respectively. For a Type II-P SN with the massive hydrogen envelope, the number density of Al atoms in the Al-rich region is estimated to be $\tilde{c}_{\rm Al}(t_{\rm on}) \simeq (0.2\text{–}8) \times 10^7$ cm^{-3} at $t_{\rm on} = 300$ days. For $\gamma \simeq 1.25$ and $T(t_{\rm on}) \simeq 2000$ K, this corresponds to $\Lambda_{\rm on} \simeq$ 70–3000, for which $a_{\rm ave,\infty} \simeq$ 0.002–0.03 μm. On the other hand, for a Type IIb SN with a small mass envelope, $\tilde{c}_{\rm Al}(t_{\rm on}) \simeq (0.3\text{–}5) \times 10^4$ cm^{-3} at $t_{\rm on} = 300$ days, resulting in $\Lambda_{\rm on} \simeq$ 0.1–2. Hence, Al_2O_3 grains are not expected to form in Type IIb SNe. Nozawa et al. (2010) reported the formation of Al_2O_3 grains in Type IIb SNe but their average radii are less than $\simeq$8 Å, which is regarded as being small clusters in this study.

Our calculations show that, in order to produce Al_2O_3 grains larger than 0.25 μm (diameter of $\geqslant$0.5μm) as measured for presolar grains, $\Lambda_{\rm on}$ should be higher than 3×10^4. Given that γ and $T(t_{\rm on})$ do not change largely, such a high $\Lambda_{\rm on}$ could be achieved by considering the gas densities that are more than one order of magnitude higher than those presented by 1D SN models (namely, $\tilde{c}_{\rm Al}(t_{\rm on}) \gtrsim 7 \times 10^8$ cm^{-3} at $t_{\rm on} = 300$ days; see Equation (4)). This strongly suggests that the discovered presolar Al_2O_3 grains were formed in dense clumps within the ejecta. Equation (4) tells us that the formation of large Al_2O_3 grains may also be possible if the formation time of dust is later than $t_{\rm on} = 3000$ days. However, it is too hard to keep the gas density as high as $\tilde{c}_{\rm Al} \simeq 10^8$ cm^{-3} in such late epochs because the gas density rapidly decreases with time (see Equation (2)).

4. DISCUSSION AND CONCLUSIONS

We have systematically investigated the formation of Al_2O_3 grains, adopting a wide variety of gas densities and cooling rates. We show that, as in the cases of C and $MgSiO_3$ grains, the average radius and condensation efficiency of Al_2O_3 grains are nicely scaled by a non-dimensional quantity $\Lambda_{\rm on}$, defined as the ratio between the timescale of the supersaturation ratio and the collision timescale of key species at dust formation. We also find that large Al_2O_3 grains with radii $\gtrsim$0.25 μm can be formed only in dense gas regions that have more than 10 times higher densities than those estimated from 1D SN models. This points out the presence of dense clumps in the ejecta of core-collapse SNe.

The formation of dust in dense clumps was deduced from various early-phase ($\leqslant$1000 days after explosion) observations of SN 1987A (e.g., Lucy et al. 1991; Meikle et al. 1993; Colgan et al. 1994), which can be classified as a Type II-P SN. The recent radiative transfer models of dust emission and absoption also suggested the necessity of optically thick clumps to account for the evolution of optical to infrared emission from

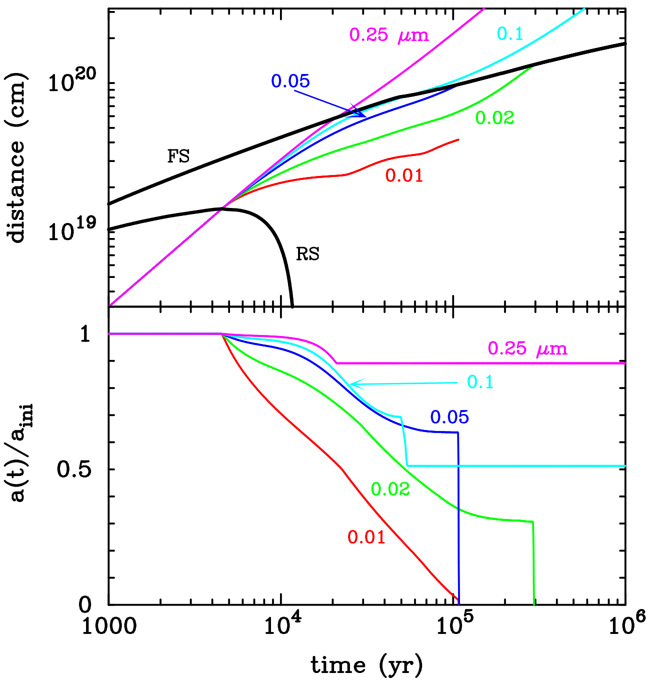

Figure 3. Time evolutions of the positions (upper) and the ratios of radii to the initial ones (lower) of Al_2O_3 grains in an SNR. The results are plotted for the initial grain radii of 0.01, 0.02, 0.05, 0.1, and 0.25 μm. In the upper panel, the thick solid curves depict the trajectories of the forward shock (FS) and reverse shock (RS).

