Molecular Dynamics Study on Evaporation Process of Adherent Molecules on Surface by High Temperature Gas

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Surface degreasing method with premixed flame is proposed as the removal method of adherent impurities on materials. Effects of adherent molecular thickness and surface potential energy on evaporation rate of adherent molecules and molecular evaporationmechanism were investigated and discussed in the present study. Evaporation processes of adherent molecules on surface molecules were simulated by the molecular dynamics method to understand thermal phenomena on evaporation processes of adherent molecules by using high temperature gas like burnt gas. The calculation system was composed of a high temperature gas region, an adherent molecular region and a surface molecular region. Both the thickness of adherent molecules and potential parameters affceted the evaporation rate of adherent molecules and evaporation mechanism in molecular scale.

Key Words : Molecular Dynamics Method, Evaporation, Surface Treatment, Adherent Molecules, Thin Film, Burnt Gas

Nomenclature

N_{col} : Number of evaporated molecules with gas interaction

N_{self} : Number of evaporated molecules without direct gas interaction

dN/dt : Evaporation rate for unit surface area (1/ns)

dN_{col}/dt : Evaporation rate with gas molecular interaction

dN_{self}/dt : Evaporation rate without gas molecular interaction

ε : Energy parameter of Lennard-Jones potential

ε_{aa} : ε between an adherent molecule and an adherent molecule

ε_{as} : ε between an adherent molecule and a surface molecule

ε_{as0} : Standard value of ε_{as}

ε_{as^*} : $\varepsilon_{as^*} = \varepsilon_{as}/\varepsilon_{as0}$

L_a : Thickness of adherent molecular layers

L_g : Length of a upper boundary region

L_s : Length of a lower boundary region

σ : Length parameter of Lennard-Jones potential

T_g : Temperature of upper boundary in a gas region

T_l : Average temperature of adherent molecules

T_s : Temperature of lower boundary in a surface region

$\phi_{(r)}$: Potential function

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1. Introduction

The molecular dynamics simulation can be useful to predict an optical surface temperature

control for complete surface cleaning process or an optical surface state control by favorable evaporation rate or removal rate of adherent molecules. From an ecological point of view, a dry-type "degreasing" method by flames was proposed and developed recently. A study of Itoh et al. (1994) was referred to a surface degreasing method by flames. Such a dry-type degreasing method by using flames can be considered as a thermal treatment in molecular scale because after such surface treatments, the adsorption of paints on base materials has been improved remarkably. Mechanisms of such improvement by flame treatments are not known clearly though some suppositions are proposed based on experimental observations. It may be true that chemical species in burnt gas at high temperature have removed almost all the adherent molecules on the materials in such processes. Therefore, these flame treatment processes involve fundamental problems of heat and mass transfer between gas molecules and liquid (adherent) molecules and also between liquid (adherent) molecules and surface molecules. These processes seem to be very complex interfacial phenomena where various polyatomic molecules on a metallic surface are decomposed thermally or evaporated by chemical reactions or collisions of various chemical species in burnt gas.

The various simulation methods have been used in order to elucidate the phenomena relating to, for example, flow field and combustion flow and so on, by using Direct Numerical Simulation (Shin, 2000 ; Na, 2003) and Large Eddy Simulation (Itoh et al., 2000 ; Kobayashi et al., 2001 ; Jang et al., 2001).

Shibahara et al.(1999) and Maruyama (1999) studied various interfacial phenomena, such as phase change and condensation and so on, by using the molecular dynamics method. Molecular states at a material surface can be predicted in the future by such a molecular dynamics simulation if concentrations, temperature and other physical or chemical conditions of burnt gas are specified beforehand.

