

Comprehensive Study of Thermal Desorption of Grain-surface Species by Accretion **Shocks around Protostars**

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Abstract

We conducted numerical simulations of the dust heating in accretion shocks induced by the interaction between the infalling envelope and the Keplerian disk surrounding a protostar, in order to investigate the thermal desorption of molecules from the dust-grain surfaces. It is thought that the surfaces of the amorphous dust grains are inhomogeneous; various adsorption sites with different binding energies should therefore exist. We assumed that the desorption energy has a Gaussian distribution and investigated the effect of the desorption energy distribution on the desorption-efficiency evaluation. We calculated the desorption fractions of the grain-surface species for wide ranges of input parameters and summarized our results in a shock diagram. The resulting shock diagram suggests that the enhanced line emissions around protostars observed using the Atacama Large Millimeter Array cannot be explained by the thermal desorption in an accretion shock if typical interstellar dust-grain sizes $(\sim 0.1 \ \mu m)$ and a single desorption energy are considered. On the other hand, if significantly smaller dust grains are the main grain-surface species carriers and the desorption energy has a Gaussian distribution, the origin of the enhanced line emission can be explained by the accretion shock heating scenario for all of the three protostars examined in this study: IRAS 04368+2557, IRAS 04365+2535, and IRAS 16293-2422. The small-grain-carrier supposition is quite reasonable when the dust grains have a power-law size distribution because the smaller grains primarily contribute to the dust-grain surface area.

Key words: ISM: clouds - ISM: molecules - protoplanetary disks - shock waves

1. Introduction

The gravitational collapse of a molecular cloud is a transient process inducing the formation of protostars and protoplanetary disks. Keplerian disks have been observed around protostars in the early evolutionary stages, such as Class I (Hogerheijde 2001; Brinch et al. 2007; Lommen et al. 2008; Jørgensen et al. 2009; Lee 2010; Yen et al. 2013, 2014; Harsono et al. 2014), Class 0/I (Tobin et al. 2012; Hara et al. 2013) and Class 0 (Choi et al. 2010; Murillo & Lai 2013; Murillo et al. 2013; Codella et al. 2014; Lee et al. 2014; Ohashi et al. 2014; Tobin et al. 2015) protostars, but the formation process is not yet well understood. Recent Atacama Large Millimeter Array (ALMA) observations have suggested that some molecular species are enhanced at the boundary between the infalling envelope and the forming Keplerian disk, suggesting thermal desorption from the grain surfaces (Sakai et al. 2014a, 2014b, 2016; Podio et al. 2015; Oya et al. 2016). Thermal desorption of the grain-surface species is one of the astrophysical processes that affects the chemical evolution of a nebula. Another important aspect of thermal desorption is that it provides a method for diagnosing the physical and chemical conditions of the forming protoplanetary disks. In order to investigate the Keplerian-disk formation process, it is therefore important to elucidate the desorption mechanism of the grain-surface species and the desorption conditions.

Previously, Sakai et al. (2014b) detected enhanced line emission of warm SO molecules around protostar IRAS 04368 +2557 using ALMA. They revealed that the warm SO

molecules only exist in a ring-like structure. One of the hypotheses to explain the origin of the enhanced SO-line emission is the following: the SO molecules are abundant on the grain surfaces in the molecular clouds; then, they are thermally desorbed in accretion shocks induced by the interaction between the infalling envelope and the forming Keplerian disk. Based on the position-velocity (PV) diagram and a simple dynamical model, Sakai et al. (2014b) confirmed that the radius of the ring-like structure corresponds to the centrifugal-barrier position. The infalling envelope, which has a specific angular momentum, cannot flow further inward beyond this barrier because of the centrifugal force. These authors also determined that the gas kinetic temperature at the emitting region is higher than the sublimation temperature of the SO, supporting the case for a thermal desorption origin.

Other possibilities that explain the origin of the enhanced line emission around protostars have also been discussed. Aota et al. (2015) investigated desorption of grain-surface species in accretion shocks not only via thermal desorption, but also by sputtering. They concluded that thermal desorption is much more efficient than sputtering. Sakai et al. (2014b) examined two possible dust-heating mechanisms other than accretion shocks: (i) an outflow shock on the disk surface, and (ii) protostellar heating. The authors discussed that the outflow shock is probably not a major cause because the enhanced line emission is localized at the centrifugal barrier and has a rotational velocity component. Furthermore, the protostellar heating does not necessarily explain the line enhancement concentrated at the centrifugal barrier; it is just a coincidence even if the distance at which grain-surface species are desorbed by the protostellar heating corresponds to the centrifugal radius. Although these other possibilities cannot be ruled out completely, thermal desorption in accretion shocks can naturally explain the enhancement of the SO emission at the centrifugal barrier.

However, the validity of the accretion shock hypothesis should be assessed more carefully. In general, the dust temperature is lower than the ambient gas because of the efficient radiative cooling; thus, the gas kinetic temperature does not constitute direct evidence of the thermal desorption. In order to determine whether thermal desorption occurs, we must obtain the dust temperature in the shocks and then evaluate the desorption-efficiency quantitatively. When molecules exist on the grain surface in the submonolayer, the thermal desorption is described by a first-order Polanyi-Wigner equation (e.g., King 1975),

$$\frac{dN}{dt} = -N\nu e^{-\frac{E_{\rm des}}{T_{\rm dust}}},\tag{1}$$

where *N* is the number of molecules on the grain surface per unit area, ν is the vibrational frequency, E_{des} is the desorption energy in units of Kelvin, and T_{dust} is the dust temperature. Aota et al. (2015) previously performed numerical simulations of the shock wave heating to obtain $T_{dust}(t)$ after the passage of the shock front and integrated Equation (1) to evaluate the thermal desorption efficiency. Their results, however, suggest that the SO molecules are only minimally desorbed from the dust surface in the accretion shock when the shock parameters speculated from the ALMA observation are considered (see Section 3.1 for details).

The previous calculation probably lacked two important factors that affect the desorption-efficiency evaluation. Aota et al. (2015) assumed a single value of the SO-molecule desorption energy, $E_{des} = 2600$ K. This value is the same as that listed in the UMIST database RATE12 (McElroy et al. 2013). However, E_{des} is not represented by a single (average) value, especially on the surfaces of amorphous substrates, as suggested by previous temperature-programed desorption (TPD) experiments (Kimmel et al. 2001; Amiaud et al. 2006; Fillion et al. 2009) and molecular dynamics calculations (Al-Halabi et al. 2004; Al-Halabi & van Dishoeck 2007). As the interstellar grains are also amorphous (Kemper et al. 2004; Henning 2010), E_{des} should be broadly distributed. The effect of the E_{des} distribution on the desorption efficiency of the grain-surface species has not been investigated. In addition, in their study, Aota et al. (2015) examined the case in which the dust-grain radius is 0.1 μ m only. However, it has been suggested that dust sizes are widely distributed from approximately 0.005 to 1 μ m for graphite and 0.025 to 0.25 μ m for other materials in the interstellar clouds (Mathis et al. 1977). If the dust grains have a power-law size distribution with an exponent of \simeq 3.5, as suggested by Mathis et al. (1977), smaller grains primarily contribute to the dustgrain surface area. The smaller dust grains have lower emissivities; thus, they are more significantly heated than the larger grains. This suggests that the grain-surface species desorption efficiency is higher than that expected from previous calculations. In this paper, we reevaluate the desorption efficiency of the grain-surface species, taking both the E_{des} and dust-size distributions into consideration, and verify the



Figure 1. (a) Schematic of dust heating in a shock wave at the shock-front rest frame. The pre-shock gas and dust grains flow into the shock front with the same velocity. The gas is compressed and decelerated suddenly behind the shock front. On the other hand, the dust grains retain their pre-shock velocity; thus, they should have a relative velocity with respect to the post-shock gas. (b) Gas and dust velocities with respect to the shock front. The horizontal axis is the distance from the shock front, *x*. The relative velocity between the gas and dust is reduced gradually by the gas friction. (c) Gas and dust temperatures. The dust grains are heated aerodynamically behind the shock front. After the gas-dust relative velocity is reduced, the thermal conduction from the ambient hot gas maintains the dust-grain temperature. Finally, they are cooled to the unshocked temperature.

shock-heating scenario as the origin of the enhanced line emission around the protostars.

2. Model

Figure 1(a) shows a schematic of the dust-heating mechanism in a shock wave. In the pre-shock region, the gas and dust move at the same velocity with respect to the shock front, $v_{\rm s}$, which is termed the shock velocity. The gas is suddenly decelerated at the shock front. In contrast, the dust passes through the shock front while retaining its pre-shock velocity because of its large inertia. Thus, a high relative velocity is induced between the gas and the dust behind the shock front. The relative velocity is gradually decreased by the gas friction (see Figure 1(b)). The dust is heated aerodynamically until the gas-dust relative velocity is reduced significantly (see Figure 1(c)). After the relative velocity is reduced, the thermal conduction from the ambient hot gas maintains the dust-grain warmth until the gas is cooled. T_{dust} reaches a maximum in response to the aerodynamic heating; however, the conductive heating continues for a longer duration.

Therefore we must consider both heating regions in order to perform a quantitative evaluation of the desorption efficiency.

We divide the calculation scheme into three steps. First, we calculate the variations of the post-shock gas quantities, such as the density, velocity, and temperature (see Section 2.1). Second, we calculate the dust thermal history using the post-shock gas quantities obtained in the first step (see Section 2.2). The first and second steps follow the conventional model adopted in previous studies. Finally, we calculate the dust thermal history obtained in the second step (see Section 2.3). We take the E_{des} distribution into account, which has not been considered previously. We describe the calculation methods in detail in Section 2.4. The ranges of input parameters that we examined in this study are discussed in Section 2.5.

2.1. Post-shock Gas Structure

We adopt the steady shock model with one-dimensional plane-parallel geometry in order to calculate the post-shock gas quantities. The same model has often been used to simulate interstellar (Shapiro & Kang 1987; Hollenbach & McKee 1989) and nebular shocks (Ruzmaikina & Ip 1994; Iida et al. 2001; Miura & Nakamoto 2005, 2006).