SN 1987A over ≃600–9000 days (Ercolano et al. 2007; Bevan & Barlow 2015; Dwek & Arendt 2015; Wesson et al. 2015). The density contrast between the clumps and interclumps considered by these works is ≃10–100, which is in good agreement with the density enhancement needed for the formation of large Al_2O_3 grains (i.e., more than 10 times that of 1D SN models). This allows us to conclude that the measured size of presolar grains is an independent and useful probe for constraining the clump density in ejecta.

Our calculations show that Al_2O_3 grains cannot form in Type IIb SNe as a result of the too low ejecta density in the 1D SN model. However, the analyses of the infrared emission spectra of Cas A, which was identified as Type IIb through a light echo (Krause et al. 2008), have suggested the presense of newly formed Al_2O_3 grains (Douvion et al. 2001; Rho et al. 2008). This contradiction can also be resolved by considering the dense gas clumps in the ejecta; from Figure 2, we can estimate that the density of gas clumps required for the formation of Al_2O_3 grains (that is, $\Lambda_{\rm on} \gtrsim 2$) is more than 10 times that of the 1D Type IIb SN model. We also note that the recent observation of near-infrared extinction implies the existence of large ($\gtrsim$0.1 μm) Si grains in Cas A, providing another indication of dust formation in dense clumps (Lee et al. 2015).

Next we discuss the survival of Al_2O_3 grains formed in the ejecta against the destruction by SN shocks on the basis of a dust evolution model in SNRs (Nozawa et al. 2007). This model assumes a spherically symmetric shock, but it has been shown that the destruction efficiency of dust is not greatly different from those by multi-dimensional hydrodynamic simulations (Silvia et al. 2010, 2012). As the initial condition of the ejecta, we here consider the core-envelope structure of $3 + 12\,M_\odot$ (implicitly assuming Type II-P SNe). The other input parameters are the explosion energy and the gas density in the ISM, for which we take reasonable values of 1.8×10^{51} erg and 1.0 cm^{-3}, respectively.

The result of the calculation is given in Figure 3, which shows that small grains with initial radii of $a_{\rm ini} \lesssim 0.01$ μm are completely destroyed in the shocked gas. Grains with 0.02 μm $\lesssim a_{\rm ini} < 0.1$ μm are eroded in the hot gas and are finally destroyed as soon as they encounter the cool dense shell that is formed behind the forward shock after $\simeq 5 \times 10^4$ years. On the other hand, Al_2O_3 grains with $a_{\rm ini} \gtrsim 0.2$ μm can be ejected from SNe without reducing their size significantly. This simple calculation illustrates that, once large Al_2O_3 grains are produced in dense clumps, they are likely to survive the destruction in SNRs and to be easily transported to the ISM.[5] Thus, we suggest that the formation of submicron-sized Al_2O_3 grains in dense clumps is also indispensable in order that newly formed Al_2O_3 grains can endure destruction by shocks and be incorporated into nearby molecular clouds and protoplanetary disks.

The identification of Al_2O_3 grains as SN in origin comes from their relatively high $^{18}O/^{16}O$ ratio (so-called Group 4 grains, Nittler et al. 1997; Choi et al. 1998) or large enrichment of ^{16}O (represented by Grain T84, Nittler et al. 1998). Since we consider the formation of Al_2O_3 grains in the O-rich layer where ^{16}O is rich, they may be categorized as T84-like grains (or Group 3 grains with the moderate enhancement of ^{16}O). On the other hand, to explain the ^{18}O-enriched composition of Group 4 grains, the extensive mixing between different layers in the ejecta is invoked with the relatively ^{18}O-rich hydrogen envelope being the dominant component (Nittler et al. 2008). However, even if large-scale mixing takes place, the molecular diffusion lengths are much smaller than the typical size of gas clumps so that the microscopic mixing of elements may be very ineffective (Deneault et al. 2003). Therefore, the origin of the oxygen isotopic composition of the Group 4 Al_2O_3 grains, as well as their formation process, is still a challenging problem.

We conclude that dense gas clumps are necessary for the formation of submicron-sized Al_2O_3 grains as discovered in meteorites. The presence of such dense clumps in the O-rich layer may also cause silicate grains to be formed with very large radii compared to those based on 1D SN models. Given that the radii of silicate grains are generally larger than those of Al_2O_3 grains by a factor of about 10 (e.g., Nozawa et al. 2003), the discovery of ^{16}O-enriched micron-sized (≃1–10 μm) silicate grains in meteorites will serve as further evidence for dense clumps in the SN ejecta.

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[5] In this calculation, we do not include the destruction of dust by non-thermal sputtering resulting from the high-velocity motion of dust after being injected into the ISM in order to focus on the survivability of dust in the SNR.

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