In the present study, the evaporation processes of adherent molecules by high temperature gas

collisions were simulated and observed in order to understand relationships between molecular behaviors at a very thin adherent molecular layers and physical conditions such as gas temperature (T_g), surface temperature (T_s), adhesion strength (ε_{as}) and thickness of adherent molecular layers (L_a). Evaporation rates, the average temperature of adherent molecules, temperature distribution in the system and molecular behaviors were investigated and discussed. A very simple simulation system was used for numerical calculation shown in Fig. 1. The calculation system consisted of a surface molecular region, an adherent molecular region and a gas region. Chemical reactions between chemical species in burnt gas and adherent molecules should play important roles in these flame treatment processes. However, as a first approach to such processes by the molecular dynamics method, chemical reactions between gas molecules and adherent molecules are ignored so as to investigate thermal mechanism in the evaporation processes of adherent molecular layers on surfaces in the present study. Macroscopic flow velocity of gas molecules is also assumed to be negligible in the present study to understand the fundamental phenomena in a simple way even though such forced convection is one of important physical factors in these processes. Energy parameters of Lennard-Jones potential between adherent molecules and surface molecules correspond to adhesion strength between adhesion and surfaces in the processes. Evaporation and removal processes of adherent molecules from the metallic surface calculated by the molecular dynamics method were discussed in the present study.

2. Numerical Method

Figure 1 shows configuration of the calculation system. T_g that is the temperature of gas region in the range of L_g Å distance from upper boundary, was controlled and kept as a gas temperature control region. Temperature of surface molecules in the range of L_s Å distance apart from bottom boundary, say a surface temperature control region, was controlled and kept at $T_s K$.

The center of mass of the bottom layer in a surface region was fixed artificially for numerical calculations. Mirror boundary condition was used as an upper boundary condition at the gas temperature control region. Periodic boundary conditions were employed in x and y directions of the calculation system in Fig. 1. Temperatures of the surface temperature control region and the gas temperature control region can be considered to be T_sK and T_gK, respectively, from a macroscopic point of view. As initial conditions, the distribution of molecular kinetic energy in a gas region was controlled in a thermally equilibrium state at T_gK. Molecules in a surface region and an adherent region were settled to be in a thermally equilibrium state at T_sK, too. Molecular dynamics calculations were conducted with these initial conditions and collision processes of gas molecules to adherent molecules and their evaporation processes were simulated in a molecular scale.

Describing in more detail, the metallic surface was regarded as thin film arranging with 3 layers (maximal molecule number : 1536, lattice constant : 3.507Å) in face-centered cubic lattice (FCC). Adherent molecules were existed on the metallic surface as thin film-type. The number of adherent molecules was 196 and the number of gas molecules was set to 160. The coordinate system was 3 dimensional Cartesian coordinate
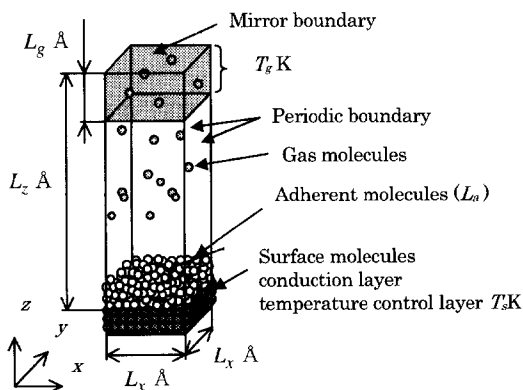
and the initial location of atom in the most upper part of surface was set to $z=0$.

In this study, as for the temperature correction, the temperature T was expressed by using mean value of kinetic energy of particle, as the following equation.

$$\frac{3}{2}kT = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}m_i|\mathbf{v}_i|^2 \qquad (1)$$

Here, N is the number of particle, m_i is mass of particle, v_i is velocity of particle and k is Boltzmann constant. In molecular dynamics, even though the system becomes thermal equilibrium state if the calculation is somewhat iterated after giving the initial state, the temperature correction is necessary to obtain the target temperature in the system. The velocity of each particle is corrected by using the following equation when the temperature T_t at time t is approached to target temperature T_o.

$$\mathbf{v}_{i0} = \mathbf{v}_{it}\sqrt{\frac{T_0}{T_t}} \qquad (2)$$

Here, $\mathbf{v}_{i0}$ is velocity after correcting the particle i and $\mathbf{v}_{it}$ is velocity before correcting the particle i. The momentum correction, which is the operation that translation velocity of whole system makes 0, was conducted by the following equation.

$$\sum_i m_i\mathbf{v}_i = 0 \qquad (3)$$

Therefore, the whole system can be regarded as stationary state.