We use the subscript "s" to denote the pre-shock gas quantities. The quantities immediately behind the shock front, denoted by subscript "gas,0," are given by the Rankine-Hugoniot relation, such that

$$\frac{\rho_{\text{gas},0}}{\rho_{\text{s}}} = \frac{v_{\text{s}}}{v_{\text{gas},0}} = \frac{(\gamma+1)M^2}{(\gamma-1)M^2+2} \text{ and}$$

$$\frac{T_{\text{gas},0}}{T_{\text{s}}} = \frac{\{2\gamma M^2 - (\gamma-1)\}\{(\gamma-1)M^2+2\}}{(\gamma+1)^2M^2}, \qquad (2)$$

where ρ is the density, v is the velocity, T is the temperature, γ is the specific-heat ratio, $M = v_s / \sqrt{\gamma k_B T_s / (\mu m_H)}$ is the Mach number, k_B is the Boltzmann constant, μ is mean molecular weight of the gas, and m_H is atomic mass unit. The gas is cooled as it moves away from the shock front. The physical quantities of the post-shock gas, denoted by subscript "gas," are determined from the hydrodynamics equations for one-dimensional plane-parallel steady flow:

$$\rho_{\rm gas,0} v_{\rm gas,0} = \rho_{\rm gas} v_{\rm gas},\tag{3}$$

$$\rho_{\rm gas,0} v_{\rm gas,0}^2 + p_{\rm gas,0} = \rho_{\rm gas} v_{\rm gas}^2 + p_{\rm gas}, \tag{4}$$

$$\frac{de_{\rm gas}}{dt} = \frac{p_{\rm gas} + e_{\rm gas}}{\rho_{\rm gas}} \frac{d\rho_{\rm gas}}{dt} - \Lambda, \tag{5}$$

where $p_{\text{gas}} = \rho_{\text{gas}} k_{\text{B}} T_{\text{gas}} / (\mu m_{\text{H}})$ is the gas pressure, $e_{\text{gas}} = p_{\text{gas}} / (\gamma - 1)$ is the gas internal energy, and Λ is the cooling function. We consider a pre-shock gas number density higher than 10^6 cm^{-3} , where the gas-dust collisional cooling dominates Λ , which is given by (Aota et al. 2015)

$$\Lambda = \frac{1}{2} \pi^{1/2} a_{\rm c}^2 n_{\rm c} \rho_{\rm gas} (T_{\rm gas} - T_{\rm c}) \frac{\gamma + 1}{\gamma - 1} \left(\frac{2k_{\rm B}}{\mu m_{\rm H}}\right)^{3/2} T_{\rm gas}^{1/2}, \quad (6)$$

where a_c , T_c , and n_c are the radius, temperature, and number density of the coolant dust grains, respectively. Note that we distinguish the coolant dust grains from the dust grains described in Section 2.2 for simplicity. The coolant grains pass through the shock front as well as other dust grains, but the relative velocity with respect to the post-shock gas is neglected in the cooling rate evaluation. Note that the same assumption was employed by Aota et al. (2015). T_c is determined by the energy balance between the energy transfer from gas to dust and the radiative cooling (see Section 2.2 for details). Furthermore, n_c satisfies the relation $(4/3)\pi a_c^3 \rho_{mat} n_c = \eta_c \rho_{gas}$, where η_c is the mass ratio of the coolant dust to the gas. We use $a_c = 0.1 \ \mu m$ and $\eta_c = 10^{-2}$ in this study. Note that our results are not affected by the choice of a_c and η_c in the low-gas-density region of interest.

2.2. Thermal History of Dust

We adopt the theory of gas-grain energy and momentum transfers in the free molecular flow approximation (Probstein 1968; Kitamura 1986) because the dust radius of interest is significantly smaller than the mean free path of the gas. This theory covers the entire range of the gas-dust relative velocity from the aerodynamic heating region to the conductive heating region. This theory has been used in previous studies of the chondrule formation in shock waves (Hood & Horanyi 1991, 1993; Iida et al. 2001; Desch & Connolly 2002; Ciesla & Hood 2002; Miura et al. 2002; Miura & Nakamoto 2005, 2006).

The variation in dust velocity with respect to the shock front, v_{dust} , is given by

$$\frac{4}{3}\pi a_{\text{dust}}^3 \rho_{\text{mat}} \frac{dv_{\text{dust}}}{dt} = -\pi a_{\text{dust}}^2 \frac{C_{\text{D}}}{2} \rho_{\text{gas}}$$
$$\times (v_{\text{dust}} - v_{\text{gas}}) |v_{\text{dust}} - v_{\text{gas}}|, \tag{7}$$

where a_{dust} is the dust radius and ρ_{mat} is the density of the material composed of the dust. C_D is the drag coefficient, given by (Probstein 1968)

$$C_{\rm D} = \frac{2}{3s_{\rm a}} \left(\frac{\pi T_{\rm dust}}{T_{\rm gas}} \right)^{1/2} + \frac{2s_{\rm a}^2 + 1}{s_{\rm a}^3 \pi^{1/2}} \exp(-s_{\rm a}^2) + \frac{4s_{\rm a}^4 + 4s_{\rm a}^2 - 1}{2s_{\rm a}^4} \operatorname{erf}(s_{\rm a}),$$
(8)

where $s_a = |v_{dust} - v_{gas}|/\sqrt{2k_BT_{gas}/(\mu m_H)}$ is the ratio of the gas-dust relative velocity to the gas-molecule thermal velocity and erf(x) is the error function defined by $erf(x) = (2/\sqrt{\pi}) \int_0^x e^{-t^2} dt$. The variation of T_{dust} is given by

$$\frac{4}{3}\pi a_{\rm dust}^3 \rho_{\rm mat} c_{\rm dust} \frac{dT_{\rm dust}}{dt} = 4\pi a_{\rm dust}^2 (\Gamma - \epsilon_{\rm em} \sigma_{\rm SB} T_{\rm dust}^4), \quad (9)$$

where c_{dust} is the dust specific heat, Γ is the rate of energy transfer from gas to dust per unit area, ϵ_{em} is the Planck mean emission efficiency, and σ_{SB} is the Stefan-Boltzmann constant. Γ is given by

$$\Gamma = \rho_{\rm gas} |v_{\rm dust} - v_{\rm gas}| (T_{\rm rec} - T_{\rm dust}) C_{\rm H}, \tag{10}$$

where $T_{\rm rec}$ and $C_{\rm H}$ are the recovery temperature and the heat transfer function, respectively, given by (Probstein 1968;

Kitamura 1986)

$$T_{\rm rec} = \frac{T_{\rm gas}}{\gamma + 1} [2\gamma + 2(\gamma - 1)s_{\rm a}^2 - \frac{\gamma - 1}{\frac{1}{2} + s_{\rm a}^2 + s_{\rm a}\pi^{-1/2}e^{-s_{\rm a}^2}/\operatorname{erf}(s_{\rm a})} \bigg],$$
(11)

and

$$C_{\rm H} = \frac{\gamma + 1}{\gamma - 1} \frac{k_{\rm B}}{8\mu m_{\rm H} s_{\rm a}^2} \bigg[\pi^{-1/2} s_{\rm a} e^{-s_{\rm a}^2} + \bigg(\frac{1}{2} + s_{\rm a}^2\bigg) \operatorname{erf}(s_{\rm a}) \bigg].$$
(12)

As described in Section 2.1, we determine the coolant grain temperature T_c assuming that the relative velocity with respect to the gas is negligibly low. For $s_a \ll 1$, we can approximate $T_{\rm rec} \rightarrow T_{\rm gas}$ and $C_{\rm H} \rightarrow (1/(4\pi^{1/2}s_{\rm a}))((\gamma + 1)/(\gamma - 1))(k_{\rm B}/(\mu m_{\rm H}))$. In this case, the energy balance equation, which is given by $\Gamma - \epsilon_{\rm em}\sigma_{\rm SB}T_c^4 = 0$, is rewritten as

$$\frac{1}{8\pi^{1/2}} \frac{\gamma+1}{\gamma-1} \rho_{\rm gas} \left(\frac{2k_{\rm B}}{\mu m_{\rm H}}\right)^{3/2} T_{\rm gas}^{1/2} (T_{\rm gas} - T_{\rm c}) - \epsilon_{\rm em} \sigma_{\rm SB} T_{\rm c}^4 = 0.$$
(13)

We solve Equation (13) for T_c using a bisection method.

Finally, we introduce a new function for ϵ_{em} , which is suitable for submicron dust grains composed of astronomical silicates, i.e.,

$$\epsilon_{\rm em} = A \ a_{\rm dust} T_{\rm dust}^2, \tag{14}$$

where A = 0.122 cm⁻¹ K⁻² (see Appendix A).

2.3. Desorption Fraction

Let us consider the scenario in which the roughness of the amorphous dust surface provides various adsorption sites with different E_{des} . The numbers of adsorption sites and adsorbed molecules per unit area, where the desorption energy ranges from E_{des} to $E_{des} + dE_{des}$, are denoted by $N_{site}(E_{des})dE_{des}$ and $N_{ad}(E_{des})dE_{des}$, respectively. We assume that each site can be occupied by one molecule at most; in other words, $N_{ad}(E_{des})$ cannot exceed $N_{site}(E_{des})$. We define the adsorption-site distribution function as

$$f_{\text{site}}(E_{\text{des}}) = \frac{N_{\text{site}}(E_{\text{des}})}{N_{\text{site,all}}},$$
(15)

where $N_{\text{site, all}} = \int_0^\infty N_{\text{site}}(E_{\text{des}}) dE_{\text{des}}$ is the total number of adsorption sites per unit area. Note that the distribution function satisfies the normalization condition $\int_0^\infty f_{\text{site}}(E_{\text{des}}) dE_{\text{des}} = 1$. We define a population $P(E_{\text{des}})$ as

$$P(E_{\rm des}) = \frac{N_{\rm ad}(E_{\rm des})}{N_{\rm site, all}}.$$
 (16)

Integration of $P(E_{des})$ over E_{des} yields the fractional coverage of molecules on the adsorption sites,

$$\theta = \int_0^\infty P(E_{\rm des}) dE_{\rm des}.$$
 (17)

We obtain $\theta = 1$ when all sites are occupied by molecules (complete adsorption). Furthermore, $P(E_{des})$ varies with time in response to the thermal desorption. Dividing Equation (1) by

 $N_{\rm site, all}$, where N is replaced by $N_{\rm ad}$, we obtain

$$\frac{dP}{dt} = -P(E_{\rm des})\nu e^{-\frac{E_{\rm des}}{T_{\rm dust}}}.$$
(18)

Although ν varies with the grain-surface species in general (Aota et al. 2015), the values are distributed around $\sim 10^{12} \text{ s}^{-1}$ for the species of interest. The change in ν has only a minor effect on our results because the desorption rate is a strong function of T_{dust} . Therefore we use a constant frequency of $\nu = 10^{12} \text{ s}^{-1}$ for simplicity. The desorption fraction is defined by

$$\xi_{\rm des} = 1 - \frac{\theta_{\infty}}{\theta_0},\tag{19}$$

where θ_0 and θ_{∞} are the fractional coverages before and after the dust-heating event, respectively. We obtain $\xi_{des} = 1$ when all grain-surface species are desorbed away (complete desorption).

In general, $f_{\rm site}$ ($E_{\rm des}$) depends on the grain-surface species and the surface structure of the host dust grains. Al-Halabi et al. (2004) have performed classical trajectory calculations of the adsorption of a CO molecule on the surface of compact amorphous water ice. They showed that CO molecules normally impacting the surface with an incident energy of 0.01 eV were adsorbed within a computational time of a few ps, even though the temperature was as high as 90 K. The CO molecules settled on the surface exhibited potential energies ranging from -0.15 to -0.04 eV with an average value of -0.094 eV. Al-Halabi & van Dishoeck (2007) have also performed the classical trajectory calculations on the adsorption of H atoms to water ice surface and found that the binding energy distributions were fitted to Gaussian functions. In this study, we adopt a Gaussian distribution

$$f_{\text{site}}(E_{\text{des}}) = \frac{1}{\sqrt{\pi}\Delta E_{\text{d}}} \exp\left[-\left(\frac{E_{\text{des}} - E_{\text{d}0}}{\Delta E_{\text{d}}}\right)^2\right], \quad (20)$$

where ΔE_d is the standard deviation and E_{d0} is the average value.

In addition, we assume that the population of the grainsurface species, i.e., $P(E_{des})$, only varies in response to the thermal desorption. However, $P(E_{des})$ can also change in response to migration of the grain-surface species along the grain surface (redistribution). In general, the surface-diffusion activation energy is lower than that of the thermal desorption; thus, the surface diffusion should occur simultaneously with the thermal desorption (Kimmel et al. 2001; Amiaud et al. 2006). We examined the effect of the redistribution on the ξ_{des} estimation and concluded that this effect is negligible (Appendix B).

2.4. Calculation Method

First, we calculate the physical quantities of the post-shock gas, ρ_{gas} , v_{gas} , and T_{gas} . The input parameters are v_{s} and n_{s} , where n_{s} is the number density of the H nuclei in the pre-shock region. We assume solar abundance for the gas-phase components, except for H₂O, as follows: $y_{\text{H}_2} = 0.5$, $y_{\text{He}} = 9.75 \times 10^{-2}$, $y_{\text{CO}} = 1.065 \times 10^{-4}$, and $y_i = 0$ for other species, where y_i is the relative abundance of species *i* to the H nuclei. We assume that H₂O is depleted onto the grain surfaces within the molecular clouds. We obtain $\mu = 2.33$ and $\gamma = 1.43$ from

the abundance (Iida et al. 2001). The pre-shock gas density is given by $\rho_s = y_t \mu m_H n_s$, where $y_t = \sum_i y_i = 0.598$, and the preshock gas temperature is set to $T_s = 10$ K. We calculate the gas quantities immediately behind the shock front using Equation (2), and then solve Equations (3)–(5) to obtain the post-shock gas quantities as functions of the time *t* that has elapsed following passage through the shock front. To obtain this solution, we use the finite-difference method presented by Shapiro & Kang (1987). Finally, we obtain the post-shock gas quantities $\rho_{gas}(x)$, $v_{gas}(x)$, and $T_{gas}(x)$ as functions of the distance from the shock front, given by

$$x = \int_0^t v_{\text{gas}}(t)dt.$$
 (21)

Second, we calculate the dust quantities in the post-shock region by solving Equations (7) and (9) for the initial conditions of $v_{dust} = v_s$ and $T_{dust} = T_s$. The gas quantities that appear in these equations are given by the linear interpolation of $\rho_{gas}(x)$, $v_{gas}(x)$, and $T_{gas}(x)$, where

$$x = \int_0^t v_{\text{dust}}(t) dt.$$
 (22)

Note that the relation x(t) for dust is different from that for gas because $v_{dust} \neq v_{gas}$ in general. We adopt a first-order Euler method for the numerical integrations. The time step is given by $\Delta t = \min[|v_{dust}/(dv_{dust}/dt)|, |T_{dust}/(dT_{dust}/dt)|] \times 10^{-3}$ in order to resolve the time variations of v_{dust} and T_{dust} . Note that this method fails when $v_{dust} - v_{gas} \rightarrow 0$ because Δt becomes excessively large. To avoid this problem, we use the following analytic integration method. When $s_a \ll 1$, Equation (7) has the solution

$$v_{\rm rel}(t + \Delta t) = v_{\rm rel}(t) e^{-\frac{\Delta t}{t_{\rm stop}}},$$
(23)

where $v_{rel} = v_{dust} - v_{gas}$ is the dust velocity with respect to the gas and

$$t_{\rm stop} = \frac{a_{\rm dust}\rho_{\rm mat}}{2\rho_{\rm gas}} \left(\frac{\pi\mu m_{\rm H}}{2k_{\rm B}T_{\rm gas}}\right)^{1/2} \left[1 + \frac{\pi}{8} \left(\frac{T_{\rm dust}}{T_{\rm gas}}\right)^{1/2}\right]^{-1}$$

is the stopping time at $s_a \ll 1$. We assume that v_{gas} , ρ_{gas} , T_{gas} , and T_{dust} are constant during the short period of Δt . In the same manner, Equation (9) can be rewritten as

$$\frac{dT_{\text{dust}}}{dt} = -\frac{3}{a_{\text{dust}}\rho_{\text{mat}}c_{\text{dust}}} \{\rho_{\text{gas}}|v_{\text{rel}}|C_{\text{H}}(T_{\text{dust}} - T_{\text{eq}}) + \epsilon_{\text{em}}\sigma_{\text{SB}}(T_{\text{dust}}^4 - T_{\text{eq}}^4)\},$$
(24)

where T_{eq} is the equilibrium dust temperature that satisfies the energy balance equation given by Equation (13). Note that $|v_{rel}|C_H$ does not depend on T_{dust} . Using an approximation of $T_{dust}^4 - T_{eq}^4 \simeq 4T_{eq}^3(T_{dust} - T_{eq})$ at $T_{dust} \simeq T_{eq}$, we obtain $dT_{rel}/dt = -T_{rel}/t_{temp}$, where $T_{rel} = T_{dust} - T_{eq}$ and

$$t_{\text{temp}} = \frac{a_{\text{dust}}\rho_{\text{mat}}c_{\text{dust}}}{3(\rho_{\text{gas}}|v_{\text{rel}}|C_{\text{H}} + 4\epsilon_{\text{em}}\sigma_{\text{SB}}T_{\text{eq}}^3)}$$

Therefore, we obtain an analytic solution of

$$T_{\rm rel}(t + \Delta t) = T_{\rm rel}(t) e^{-\frac{\Delta t}{t_{\rm temp}}}.$$
(25)

Equations (23) and (25) do not constrain Δt . We set Δt to be 1.01 times the previous time step and set $\rho_{\text{mat}} = 3 \text{ g cm}^{-3}$ and $c_{\text{dust}} = 10^7 \text{ erg g}^{-1} \text{ K}^{-1}$.

Finally, we calculate ξ_{des} using the $T_{dust}(t)$ obtained above. We take an E_{des} range of 0 to 10⁴ K, and divide this range into 10⁴ bins of the same width, $dE_d = 1$ K. The desorption energy of the *k*th bin is given by $E_k = (k - 1/2)dE_d$. We assume that all adsorption sites are occupied by molecules before heating; thus, the initial population of the *k*th bin is given by $P_k = f_{site}(E_k)$. The time variation of P_k is calculated using Equation (18), and ξ_{des} is finally obtained from Equations (17) and (19).

2.5. Input Parameters

We set E_{d0} between 1000 and 5000 K, which covers typical values for grain-surface species such as CH₄ (1090 K), CO (1150 K), H₂CO (2050 K), SO (2600 K), H₂S (2743 K), CO₂ (2990 K), HCOOCH₃ (4000 K), H₂O (4800 K), and CH₃OH (4930 K) (McElroy et al. 2013).

We chose $\Delta E_d/E_{d0}$ between 0 and 0.3 based on the result of classical trajectory calculations (see Table 1). The typical value is $\Delta E_d/E_{d0} \simeq 0.2 - 0.3$ for H atoms and CO molecules on water ice surfaces (Al-Halabi et al. 2004; Al-Halabi & van Dishoeck 2007). Unfortunately, the ΔE_d values for other molecules and substrates were not available in the literature. We assume that $\Delta E_d/E_{d0}$ does not depend on molecular or substrate species for simplicity. We also performed calculations with $\Delta E_d/E_{d0} < 0.2$ to see the effect of the desorption energy distribution on the desorption efficiency.

It has been suggested that dust sizes are distributed approximately from 0.005 to 1 μ m for graphite and 0.025 to 0.25 μ m for other materials in the interstellar clouds (Mathis et al. 1977). We examined a_{dust} between 0.01 μ m and 1 μ m in order to cover the size range.

3. Results

3.1. Molecular Desorption

Figure 2 shows an example of the numerical results for the physical quantities in the post-shock region. In this calculation, we consider the typical interstellar grain size $(a_{dust} = 0.1 \ \mu m)$ and the shock parameters speculated from the observation of a protostar, namely, IRAS 04368+2557 (Sakai et al. 2014b, $n_{\rm s} = 10^8 \ {\rm cm}^{-3}$ and $v_{\rm s} = 2 \ {\rm km} \ {\rm s}^{-1}$). The gas velocity is reduced from $v_{\rm gas} = 2 \ {\rm km} \ {\rm s}^{-1}$ to $\simeq 0.4 \ {\rm km} \ {\rm s}^{-1}$ at the shock front. In contrast, $v_{\rm dust}$ retains its pre-shock value (panel a). $T_{\rm dust}$ increases a potential maximum of 53 K under the influence of the aerodynamic heating, and then decreases with the decrease in $v_{\rm rel}$ (panel b). Although $v_{\rm rel}$ is reduced to almost zero at $x \simeq 3 \times 10^5 \ {\rm km}$, the $T_{\rm dust}$ remains high ($\simeq 44 \ {\rm K}$) because of the thermal conduction from the ambient hot gas. Finally, $T_{\rm dust}$ decreases as the gas is cooled.

The dust heating induces thermal desorption of the grainsurface species. The desorption is likely to occur from adsorption sites with lower E_{des} . Figure 3 shows the variation of $P(E_{des})$ during the shock heating in Figure 2 for the case of $E_{d0} = 2000$ K and $\Delta E_d = 400$ K. The solid curve represents the initial $P(E_{des})$, which is given by Equation (20). At $x = 5.9 \times 10^3$ km, molecules at the sites of $E_{des} \lesssim 1600$ K are desorbed almost completely. At $x = 1.9 \times 10^4$ km, the desorption proceeds further. The final $P(E_{des})$ is shown by the dotted curve. The desorption fraction calculated from the final

 Table 1

 Desorption Energies of Molecules from Water Ice Surface (Substrate) Inferred from Molecular Dynamics Simulations

Molecule	Substrate	<i>E</i> _{d0} (K)	$\Delta E_{\rm d}$ (K)	$\Delta E_{\rm d}/E_{\rm d0}$	References
H atom	amorphous	650	117	0.18	Al-Halabi & van Dishoeck (2007)
H atom	crystalline	400	66.7	0.17	Al-Halabi & van Dishoeck (2007)
CO	amorphous	1091	373	0.34	Al-Halabi et al. (2004)

Note. The desorption energy is represented by the Gaussian distribution of its center at E_{d0} and the standard deviation of ΔE_d . The ΔE_d for CO is calculated from the potential energy distribution histogram (Figure 6 of the reference).



Figure 2. Sample of numerical results of dust thermal histories. The velocities with respect to the shock front (a) and temperatures (b) of the dust (solid curve) and gas (dashed curve) are plotted as functions of the distance from the shock front, *x*. The input parameters are $n_s = 10^8 \text{ cm}^{-3}$, $v_s = 2 \text{ km s}^{-1}$, and $a = 0.1 \ \mu\text{m}$.