In order to give the initial state at $t=0$ to surface atoms, adherent molecules and gas molecules, a thermal equilibrium state was prepared by dividing the surface atoms, adherent molecules and gas molecules, respectively. The surface atoms and adherent molecules were arranged on surface side, the only surface atoms were given initial velocity vector by using random numbers. As making stationary state by performing the momentum correction for the most lower 1 layer of surface atoms, the temperature was calculated from its velocity vector. Then the temperature correction was performed by approaching its

Fig. 1   Configuration of the simulation system for evaporation processes of adherent molecules on a surface by high temperature gas collisions

mean temperature to surface boundary temperature $T_s(K)$. At this time, adherent molecules, which were not given initial velocity vector, were prepared to be thermal equilibrium with surface atoms, by thermal conduction from surface atoms. As like the surface atoms, the gas molecules were also given the initial velocity vector using the random numbers. After calculating the temperature from whole velocity vector, the temperature correction was conducted by approaching its mean temperature to gas boundary temperature $T_g(K)$. As for the surface molecule side, the periodic boundary condition was applied to x, y direction and the mirror boundary condition was applied to $L_g = 40\,\text{Å}$ in z direction. The periodic boundary condition was applied to the gas molecule side in the range of $50\,\text{Å} \leq z \leq 280\,\text{Å}$.

Two methods are well-known to realize an unsteady molecular system where a substantial energy flux exists as a calculation condition. One method is to control temperatures of two boundary regions at constant temperatures, here, studies of Watanabe et al. (1993), Ohara et al. (1998) and Ohara et al. (1999) were referred, and the other is to control the magnitudes of heat flux at boundary conditions, as referring studies of Kotake et al. (1994) and Maruyama et al. (1999). In the present study, temperature control method is used so as to investigate effects of boundary temperature (T_g, T_s) clearly on the interfacial phenomena near adhesion materials with very steep temperature gradients and to model burnt gas collision to the metallic surface kept at room temperature.

As mentioned above, molecular dynamics was used in this study to solve the motion of atoms or molecules. It has two equations of motion, namely one is for monoatomic molecules and the other is for polyatomic molecules. Basically, the equation of Newton is applied for calculating molecular motions of all molecules. The following equation was solved in the case of monoatomic molecules.

$$\mathbf{F}_i = -\sum_j \nabla_i \phi(r_{ij}) \qquad (4)$$

Here, $\phi(r_{ij})$ is a potential energy between molecule i and j.

The intermolecular potential function used 12-6 Lennard-Jones potential function as follows,

$$\phi(r) = 4\varepsilon\left\{\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right\} \qquad (5)$$

Table 1 shows the potential parameters ε and σ used in the present study. The potential parameters of a gas molecule, an adherent molecule and a surface molecule correspond to those of an oxygen molecule, an acetone or a methanol molecule and an iron atom, respectively. A methanol molecule as an adherent molecule was employed only for checking molecular structure effect on evaporation rate. For the determination of 12-6 Lennard-Jones potential parameters, the study of Reid (1977) was referred. Length parameter σ is kept constant between different molecules A and B as $\sigma_{AB} = (\sigma_A + \sigma_B)/2.0$ based on the simple combination rule. Energy parameter ε is also kept constant as $\varepsilon_{AB} = \sqrt{\varepsilon_A \times \varepsilon_B}$. These combination rules are called as Lorentz-Berthelot combination rule. Energy parameter ε_{as} between an adherent molecule and a surface molecule is one of important parameters because it represents adhesion conditions on a surface such as physical adsorption or chemisorption. In the present study, energy parameter between an adherent molecule and a surface molecule (ε_{as}) is expressed as a non dimensional value ($\varepsilon_{as}*$) divided by the standard value (ε_{as0}: 9.130×10^{-21} J). Effects of adhesion strength ($\varepsilon_{as}*$) on evaporation processes were investigated by changing the magnitude of $\varepsilon_{as}*$ from 0.333 to 3.000. When energy parameter between an adherent molecule and a surface molecule was equal to the energy parameter between an adherent molecule and another adherent molecule, $\varepsilon_{as}*$ is equal to the value of 0.906 ($\varepsilon_{aa}/\varepsilon_{as0}=0.906$). Therefore, when $\varepsilon_{as}*$ was equal to 1.000, the adhesion was not strong such as weak physical adsorption. In the case of $\varepsilon_{as}*=3.000$, the adhesion strength became stronger than usual physical adsorption and it can be considered to be a kind of chemisorption.