 $P(E_{des})$ is $\xi_{des} = 0.537$; that is, approximately half of the grainsurface species are desorbed.

3.2. Effect of Desorption Energy Distribution

The calculated results of ξ_{des} for various input parameters, a_{dust} , E_{d0} , and ΔE_d , are summarized in Table 2. The shock parameters are fixed at $n_s = 10^8 \text{ cm}^{-3}$ and $v_s = 2 \text{ km s}^{-1}$. In the case of $a_{dust} = 0.1 \ \mu\text{m}$ and $E_{d0} = 3000 \text{ K}$, we obtain $\xi_{des} \sim 4 \times 10^{-9}$ when $\Delta E_d / E_{d0} = 0$, suggesting that the molecules are only minimally desorbed. However, ξ_{des} is increased by orders of magnitude when $\Delta E_d / E_{d0} = 0.1$, 0.2, and 0.3. This dramatic increase is due to the contribution of the desorption from weak adsorption sites with $E_{des} \ll E_{d0}$. This



Figure 3. Variation of grain-surface species population, $P(E_{des})$, during shock heating, where E_{des} is the desorption energy. The data are taken from the numerical results shown in Figure 2 at x = 0 (initial), 5.9×10^3 , 1.9×10^4 and 1.2×10^7 km. The initial population is given by Equation (20), with $E_{d0} = 2000$ K and $\Delta E_d = 400$ K.

suggests that the E_{des} distribution can enhance the thermal desorption considerably, even if the desorption is negligible when E_{des} is represented by a single value.

In contrast, in the case of $a_{dust} = 0.1 \ \mu m$ and $E_{d0} = 2000 \text{ K}$, ξ_{des} decreases slightly with increased ΔE_d . The opposite trend is due to the contribution of strong adsorption sites with $E_{des} \gg E_{d0}$; the fraction of such sites is increased with increased ΔE_d . However, ξ_{des} dependence on ΔE_d is negligibly small in the opposite trend.

The ξ_{des} dependence on E_{d0} is also notable. When $\Delta E_d/E_{d0} = 0$, ξ_{des} decreases by orders of magnitudes as E_{d0} is increased. For example, when $a_{dust} = 0.1 \ \mu\text{m}$, we obtain $\xi \simeq 0.6$, $\sim 10^{-9}$, and $< 10^{-16}$ for $E_{d0} = 2000$, 3000, and 4000 K, respectively. However, the strong dependence becomes milder for larger ΔE_d ; for the same setup except of $\Delta E_d/E_{d0} = 0.2$, we obtain $\xi \simeq 0.5$, $\sim 10^{-2}$, and $\sim 10^{-4}$ for $E_{d0} = 2000$, 3000, and 4000 K, respectively. This suggests that the desorption-efficiency difference between different species becomes less remarkable when we consider the desorption energy distribution.

The $\xi_{\rm des}$ is increased significantly as $a_{\rm dust}$ is decreased. For example, when $E_{\rm d0} = 3000$ K and $\Delta E_{\rm d}/E_{\rm d0} = 0$, we obtain $\xi < 10^{-16}$, $\sim 10^{-9}$, and $\sim 10^{-2}$ for $a_{\rm dust} = 1$, 0.1, and 0.01 μ m, respectively. This is due to the $\epsilon_{\rm em}$ dependence on $a_{\rm dust}$ (see Equation (14)); the smaller grain has smaller $\epsilon_{\rm em}$, and so reaches a higher peak temperature in the same shock. The desorption-efficiency difference on different-sized grains is also less remarkable when $\Delta E_{\rm d} > 0$, but still important in the $\xi_{\rm des}$ evaluation.
 Table 2

 Calculated Results for the Desorption Fraction ξ_{des} for Various Cases of Dust-grain Radius a_{dust} , Average Desorption Energy E_{d0} , and Standard Deviation ΔE_d

a _{dust} (µm)	E 10	$\xi_{\rm des}$ for different $\Delta E_{\rm d}/E_{\rm d0}$				
	(\mathbf{K})	$\Delta E_{\rm d}/E_{\rm d0}=0$	0.1	0.2	0.3	
1	1000	>0.99999	>0.99999	0.999	0.987	
	2000	3.06×10^{-7}	3.36×10^{-4}	3.50×10^{-2}	0.112	
	3000	$< 10^{-16}$	8.28×10^{-12}	1.87×10^{-4}	8.62×10^{-3}	
	4000	$< 10^{-16}$	$< 10^{-16}$	4.55×10^{-6}	1.51×10^{-3}	
	5000	$< 10^{-16}$	$< 10^{-16}$	3.42×10^{-7}	4.57×10^{-4}	
0.1	1000	>0.99999	>0.99999	>0.99999	>0.99999	
	2000	0.617	0.565	0.537	0.525	
	3000	4.08×10^{-9}	1.25×10^{-5}	1.18×10^{-2}	6.42×10^{-2}	
	4000	$< 10^{-16}$	4.44×10^{-11}	2.70×10^{-4}	1.02×10^{-2}	
	5000	$< 10^{-16}$	6.66×10^{-16}	1.44×10^{-5}	2.57×10^{-3}	
0.01	1000	>0.99999	>0.99999	>0.99999	>0.99999	
	2000	>0.99999	>0.99999	0.996	0.966	
	3000	2.51×10^{-2}	0.178	0.313	0.370	
	4000	2.61×10^{-8}	3.90×10^{-5}	1.73×10^{-2}	7.75×10^{-2}	
	5000	4.44×10^{-14}	3.42×10^{-9}	9.71×10^{-4}	1.88×10^{-2}	

Note. The shock parameters are $n_s = 10^8 \text{ cm}^{-3}$ and $v_s = 2 \text{ km s}^{-1}$.

3.3. Shock Diagram

We are interested in the shock condition that induces significant thermal desorption of the grain-surface species. The shock condition is primarily characterized by two parameters, n_s and v_s ; thus, a contour map of ξ_{des} on the density-velocity plane would be convenient to demonstrate the shock condition. Note that the contour map is termed the shock diagram hereafter. The same diagram has been used to investigate the grain vaporization induced by dense molecular shocks (Neufeld & Hollenbach 1994), chondrule formation induced by shock waves (Iida et al. 2001; Miura et al. 2002), and the thermal desorption of grain-surface species (Aota et al. 2015).

Figure 4 is the shock diagram obtained for $a_{dust} = 0.1 \ \mu m$ and $\Delta E_{\rm d} = 0$ K. The solid, dashed, and dotted curves indicate shock conditions above which ξ_{des} is greater than 10^{-1} , 10^{-2} , and 10^{-3} , respectively. All contours are downward to the right in the low-density region, suggesting that the lower the preshock gas density, the higher the shock velocity that is required to cause the same degree of desorption. The ξ_{des} in the lowdensity region can also be calculated analytically using an approximation formula (see Appendix C.1). On the other hand, in the higher-density region, the contours are almost vertical, suggesting that the minimum v_s necessary to cause the thermal desorption does not depend significantly on n_s . This is because the peak T_{dust} and the heating duration do not depend on n_s at the high-density limit (see Appendix C.2). In addition, it is found that a stronger shock is required in order to cause desorption from stronger adsorption sites.

The stronger shock yields larger ξ_{des} ; however, the contours of $\xi_{des} = 10^{-1}$, 10^{-2} , and 10^{-3} are very close on the shock diagram. This suggests that the dependence of ξ_{des} on v_s and n_s is very strong. In other words, a slight change in v_s or n_s varies ξ_{des} significantly. For example, when $E_{d0} = 2000$ K and $n_s = 10^8$ cm⁻³, the shock velocities required to achieve $\xi_{des} = 10^{-1}$, 10^{-2} , and 10^{-3} are very similar, being $v_s = 1.8$, 1.6, and 1.5 km s⁻¹, respectively. Hereafter, we adopt $\xi_{des} = 10^{-1}$ as the criterion for determining whether thermal desorption occurs (the 10%—desorption condition).



Figure 4. Shock conditions required to achieve the desorption fraction $\xi_{\text{des}} = 10^{-1}$ (solid curve), 10^{-2} (dashed curve), and 10^{-3} (dotted curve) when the desorption energy is represented by a single value, i.e., $E_{d0} = 1000$ (red), 2000 (green), 3000 (blue), 4000 (pink), and 5000 K (light blue). The dust radius is $a_{\text{dust}} = 0.1 \ \mu\text{m}$.

4. Implications

4.1. Desorbed-molecule Column Density: The Case of IRAS 04368+2557

Enhanced line emission of SO molecules around the IRAS 04368+2557 protostar was detected using ALMA (Sakai et al. 2014a, 2014b). One of the interpretations of the origin of this enhanced emission is that the SO molecules are thermally desorbed from the dust surface in accretion shocks at the centrifugal barrier. If this interpretation is valid, the emitted SO molecules should be localized immediately behind the shock front, at which point the desorbed SO molecules are in thermal equilibrium with the ambient shocked gas. Sakai et al. (2014a) estimated the column density of the warm SO molecules as $N_{\rm SO} \sim 5 \times 10^{13}$ cm⁻², and extracted the component localized at the centrifugal barrier only using the PV diagram.

In the following, we assess whether the accretion shock scenario meets the observational constraint based on our numerical results. For simplicity, we assume that the gas density



Figure 5. Desorption fraction ξ_{des} for $a_{dust} = 0.1$ (panel a) and 0.01 μ m (panel b) as a function of shock velocity v_s for $\Delta E_d / E_{d0} = 0$ (solid curve), 0.1 (dashed curve), 0.2 (dash-dotted curve), and 0.3 (dotted curve). We use $n_s = 10^8$ cm⁻³ and $E_{d0} = 2600$ K. The gray region denotes the maximum rotation velocity at the centrifugal barrier estimated using ALMA (Sakai et al. 2014b).

and its temperature are constant at the warm region behind the shock front. The column density of the SO molecules in the warm region is given by $N_{\rm SO} \sim n_{\rm SO}L_{\rm warm}$, where $n_{\rm SO}$ is the number density of the SO molecules and $L_{\rm warm}$ is the extent of the warm region. Let us assume that all SO molecules in the pre-shock region are adsorbed on the dust surface. We obtain $n_{\rm SO} \simeq \xi_{\rm des} y_{\rm SO} n_{\rm gas}$, where $y_{\rm SO}$ is the abundance of SO in the pre-shock region and $n_{\rm gas}$ is the number density of H nuclei in the post-shock region. The $n_{\rm gas}$ can be calculated using the Rankine-Hugoniot relation, i.e., $n_{\rm gas} = [(\gamma + 1)(\gamma - 1)]n_s$, at the strong shock limit ($M \gg 1$). Aota et al. (2015) have estimated $L_{\rm warm} \sim 0.06 (n_s/10^8 \,{\rm cm}^{-3})^{-1}$ au, from their numerical results. Substituting these values, we obtain

$$N_{\rm SO} \sim 5 \times 10^{15} \xi_{\rm des} \left(\frac{y_{\rm SO}}{10^{-5}} \right) {\rm cm}^{-2}.$$
 (26)

The evaluation of y_{SO} is difficult in general because the main carrier of S in dense clouds is unknown (Bilalbegović & Baranović 2015). Jiménez-Serra et al. (2005) have derived the abundances of various gas-phase species in the L1448 mm outflow based on observation. The estimated SO abundance in the post-shock component is $y_{SO} \sim 10^{-7}$, which is significantly higher than that for the ambient quiescent clouds. These researchers proposed that the SO molecules, rather than H₂S or OCS molecules, may be abundant on the dust grains, depending on the chemical history of the grain mantles, and may be directly released from the grains in the outflow internal shocks. The estimated abundance is only determined based on the SO molecules released into the gas phase; therefore the total SO abundance, including that on the grain surfaces, may be significantly higher. Kalvans & Shmeld (2010) have calculated the abundances of various species in interstellar molecular clouds based on their simple kinetic model, in which the gas phase, grain surface, and H-poor subsurface pore reactions are included. These researchers demonstrated that $y_{\rm SO} \sim 10^{-6}$ in the icy mantle on grains. From this evidence, the assumable maximum abundance is $y_{\rm SO} \sim 10^{-6}$. In this case, the observational constraint can be satisfied when $\xi_{\rm des} \sim 10^{-1}$.

The desorption energy of the SO molecules was estimated as $E_{des} = 2600$ K in the UMIST database RATE12 (McElroy et al. 2013). Figure 5 shows the calculated results of ξ_{des} as a function of v_s . The number density of H molecules in the infalling envelope was estimated as $\simeq 10^8$ cm⁻³ at most (Sakai

et al. 2014b). Panel (a) shows the calculation result for $n_{\rm s} = 10^8 {\rm ~cm^{-3}}$ and $a_{\rm dust} = 0.1 \ \mu{\rm m}$. The solid curve is the result for the case of $\Delta E_{\rm d}/E_{\rm d0} = 0$, which agrees with the previous calculation (Aota et al. 2015). The gray region denotes the maximum rotation velocity of the infalling rotating envelope at the centrifugal barrier (Sakai et al. 2014b, $v_{\theta}^{\text{max}} = 1.8 \pm 0.2 \text{ km s}^{-1}$), which gives the upper limit of the expected $v_{\rm s}$. We obtain $\xi_{\rm des} < 10^{-5}$ in the case of $\Delta E_{\rm d}/E_{\rm d0} = 0$, which does not satisfy the observational constraint. On the other hand, we obtain $\xi_{\rm des} \sim 10^{-1}$ in the case of $\Delta E_d/E_{d0} = 0.3$. Thus, the origin of the enhanced SO-line emission may be explained if v_s is almost equal to v_{θ}^{\max} . However, v_{s} is most likely smaller than v_{θ}^{\max} because the infalling rotating envelope flows diagonally in the inner disk. If we consider the oblique shock effect, the observational constraint is not satisfied for the case shown in panel (a) even for $\Delta E_{\rm d}/E_{\rm d0} = 0.3$.

When we consider significantly smaller dust grains to be the interstellar-molecule carriers, the observational constraint is satisfied even when the oblique shock effect is considered. Panel (b) shows the results for $a_{dust} = 0.01 \ \mu m$. Smaller dust grains have lower emissivities, therefore they are heated more significantly than the larger grains for the same shock parameters. In the case of $\Delta E_d / E_{d0} \ge 0.2$, we obtain $\xi_{\rm des} \sim 10^{-1}$ or larger at $v_{\rm s} \simeq 1.3$ km s⁻¹. This shock velocity is achieved even for the oblique shock for which the pre-shock gas flow is inclined by $\simeq 45^{\circ}$ relative to the shock front (see Appendix D). The existence of such small dust grains has been supported by studies of interstellar extinction. Mathis et al. (1977) have revealed that the interstellar extinction spectrum is reproduced by dust grains with a power-law size distribution with an exponent of approximately -3.3 to -3.6. In the powerlaw size distribution, smaller grains primarily contribute to the dust-grain surface area. This suggests that the smaller dust grains are the main interstellar-molecule carriers if the number of molecules is simply proportional to the surface area. Mathis et al. (1977) have shown that the size range is approximately 0.005–1 μ m for graphite and approximately 0.025–0.25 μ m for other materials. Weingartner & Draine (2001) have demonstrated the existence of very small carbonaceous grains with $a < 0.005 \ \mu m$. We conclude that the enhanced SO-line emission around the IRAS 04368+2557 protostar may

Physical Quantities of Protostars for Which Thermal Desorption of the Grain-surface Species in the Accretion Shocks is Indicated by ALMA Observations v_{θ}^{max} (km s⁻¹) $n_{\rm s}~({\rm cm}^{-3})$ Protostar $M_*~(M_\odot)$ $R_{\rm CB}$ (au) Observed Species IRAS 04368+2557 0.18 ± 0.05 100 ± 20 1.8 ± 0.2 $1.2 \times 10^{7} - 2 \times 10^{8}$ SO IRAS 04365+2535 0.20-0.30 50 ± 10 2.4 - 3.7 $1 \times 10^{6} - 1 \times 10^{8}$ SO $10^{7} - 10^{9}$ CH₃OH, HCOOCH₃ IRAS 16293-2422 0.5 - 1.0 50 ± 10 4.5

Table 3

Note. M_* , protostar (plus inner disk) mass; R_{CB} , centrifugal barrier radius; v_{θ}^{max} , maximum rotation velocity of infalling rotating envelope; n_s , H-nucleus number density in pre-shock region. The IRAS 04368+2557 data are from Sakai et al. (2014a, 2014b). n_s was estimated as twice the inferred value of the H-molecule number density. The IRAS 04365+2535 data are from Sakai et al. (2016). The maximum rotation velocity is given by $v_{\theta}^{max} = (2GM_*/R_{CB})^{1/2}$, where *G* is the gravitational constant. Sakai et al. (2016) obtained the H-molecule number density at the centrifugal barrier, $n_{H_2} = 3 \times 10^6 - 3 \times 10^8 \text{ cm}^{-3}$, which represents the post-shock gas density. n_s was estimated using the Rankine-Hugoniot relation at the strong shock limit, $n_s = 2 n_{H_2}/[(\gamma + 1)/(\gamma - 1)]$. The IRAS 16293–2422 data are from Oya et al. (2016). These researchers obtained an H-molecule number density in the infalling rotating envelope of 10^7 – 10^9 cm^{-3} .

originate from the SO molecules that are thermally desorbed from $\sim 0.01 \,\mu\text{m}$ sized or smaller dust grains.

4.2. Comparison of the Calculations with the Observations

Enhanced line emission at the centrifugal barrier has been observed around some protostars. For example, Sakai et al. (2016) have detected enhanced SO-line emission around the class I protostar labeled IRAS 04365+2535. Furthermore, Oya et al. (2016) have observed enhanced line emissions of HCOOCH₃ and CH₃OH molecules around the class 0 protostar known as IRAS 16293–2422. The SO, HCOOCH₃, and CH₃OH desorption energies are 2600, 4000, and 4930 K, respectively, according to the UMIST database RATE12 (McElroy et al. 2013). Here, we show that these enhanced line emissions can be explained by the accretion shock heating that occurs for all of these protostars.

The observed physical properties of these protostars are summarized in Table 3. The parameters, such as M_* , R_{CB} , v_{θ}^{\max} , and n_{s} , differ for each protostar, indicating that a variety of molecules are desorbed by the accretion shock heating. Figure 6 shows the expected shock parameters for three protostars based on the 10% desorption criterion. It is found that IRAS 16293–2422 causes a stronger accretion shock than IRAS 04368+2557, therefore the grain-surface species with large E_{des} are desorbed in the former. Panel (a) shows the result for $a_{dust} = 1 \ \mu m$. It is apparent that no significant desorption of molecules with $E_{d0} > 2000$ K, including SO, occurs in the protostars IRAS 04368+2557 and IRAS 04365 +2535. It is also found that no significant desorption of molecules with $E_{d0} > 4000$ K, including HCOOCH₃ and CH₃OH, occurs in the protostar IRAS 16293-2422. If the main carriers of these molecules are $\sim 1 \,\mu m$ sized dust grains, the enhanced line emissions observed for these protostars therefore cannot be explained by accretion shock heating. This conclusion is valid even if the E_{des} distribution or 0.1 μ m sized dust grains are taken into consideration (see panel b). On the other hand, the negative conclusion turns out to be positive when we regard significantly smaller grains as being the main interstellar-molecule carriers. Panel (c) shows the result for $a_{dust} = 0.01 \ \mu m$. It is found that molecules with $E_{\rm des} \lesssim 3000$ K, including SO, are desorbed in the protostars IRAS 04368+2557 and IRAS 04365+2535. It is also found that molecules with $E_{\rm des} \lesssim 5000$ K, including HCOOCH₃ and CH₃OH, are desorbed in the protostar IRAS 16293-2422. This means that the enhanced line emissions in these protostars can be explained by the accretion shock heating mechanism if the main carriers of these molecules are $\sim 0.01 \,\mu m$ sized dust grains.

4.3. Possibility of Protostar Heating

We discuss the protostellar heating as another mechanism that can induce the thermal desorption of grain-surface species. The dust temperature is determined by the energy balance between the protostellar heating and the radiative cooling of the grain. The equilibrium temperature, T_{eq} , is given by

$$T_{\rm eq} = \left(\frac{\epsilon_{\rm abs}L_*}{16\pi\epsilon_{\rm em}R^2\sigma_{\rm SB}}\right)^{1/4} \tag{27}$$

for optically thin disks, where L_* is the system luminosity, R is the distance from the protostar, and ϵ_{abs} is the Planck mean absorption efficiency. We use ϵ_{em} given by Equation (14) and $\epsilon_{abs} \simeq A'a_{dust}$ for a visible wavelength with $A' \simeq 3 \times 10^3$ cm⁻¹ (see Appendix A). The factor of $(\epsilon_{abs}/\epsilon_{em})^{1/4}$ is due to the difference in wavelength between the protostar radiation and the grain thermal radiation and does not depend on a_{dust} because both ϵ_{em} and ϵ_{abs} are proportional to a_{dust} in the parameter range of interest ($a_{dust} \leq 1 \ \mu m$ and $T < 10^4$ K). For optically thick disks the protostar radiation does not reach the disk midplane directly, so the dust temperature should be lower than T_{eq} given by Equation (27) (Chiang & Goldreich 1997; Chiang et al. 2001; Tanaka et al. 2005).

The T_{eq} becomes higher as the grain approaches the protostar, so the desorption proceeds more rapidly, as suggested by Equation (1). When T_{eq} is constant, N decreases exponentially with time. We define a sublimation temperature, T_{sub} , such that N decreases 1/e times the initial value at the temperature T_{sub} during a given time interval t_{sub} . Namely,

$$T_{\rm sub} = \frac{E_{\rm des}}{\ln\left(\nu t_{\rm sub}\right)}.$$
 (28)

When we adopt $t_{sub} = 100$ year, which is a typical orbital period at 100 au, T_{sub} is simply equal to E_{des} divided by 49.5. The choice of t_{sub} does not affect the T_{sub} evaluation significantly. If $T_{eq} \simeq T_{sub}$ at $R = R_{CB}$, the protostar heating can explain the molecular enhancement at the centrifugal barrier by coincidence. We summarize T_{eq} and T_{sub} in each protostar in Table 4. For comparison, we display the disk temperature, T_{disk} , which is obtained by detailed model fitting (Crimier et al. 2010; Green et al. 2013; Tobin et al. 2013).