Thickness of adherent molecules was changed from 1 molecular layer to 6 molecular layers in order to discuss effects of adhesion thickness on interfacial phenomena between a gas region and

Table 1 Potential parameters

	$\varepsilon[\times 10^{-21}\,J]$	$\sigma[\mathring{A}]$
gas–gas	1.779 (ε_{gg})	3.362
gas–adherent	3.836 (ε_{ga})	3.664
gas–surface	2.823 (ε_{gs})	2.803
adherent–adherent	8.271 (ε_{aa})	3.966
adherent–surface	9.130 (ε_{as0})	3.105
surface–surface	40.00 (ε_{ss})	2.243

Table 2 Calculation conditions

$T_g(K)$	$500 \sim 2000$
$T_s(K)$	$250 \sim 500$
$L_a(\mathring{A})$	$4.0 \sim 25$ $(1 \sim 6$ layers$)$
$L_z(\mathring{A})$	$180 \sim 280$
$L_x(\mathring{A})$	$28.6 \sim 56.11$
$\varepsilon_{as}*$	0.333, 1.0, 1.5, 2.0, 3.0

Fig. 2(a)   Evaporation rate of surface adherent molecules depending on adherent molecular structures in comparison between a monoatomic molecular model and a polyatomic molecular model of CH_3OH

Fig. 2(b)   Typical adherent state of surface adherent molecules in the case of polyatomic molecular adhesion

an adherent region. Adherent molecules were regarded to be evaporated when they reached several angstrom apart from an adhesion surface and more than two adherent molecules were not found within 6 Å distance from the molecule.

Table 2 shows calculation conditions used in the present study. Total calculation time is variable from 100 ps to 200 ps. The Verlet integration and the Leap-frog method were used for numerical calculation of Newton's equations with time step of 2 fs. For these purposes, the study of Kotake (1990) was referred.

3. Effects of Adherent Molecular Structures on Evaporation Rate

In order to investigate the effects of adherent molecular structures on evaporation, the evaporation processes of adherent molecules of methanol molecules were discussed in the present section. A methanol molecule was used as a monoatomic molecule of 12-6 Lennard Jones potential molecules and two site Lennard-Jones potential for a CH_3-OH molecule was used as a polyatomic molecule model. Figure 2(a) shows the typical example of evaporation ra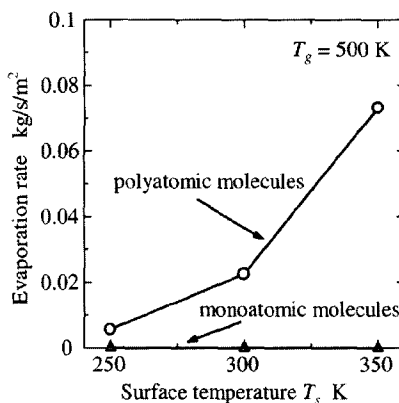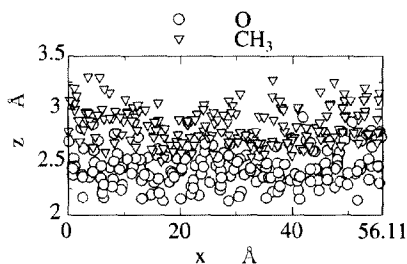te of surface adhesion molecules with respect to surface temperature. From the result in Fig. 2(a), the evaporation rate of adherent molecules in case of a polyatomic molecular model is higher than that of a monoatomic molecular model.

Figure 2(b) shows typical state of surface adhesion of a polyatomic molecular model of CH_3-OH. The most of CH_3 among adhesion molecules were located at upper position in z-direction. This is because the characteristic distance of a potential function between CH_3 and the surface is longer than that between an oxygen atom in OH and a surface. On the other hand, a potential energy of CH_3 to the surface is larger than that in the case of a monoatomic molecular model. By considering that adhesion strength for the surface was expressed as potential energy parameter,

if an adherent molecule on surface was expressed as a polyatomic molecular model instead of a monoatomic molecular model, adhesion strength between surface molecules and adherent molecules became weaker consequently. Therefore, a molecular structure and adhesion state of adherent molecules were much related to the degree of evaporation and removal of adherent molecules from the surface.