In IRAS 04368+2557, we found that $T_{eq} \simeq 59$ K at the centrifugal barrier, which is almost equal to T_{sub} for SO molecules. On the other hand, a radiative transfer calculation by Tobin et al. (2013) obtained that $T_{disk} \simeq 30$ K at R = 100 au. The difference in the temperature suggested that



Figure 6. Shock conditions necessary to achieve $\xi_{des} = 10^{-1}$ (10% desorption condition) for various desorption energy distributions: $E_{d0} = 1000$ (red), 2000 (green), 3000 (blue), 4000 (pink), and 5000 K (light blue) and $\Delta E_d / E_{d0} = 0$ (solid curve), 0.1 (dashed curve), 0.2 (dash-dotted curve), and 0.3 (dotted curve). Panels (a)–(c) are the results for $a_{dust} = 1.0$, 0.1, and 0.01 μ m, respectively. The black crosses (or vertical line) indicate shock parameters speculated from ALMA observations of protostars (see Table 3).

the region at R = 100 au is obscured from the protostar radiation in this system. For $T_{sub} \simeq 30$ K, the SO desorption by the protostar heating is excluded because T_{disk} at the centrifugal barrier is sufficiently lower than T_{sub} . This conclusion is supported by the ALMA observation that showed that the gas kinetic temperature outside the centrifugal barrier is 23–33 K (Sakai et al. 2014b). Other heating mechanisms are therefore required to explain the SO-line enhancement. We conclude that the accretion shock is the most plausible mechanism in this system. On the other hand, SO desorption by the protostar heating cannot be ruled out in the protostar IRAS 04365+2535 because R_{CB} is smaller than that in the protostar IRAS 04368+2557, leading to a higher grain temperature at the centrifugal barrier. The reported model (Brown & Chandler 1999) evaluated T_{disk} to be 332 ± 235 K at the centrifugal barrier, but it contains a large uncertainty. Assuming the optically thin disk, we obtain $T_{eq} \simeq 72$ K, so the grain-surface SO molecules will be desorbed only by the protostar heating because $T_{eq} > T_{sub}$. Sakai et al. (2016) found that the SO distribution is slightly extended outward of the centrifugal barrier in a certain direction up to ~100 au, which can also be explained by the strong protostar heating. This means that the protostar heating can explain the enhanced line emission at the centrifugal barrier.

We cannot rule out the possibility of protostar heating in IRAS 16293–2422. Because of the large L_* , the dust temperature at the centrifugal barrier will be much higher than other protostars. The spherical model by Crimier et al. (2010) suggested that $T_{\text{disk}} \simeq 130$ K at the centrifugal barrier, which is slightly higher than the dust temperature in an optically thin disk ($T_{eq} \simeq 104$ K). Since these estimates are equal to or higher than T_{sub} of the grain-surface species, the protostar heating is a possible mechanism for the molecular line enhancement in this system. However, both the spherical model and Equation (27) are too simplified to evaluate the dust temperature at the centrifugal barrier because it did not consider the optically thick disk. When the shading effect is taken into consideration, the dust temperature may be lower than T_{sub} . In this case, other heating sources, such as accretion shocks, are required to explain the molecular enhancement.

5. Conclusion

We performed a comprehensive study of thermal desorption of grain-surface species in a shock wave. We calculated the desorption fraction based on the following two factors: (i) a Gaussian distribution of the desorption energy, and (ii) dust grains with various sizes. We summarized our results on the corresponding shock diagram, which clearly demonstrates the shock conditions required to induce thermal desorption as functions of the pre-shock gas density and shock velocity. We compared our results with recent ALMA observations of enhanced line emissions around young protostars, namely, IRAS 04368+2557, IRAS 04365+2535, and IRAS 16293–2422. Our findings are summarized as follows:

1. The enhanced line emissions observed in all of these protostars can be explained by considering the thermal desorption of the grain-surface species in the accretion shock if $\sim 0.01 \,\mu\text{m}$ sized dust grains are the main carriers of these species. This assumption is consistent with the power-law size distribution $a^{-3.5}$ because in this case the smaller grains primarily contribute to the dust-grain surface area. Note that if the main carriers are $\sim 0.1 \, \mu m$ sized dust grains, which is the case investigated previously (Aota et al. 2015), the accretion shock parameters inferred from the ALMA observations are insufficient to cause significant desorption if we consider the oblique shock effect. This conclusion is not robust, however, because of the uncertainty regarding the grainsurface species desorption energies. To render this conclusion more reliable, precise measurements of the

Table 4Disk Temperatures at Centrifugal Barriers

Protostar	$L_*~(L_{\odot})$	R _{CB} (au)	$T_{\rm eq}$ (K)	T _{disk} (K)	T _{sub} (K)
IRAS 04368+2557	2.75 ^a	100 ± 20	\simeq 59	$\simeq 30^{a}$	53 (SO)
IRAS 04365+2535	2.47 ^b	50 ± 10	\simeq 72	$332 \pm 235^{\circ}$	53 (SO)
IRAS 16293–2422	22 ^d	50 ± 10	$\simeq 104$	$\simeq 130^{d}$	81 (HCOOCH ₃), 100 (CH ₃ OH)

Notes. L_* is the system luminosity. T_{eq} is the equilibrium temperature of dust grains in an optically thin disk (see Equation (27)). T_{disk} is the disk temperature obtained by the model fitting. The T_{disk} of IRAS 04365+2535 is calculated by using the relation $T_{disk} = T_{100au}(R/100 \text{ au})^{-q}$, where $T_{100au} = 155 \pm 99$ K and $q = 1.1 \pm 0.3$ (Brown & Chandler 1999). T_{sub} is the sublimation temperature of each grain-surface species (see Equation (28)). The R_{CB} values are taken from Table 3. ^a Tobin et al. (2013).

^b Green et al. (2013).

^c Brown & Chandler (1999).

^d Crimier et al. (2010).

desorption energy and its distribution together with the characterization of the dust surface are quite important.

- 2. The desorption fraction depends on the desorption energy distribution. Even if the desorption occurred only minimally when the desorption energy were represented by a single (average) value, the desorption fraction is increased by some orders of magnitude when the desorption energy is broadly distributed. In the case, for example, that pre-shock gas number density, shock velocity, dust radius, and average desorption energy are $n_{\rm s} = 10^8 \text{ cm}^{-3}, \ v_{\rm s} = 1.8 \text{ km s}^{-1}, \ a_{\rm dust} = 0.1 \ \mu\text{m}, \ \text{and}$ $E_{d0} = 2600$ K estimated for SO molecules, respectively, the desorption fractions are $\xi_{\rm des} \sim 10^{-6}, \sim 10^{-4}, \sim 10^{-2},$ and $\sim 10^{-1}$ for $\Delta E_d / E_{d0} = 0$, 0.1, 0.2, and 0.3, respectively. The desorption energy distribution reduces the shock velocity required to cause the same degree of desorption at a fixed pre-shock gas density. This behavior suggests that thermal desorption occurs even in an oblique shock with a lower effective shock velocity than in a normal shock.
- 3. The shock diagram is useful for determining the possibility of thermal desorption of grain-surface species in a shock wave, based on the observed protostar quantities.
- 4. Desorption of grain-surface species by protostar heating cannot be ruled out for the protostars IRAS 04365+2535 and IRAS 16293-2422. In these systems, the dust temperature at the centrifugal radius is estimated to be almost equal to or higher than the sublimation temperature of the grain-surface species. Therefore, no other mechanism is required to cause the substantial desorption of grain-surface species. We cannot specify the molecular desorption mechanism in these two systems at present: accretion shock, protostar radiation, or a combination of these two mechanisms.

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Appendix A Emissivity

We calculate the dust-grain emissivity using the optical constant of astronomical silicate (Draine & Lee 1984). Let us denote the complex dielectric function as $\epsilon = \epsilon_1 + i\epsilon_2$, where ϵ_1 and ϵ_2 are the real and imaginary parts, respectively. At the long wavelength limit, ϵ_1 is constant and ϵ_2 is inversely proportional to the wavelength λ , i.e., $\epsilon_2 = \epsilon_i / \lambda$, where ϵ_i is constant. The absorption coefficient of a spherical dust grain of radius *a* is given by

$$Q_{abs}(\lambda, a) = \frac{8\pi a}{\lambda} \Im\left(\frac{\epsilon - 1}{\epsilon + 2}\right) = \frac{24\pi a}{\lambda} \frac{\epsilon_2}{(\epsilon_1 + 2)^2 + \epsilon_2^2}$$
$$\simeq \frac{24\pi\epsilon_i}{(\epsilon_1 + 2)^2} \frac{a}{\lambda^2},$$
(29)

where we use the relation $\epsilon_1 \gg \epsilon_2$ for large λ . Finally, we obtain the Planck mean absorption coefficient

$$\langle Q_{\rm abs} \rangle(T, a) = \frac{\int_0^\infty Q_{\rm abs} B(\lambda, T) d\lambda}{\int_0^\infty B(\lambda, T) d\lambda} = AaT^2,$$
 (30)

where $B(\lambda, T)$ is the Planck function,

$$A = \frac{320\pi^3}{7} \frac{\epsilon_i}{(\epsilon_1 + 2)^2} \left(\frac{k_{\rm B}}{hc}\right)^2$$

is a constant, *h* is the Planck constant, and *c* is the light speed. Substituting $\epsilon_1 = 11.8$ and $\epsilon_i = 3.4 \times 10^{-2}$ cm (Draine & Lee 1984), we obtain A = 0.122 cm⁻¹ K⁻².

In order to confirm the validity of Equation (30), we compare the results obtained using this equation with the numerical solution based on the Mie theory (Bohren & Huffman 1983). Figure 7 shows the Planck mean absorption coefficients for a = 1, 0.1, and 0.01 μ m as functions of *T*. When the optical property of astronomical silicate is considered, Equation (30) agrees with the numerical solution at $T \leq 200$ K. We also examine dust grains composed of H₂O ice (Warren 1984) or dirty ice (Preibisch et al. 1993), finding that the Planck mean absorption coefficient agrees with Equation (30) at $T \leq 100$ K. This suggests that Equation (30) is a good approximation of the Planck mean absorption coefficient of submicron-sized silicate dust grains at $T \leq 100$ K, even if the grains are covered by an icy mantle.



Figure 7. Temperature dependence of Planck mean absorption coefficient for a spherical particle of radius a = 1, 0.1, and $0.01 \ \mu\text{m}$. The solid line is that adopted in this study (see Equation (14)). The dashed, dash-dotted, and dotted curves are the numerical results based on the Mie theory (Bohren & Huffman 1983) using the optical properties of astronomical silicate (Draine & Lee 1984), H₂O ice (Warren 1984), and dirty ice (Preibisch et al. 1993), respectively.

For T > 1000 K, on the other hand, $\langle Q_{abs} \rangle$ given by Equation (30) is overestimated. This means that this approximation formula cannot be applied to estimate the Planck mean adsorption coefficient of dust grains irradiated by protostars with effective temperatures of thousands of Kelvin. The temperature dependence of $\langle Q_{abs} \rangle$ at T > 1000 K is weaker than that given by Equation (30), and is roughly independent of the effective temperatures of protostars.

Appendix B Redistribution of Grain-surface Species

We examine the effect of the grain-surface species redistribution on the ξ_{des} estimation based on the model proposed by Amiaud et al. (2006). The adsorption sites on the grain surface have a certain adsorption energy distribution $f(E_{des})$. Each adsorption site allows only one molecule to be adsorbed at most. Under such an exclusion constraint, the appropriate statistical law is the Fermi-Dirac distribution function. We therefore obtain

$$P(E_{\rm des}, T_{\rm dust}, \mu) = \frac{f(E_{\rm des})}{1 + e^{-\frac{E_{\rm des}-\mu}{T_{\rm dust}}}},$$
(31)

where μ is the chemical potential that can be obtained by the closing relation,

$$\int_0^\infty P(E_{\rm des}, T_{\rm dust}, \mu) dE_{\rm d} = \theta.$$
(32)

Figure 8 shows an example of the redistribution effect. The solid and dashed curves correspond to the initial $P(E_{des})$ and that after isothermal desorption without redistribution, respectively. The dotted curve is the $P(E_{des})$ after complete redistribution from the dashed curve. The total number of adsorbed molecules is conserved during the redistribution procedure. As a result of the redistribution, a low-energy tail appears in $P(E_{des})$. The low-energy tail is likely to promote the molecular desorption, but this effect is minor. We summarize the calculated results of the isothermal desorption in Table 5. In



Figure 8. Effect of redistribution on grain-surface species population. The solid curve is the initial population with $E_{d0} = 2000$ K and $\Delta E_d / E_{d0} = 0.1$. The dashed curve is the population after isothermal desorption at T = 60 K for 10^3 s. The dotted curve is the population after redistribution from the dashed curve.

all cases, ξ_{des} exhibits relatively minor variation, even if the redistribution is considered. Therefore we can ignore the redistribution in order to evaluate the molecular ξ_{des} due to shock heating.

Appendix C Approximation Formulae for the Desorption Fraction

We derive approximation formulae for the grain-surface species ξ_{des} due to shock heating. Using these formulae, one can estimate ξ_{des} for any values of E_{d0} and ΔE_{d} without conducting numerical simulations.

The derivation is conducted independently for the following two different regions: the aerodynamic (Appendix C.1) and conductive (Appendix C.2) heating regions. In the former region, the dust temperature is primarily determined by the aerodynamic heating, therefore the thermal desorption after the dust grains come to rest against the ambient shocked gas is neglected. In the latter region, the thermal desorption occurs because of the thermal conduction from the hot gas to the dust grains. As the latter region continues for a significantly longer period than the former, this contribution to ξ_{des} is not negligible when the gas density is quite high. We compare the approximation formulae with numerical results in Appendix C.3.

C.1. Aerodynamic Heating Region

We assume that the gas quantities are unchanged from the quantities immediately behind the shock front, that is, $\rho_{\text{gas}} = \rho_{\text{gas},0}$, $v_{\text{gas}} = v_{\text{gas},0}$, and $T_{\text{gas}} = T_{\text{gas},0}$, for simplicity.

C.1.1. Equation of Motion

The dust-grain equation of motion is given by Equation (7). Using $C_D \rightarrow 2$ at $s_a \gg 1$, we obtain the analytic solution of

$$v_{\rm rel}(t) = \frac{v_{\rm rel,0}}{1 + \frac{t}{t_{\rm ren}}},$$
 (33)

 Table 5

 Effect of the Redistribution on the Estimation of Grain-surface Species Desorption Fraction, ξ_{des}

T.		ξ_{des} after isothermal desorption for 10 ³ s					
(K)	No redist.	100 s	10 s	1 s	0.1 s		
40	8.08×10^{-5}	8.24×10^{-5}	8.29×10^{-5}	8.30×10^{-5}	8.30×10^{-5}		
50	5.95×10^{-2}	6.46×10^{-2}	6.69×10^{-2}	6.74×10^{-2}	6.75×10^{-2}		
60	0.745	0.809	0.846	0.858	0.860		

Note. We calculated ξ_{des} for 10³ second-isothermal heating at temperatures of 40, 50, and 60 K, respectively. The redistribution procedures were inserted at regular intervals of 10³ (no redistribution), 10², 10, 1, and 0.1 s. A shorter interval means more efficient redistribution.

where $v_{rel} = v_{dust} - v_{gas}$ is the gas-dust relative velocity, $v_{rel,0}$ is the value of v_{rel} immediately behind the shock front, and

 $t_{\rm stop} = \frac{4\rho_{\rm mat}a_{\rm dust}}{3\rho_{\rm gas,0}v_{\rm rel,0}}$ (34)

is the stopping time at $s_a \gg 1$.

C.1.2. Thermal History of Dust

 T_{dust} is determined from the energy Equation (9). If the specific heat of the dust, c_{dust} , is extremely low (small thermal inertia approximation), T_{dust} is determined by the energy balance equation, which is given by $\Gamma - 4\epsilon_{\text{em}}\sigma_{\text{SB}}T_{\text{dust}}^4 = 0$. Ida et al. (2001) used the small thermal inertia approximation to derive the peak temperature of the dust grains in the post-shock region. They also considered a limit of $s_a \gg 1$ for simplicity, which is valid for shocks that are sufficiently strong for the post-shock gas to cool rapidly. However, in this study, we consider significantly weaker shocks for which the limit $s_a \gg 1$ is invalid.

The energy balance condition can be rewritten as

$$\frac{1}{8}\rho_{\text{gas},0}v_{\text{rel}}^{3}\alpha_{1}(s_{a})\alpha_{2}(s_{a}) - \frac{1}{8}\frac{\gamma+1}{\gamma-1}\frac{k_{\text{B}}}{\mu m_{\text{H}}}\rho_{\text{gas},0}T_{\text{dust}}v_{\text{rel}}\alpha_{2}(s_{a}) - A\sigma_{\text{SB}}a_{\text{dust}}T_{\text{dust}}^{6} = 0,$$
(35)

substituting Equation (14) and

$$\alpha_{1}(s_{a}) = 1 + \frac{\gamma}{\gamma - 1} s_{a}^{-2} - \frac{s_{a}^{-2}}{1 + 2s_{a}^{2} + 2\pi^{-1/2} s_{a} e^{-s_{a}^{2}} / \operatorname{erf}(s_{a})}, \quad (36)$$

$$\alpha_2(s_{\rm a}) = \left(1 + \frac{0.5}{s_{\rm a}^2}\right) \operatorname{erf}(s_{\rm a}) + \pi^{-1/2} s_{\rm a}^{-1} e^{-s_{\rm a}^2}, \quad (37)$$

which are correction terms satisfying $\alpha_1 \rightarrow 1$ and $\alpha_2 \rightarrow 1$ at $s_a \gg 1$. Hereafter, we approximate $s_a = s_{a,0} \equiv |v_{rel,0}| / \sqrt{2k_B T_{gas,0}/(\mu m_H)}$ for simplicity. The left-hand side of Equation (35) contains two cooling terms. The second term is proportional to $\rho_{gas,0}$; on the other hand, the third term is density independent. Therefore we can define a critical density, $\rho_{gas,cr}$, above which the second term dominates the third. At $\rho_{gas,0} > \rho_{gas,cr}$, T_{dust} is obtained by equating the first term with the second. Then

$$T_{\text{dust}}(t) = \frac{\gamma - 1}{\gamma + 1} \frac{\mu m_{\text{H}}}{k_{\text{B}}} \alpha_1(s_{\text{a},0}) v_{\text{rel}}^2(t) \quad \text{(for } \rho_{\text{gas},0} > \rho_{\text{gas},\text{cr}}\text{)}.$$
(38)

At $\rho_{\text{gas},0} < \rho_{\text{gas,cr}}$, on the other hand, T_{dust} is given by equating the first term with the third one. Then

$$T_{\rm dust}(t) = \left(\frac{\rho_{\rm gas,0} \alpha_1(s_{\rm a,0}) \alpha_2(s_{\rm a,0})}{8A \sigma_{\rm SB} a_{\rm dust}}\right)^{1/6} v_{\rm rel}^{1/2}(t).$$

(for $\rho_{\rm gas,0} < \rho_{\rm gas,cr}$) (39)

Substituting Equation (33) into Equations (38) and (39), we obtain

$$T_{\rm dust}(t) = \frac{T_0}{(1 + t/t_{\rm stop})^m},$$
(40)

where $T_0 = T_{dust}(0)$ is the peak temperature of the dust and *m* is a constant, with m = 2 and 1/2 for high- and low-density cases, respectively. An expression for $\rho_{gas,cr}$ is obtained by equating Equations (38) and (39), such that

$$\rho_{\text{gas,cr}} = \frac{8\alpha_1^5(s_{a,0})A\sigma_{\text{SB}}a_{\text{dust}}}{\alpha_2(s_{a,0})} \left(\frac{\gamma-1}{\gamma+1}\right)^6 \left(\frac{\mu m_{\text{H}}}{k_{\text{B}}}\right)^6 v_{\text{rel},0}^9.$$
 (41)

C.1.3. Desorption Fraction

Substituting Equation (40) into (18) and integrating the resulting expression over *t* from 0 to ∞ , we obtain

$$P_{\infty}(E_{\rm des}) \simeq P_0(E_{\rm des}) \exp\left(-\frac{\nu t_{\rm stop}}{m} \frac{T_0}{E_{\rm des}} e^{-\frac{E_{\rm des}}{T_0}}\right),\tag{42}$$

where $P_0(E_{des})$ is the initial population and $P_{\infty}(E_{des})$ is the final population after heating. Here, we use an approximation of $(1 + t/t_{stop})^m \simeq 1 + mt/t_{stop}$ because the thermal desorption primarily occurs when the shock heating is initiated $(t/t_{stop} \ll 1)$. In the case of $\Delta E_d/E_{d0} = 0$, E_{des} can be represented by a single value, therefore the fractional coverage at the end of the shock heating is given by

$$\theta_{\infty} = \frac{P_{\infty}(E_{\rm d0})}{P_0(E_{\rm d0})} = \exp\left(-\frac{\nu t_{\rm stop}}{m} \frac{T_0}{E_{\rm d0}} e^{-\frac{E_{\rm d0}}{T_0}}\right) \quad (\text{for } \frac{\Delta E_{\rm d}}{E_{\rm d0}} = 0).$$
(43)