4. Temperature Distributions in a Simulation System

A typical temperature distributions in the calculation system in the cases of the adhesion thickness of 6 adherent layers were shown in Fig. 3. Adhesion strength (ε_{as}^*) are 0.333 and 3.000 in Figs. 3(a) and (b), respectively. For numerical calculation of temperature distribution, the calculation domain in the gas region was divided into 25 regions along to z-axis direction. Kinetic energy of all molecules in the divided region was averaged over during 50 ps and converted into temperature as a representative temperature of each divided region. Temperature distributions in a surface molecular region, an adherent molecular region and a gas molecular region do not always become linear in the calculation system and the magnitudes of temperature gradients in the regions are different each other. Temperature gaps at the interfaces between a gas region and an adhesion region and those between

an adhesion region and a surface region were observed clearly. Temperature gaps between an adhesion region and a surface region increased with the reduction of ε_{as}^*. Such relationships between potential parameters and thermal resistance at solid–liquid interface were predicted and discussed in a report by Maruyama et al.(1999). Results in the present study coincided with the results in Maruyama et al.(1999) qualitatively.

5. Molecular Dynamics Behaviors of Evaporated Molecules at Very Thin Adherent Layers

5.1 Effects of gas temperature, surface temperature and adhesion strength on evaporation rate at 1~2 adherent molecular layers

Effects of surface temperature (T_s), gas temperature (T_g) and adhesion strength (ε_{as}^*) on evaporation rates of adhesion molecules (dN/dt) in the case of 1~2 adherent molecular layers were shown in Fig. 4. Evaporation rates (dN/dt) were estimated by the molecular dynamics simulation during 200 ps in larger calculation systems than those used in the previous sections so as to discuss removal and evaporation phenomena in a very thin adherent layers precisely. The gradients of lines in Fig. 4 were changed
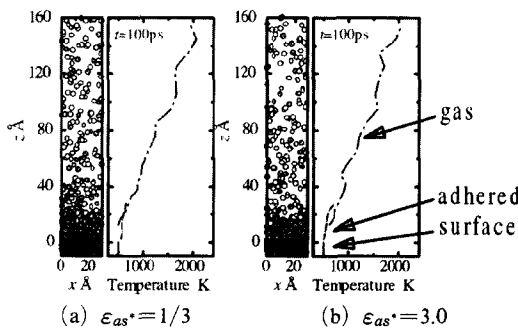
Fig. 3 Effects of adhesion strength (ε_{as}^*) on temperature distributions in the system and snapshots of the system $(L_a=6,\ T_g=2000\ \text{K},\ T_s=500\ \text{K})$
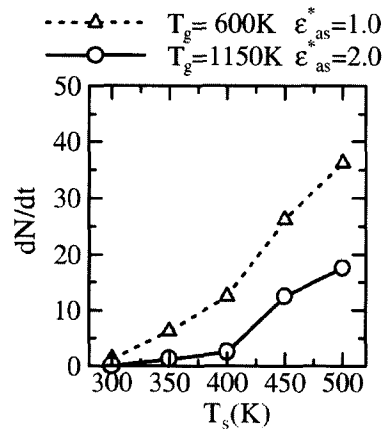
(a) $\varepsilon_{as}^*=1/3$　　　(b) $\varepsilon_{as}^*=3.0$

Fig. 4 Effects of surface temperature (T_s), gas temperature (T_g) and adhesion strength (ε_{as}^*) on evaporation rate (dN/dt); $L_a=1~2$

at the points of 400 K in both cases shown in Fig. 4. Adding these facts, evaporation of adherent molecules started at 300 K and removal rates (dN/dt) increased in accordance with the increase of surface temperature (T_s) in both cases. Gradients of the lines in Fig. 4 became large with the decrease of the magnitude of adhesion strength (ε_{as}). The gradients can be considered to be in inverse proportion to the magnitude of ε_{as} when adhesion thickness was very thin such as $1 \sim 2$ molecular layers.

5.2 Molecular dynamics behaviors of adherent molecules in evaporation processes by high temperature gas collisions

In order to discuss molecular behaviors in the vicinity of surface and adherent molecular layers, here, the study of Matsumoto et al.(1994) was referred, evaporation processes of adherent molecules were observed in detail at the time when adherent molecules just separated from adherent layers.