In the case of $\Delta E_d/E_{d0} \neq 0$, substituting Equation (42) into (17) and integrating the resulting expression over E_{des} , we

obtain

$$\theta_{\infty} = \int_{0}^{\infty} P_{0}(E_{\text{des}}) \exp\left(-\frac{\nu t_{\text{stop}}}{m} \frac{T_{0}}{E_{\text{des}}} e^{-\frac{E_{\text{des}}}{T_{0}}}\right) dE_{\text{des}}$$
$$\times (\text{for } \frac{\Delta E_{\text{d}}}{E_{\text{d0}}} \neq 0). \tag{44}$$

The integral can be calculated by noting that

$$g(E_{\rm des}) = \exp\left(-\frac{\nu t_{\rm stop}}{m} \frac{T_0}{E_{\rm des}} e^{-\frac{E_{\rm des}}{T_0}}\right)$$

is a monotonically increasing function of E_{des} that increases rapidly from 0 to 1 within a narrow region. Thus, this function can be approximated as a step function, such that

$$g(E_{\rm des}) \simeq \begin{cases} 0, & \text{when } E_{\rm des} < E_{\rm th}, \\ 1, & \text{when } E_{\rm des} > E_{\rm th}, \end{cases}$$
(45)

where E_{th} is the threshold desorption energy. Using this step function, Equation (44) is rewritten as

$$\theta_{\infty} \simeq \frac{1}{2} \operatorname{erfc}\left(\frac{E_{\rm th} - E_{\rm d0}}{\Delta E_{\rm d}}\right) \quad \left(\operatorname{for}\frac{\Delta E_{\rm d}}{E_{\rm d0}} \neq 0\right),$$
(46)

where $\operatorname{erfc}(x)$ is the complementary error function defined by $\operatorname{erfc}(x) = 1 - \operatorname{erf}(x)$. E_{th} can be approximately determined from $d^2g/dE_{\text{des}}^2 = 0$ at $E_{\text{des}} = E_{\text{th}}$. Therefore we obtain

$$E_{\rm th} = T_0 \ln\left(\frac{\nu t_{\rm stop}}{m} \frac{T_0}{E_{\rm d0}}\right),\tag{47}$$

where we employed the approximation

$$g(E_{\rm des}) \simeq \exp\left(-\frac{\nu t_{\rm stop}}{m} \frac{T_0}{E_{\rm des,0}} e^{-\frac{E_{\rm des}}{T_0}}\right)$$

C.1.4. Scaling Law

For given E_{d0} and ΔE_d , θ_{∞} is determined by $\beta \equiv \nu t_{stop}/m$ and T_0 only (see Equations (43) and 44). The t_{stop} is proportional to $(n_s/a_{dust})^{-1}$ (see Equation (34)). T_0 is independent of n_s or a_{dust} for the high-density case (see Equation (38)), whereas it is proportional to $(n_s/a_{dust})^{1/6}$ for the low-density case (see Equation (39)). The scaling law in the low-density case is based on the fact that $\epsilon_{em} \propto a_{dust}$ (see Equation (14)). Therefore, we find that θ_{∞} is scaled by (n_s/a_{dust}) when the thermal desorption is primarily caused within the aerodynamic heating region.

C.2. Conductive Heating Region

When $\rho_{\rm gas}$ is sufficiently high, the dust grains are in thermal equilibrium with the gas in the post-shock region ($T_{\rm dust} \simeq T_{\rm gas}$). The thermal equilibrium is also derived from Equation (13), that is, $T_{\rm dust}$ should be equal to $T_{\rm gas}$ when $\rho_{\rm gas}$ is sufficiently large. The thermal history of the dust grains is therefore not determined by the aerodynamic heating, but instead by the cooling of the post-shock gas. Deleting ($T_{\rm gas} - T_{\rm c}$) from Equations (6) and (13), we obtain

$$\Lambda = 4\pi a_{\rm c}^2 n_{\rm c} \epsilon_{\rm em} \sigma_{\rm SB} T_{\rm c}^4 \simeq 4\pi a_{\rm c}^2 n_{\rm c} \epsilon_{\rm em} \sigma_{\rm SB} T_{\rm gas}^4.$$
(48)

The thermal energy of the gas is transferred to the dust grains by the thermal collisions of the gas molecules, and then



Figure 9. Comparison of 10% desorption condition for numerical results and approximation formulae. We use $\Delta E_d / E_{d0} = 0.2$. The solid curves are the numerical results and the other curves correspond to the approximation formulae: approximation for aerodynamic heating in low- (dashed) and high-density (dash-dotted) cases, and approximation for conductive heating case (dotted). Red, green, blue, pink, and light blue indicate $E_{d0} = 1000$, 2000, 3000, 4000, and 5000 K, respectively. Panels (a), (b), and (c) are the results for $a_{dust} = 1.0, 0.1$, and 0.01 μ m, respectively.

is directly removed from the optically thin region by the thermal radiation of the dust grains.

For a one-dimensional plane-parallel shock, the post-shock region becomes almost isobaric when the flow is steady (Susa et al. 1998, $dp_{gas}/dt \simeq 0$). The energy Equation (5) can therefore be rewritten as

$$-\frac{1}{T_{\rm gas}}\frac{dT_{\rm gas}}{dt} = \frac{\gamma - 1}{\gamma}\frac{\Lambda}{p_{\rm gas}},\tag{49}$$





Figure 10. (a) Schematic of an oblique shock. The shock front is parallel to the *y*-axis. ϕ is the angle between the streamline in the pre-shock region and the shock front ($\phi = 90^{\circ}$ for normal shock). The pre-shock gas velocity is v_1 , and its *x*- and *y*-components are v_{1x} and v_{1y} , respectively. The post-shock gas velocity is v_2 , and its *x*- and *y*-components are v_{2x} and v_{2y} , respectively. The angle between the gas streamlines in the pre- and post-shock regions is χ . (b) Dust velocity with respect to gas behind the shock front, v_{rel} .

using the equation of state, $p_{\text{gas}} = (k_{\text{B}}/\mu m_{\text{H}})\rho_{\text{gas}}T_{\text{gas}}$. When Λ is evaluated by the value immediately behind the shock front, Λ_0 , for simplicity, we obtain the solution

$$T_{\rm gas} = T_{\rm gas,0} e^{-\frac{t}{t_{\rm cool}}},\tag{50}$$

where

$$t_{\rm cool} = \frac{\gamma}{\gamma - 1} \frac{p_{\rm gas,0}}{\Lambda_0},\tag{51}$$

is the post-shock gas cooling time. At $t/t_{cool} \ll 1$, under which the thermal desorption primarily occurs, Equation (50) can be approximated as

$$T_{\rm gas} \simeq \frac{T_{\rm gas,0}}{1 + \frac{t}{t_{\rm real}}}.$$
 (52)

This formula corresponds to Equation (40) with the following substitutions: $T_0 \rightarrow T_{\text{gas},0}$, $t_{\text{stop}} \rightarrow t_{\text{cool}}$, and $m \rightarrow 1$. Therefore we can calculate the desorption fraction in the same manner in Appendix C.1.3.

C.3. Comparison with Numerical Results

The approximation formulae are compared with the corresponding numerical results in Figure 9. Panel (a) shows the 10% desorption condition in the case of $a_{dust} = 1 \ \mu m$ obtained from the numerical simulation (solid), the approximations for aerodynamic heating in the low- (dashed) and high-density (dash-dotted) cases, and the approximation for the conductive heating case (dotted). We adopt $\Delta E_d / E_{d0} = 0.2$. It is found that the behaviors of the numerical results at low and high densities agree with the dashed and dotted curves, respectively. The dash-dotted curves make minor contributions to explain the behaviors of the numerical results in any of the density regions. The good agreement between the numerical results and the approximation formulae is confirmed for $a_{dust} = 0.1 \ \mu m$ (panel b) and 0.01 μm (panel c).

Appendix D Oblique Shock

In this study, we imply a normal shock in our calculation, that is, the gas and dust-grain streamlines in the preshock region are perpendicular to the shock front. However, the normal shock assumption is not necessarily valid because the infalling rotating envelope in principle has only an azimuthal velocity component at the centrifugal barrier. In this section, we consider the effect of the obliquity on the ξ_{des} estimation.

The degree of shock heating is primarily determined by $\rho_{\text{gas},0}$ and v_{rel} in the post-shock region. Figure 10(a) is a schematic of the gas velocity before and behind the oblique shock front. The gas-velocity tangential component is unchanged, that is, $v_{1y} = v_{2y} = v_{\parallel}$. On the other hand, the normal component is decreased. Therefore the relative velocity behind the shock front is given by $v_{\text{rel}}^{\text{obl}} = v_{1x} - v_{2x}$ (see panel b). Using the relationships $v_{1x} = v_1 \sin \phi$, $v_{2x} = v_{\parallel} \tan(\phi - \chi)$, and $v_{\parallel} = v_1 \cos \phi$, we obtain

$$v_{\rm rel}^{\rm obl} = v_1 [\sin \phi - \cos \phi \tan(\phi - \chi)], \tag{53}$$

where the angle of deviation χ of the velocity is given by (Landau & Lifshitz 1987)

$$\cot \chi = \tan \phi \left[\frac{(\gamma + 1)M^2}{2(M^2 \sin^2 \phi - 1)} - 1 \right].$$
 (54)

On the other hand, $\rho_{\text{gas},0}$ is not significantly affected by the obliquity. The equation of continuity is given by $\rho_s v_{1x} = \rho_{\text{gas},0}v_{2x}$; therefore we obtain $\rho_{\text{gas},0}/\rho_s = \tan \phi/\tan(\phi - \chi)$. Substitution of Equation (54) in the limit $M \gg 1$ yields $\rho_{\text{gas},0}/\rho_s = (\gamma + 1)/(\gamma - 1)$, which corresponds to the normal shock case (see Equation (2)).

In the case of normal shock, the relative velocity is given by (see Equation (2))

$$v_{\rm rel}^{\rm nor} = v_{\rm s} - v_{\rm gas,0} = v_{\rm s} \frac{2(M^2 - 1)}{(\gamma + 1)M^2}.$$
 (55)



Figure 11. Effective shock velocity, veff, of an oblique shock as a function of the angle between the shock front and the streamline in the pre-shock region, ϕ . The normal shock corresponds to the case with $\phi = 90^{\circ}$.

Here, the value of v_s that satisfies $v_{rel}^{obl} = v_{rel}^{nor}$ is defined as the effective shock velocity, v_{eff} . From Equations (53) and (55), we obtain

$$\frac{v_{\text{eff}}}{v_1} = \frac{\gamma + 1}{2} [\sin \phi - \cos \phi \tan(\phi - \chi)], \qquad (56)$$

at the strong shock limit ($M \gg 1$). Thus, the oblique shock with veff realizes the same degree of shock heating as the normal shock with $v_{\rm s} = v_{\rm eff}$. Figure 11 shows $\frac{v_{\rm eff}}{v_{\rm l}}$ as a function of ϕ . For example, we obtain $\frac{v_{\text{eff}}}{v_1} = 0.5$ at $\phi = 30^\circ$. In that case, if $v_1 =$ 2 km s⁻¹, we can expect the same ξ_{des} as for a normal shock with $v_{s} = 1 \text{ km s}^{-1}$.

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