Figure 5 shows typical snapshots of an evaporation process of an adherent molecule assisted by a gas molecular collision (case 1). In Fig. 5 (a), an adherent molecule A stayed at the second adherent layer on the adherent molecular surface. In Fig. 5(b), a gas molecule B which had large amount of kinetic energy collided with an adherent molecule A. In Fig. 5(c), after the molecular collision between an adherent molecule A and a gas molecule B, an adherent molecule A collided with adherent molecular surface again, and a gas molecule B lost its kinetic energy and started to migrate on the surface. In Fig. 5(d), a molecule A has finally separated from the surface and the evaporation of a molecule A has completed. A characteristic time for these processes from Fig. 5(b) to Fig. 5(d) corresponds to about 2 ps in the present case.

Figure 6 shows typical snapshots of an evaporation process of an adherent molecule without a gas molecular collision (case 2). In Fig. 6(a), an adherent molecule A stayed at the second layer and migrated on the adherent molecular surface. In Fig. 6(b), an adherent molecule A collided with another adherent molecule in the first layer of adhesion. In Figs. 6(c) and (d), a molecule A has separated from surface molecules without any direct interaction of gas molecular collision.

Figures 7(a) and (b) show time history of molecular trajectories and velocities in z-axis direction for evaporated molecules shown in Fig. 5 and Fig. 6, respectively. In Fig. 7(a), z-coordinates of the evaporated molecule once decreased and then increased linearly. In the present
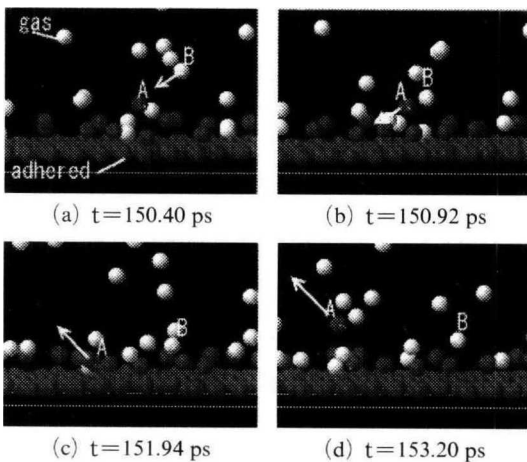

(a) t=150.40 ps (b) t=150.92 ps

(c) t=151.94 ps (d) t=153.20 ps

Fig. 5 Snapshots of an evaporation process of an adherent molecule with gas molecular interaction : case 1

(a) t=153.20 ps (b) t=154.00 ps

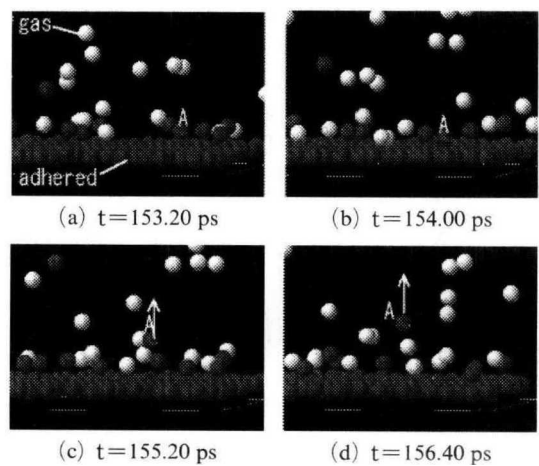(c) t=155.20 ps (d) t=156.40 ps

Fig. 6 Snapshots of an evaporation process of an adherent molecule with gas molecular interaction : case 2

case, the evaporated molecule was bouncing up on the surface and collided with a gas molecule. And the evaporated molecule collided against the surface again and has separated into gas region. The velocity in z-direction once decreased than before by a gas molecular collision. In Fig. 7(b), the evaporated molecule separated from surface suddenly and its velocity in z-direction did not decrease before the evaporation. In other cases, a gas molecule and an adherent molecule have formed a molecular cluster (a dimer) and evaporated from surface. There are many patterns in evaporation processes of adherent molecules and such patterns can be classified into the following two ways. One is an evaporation process of an adherent molecule assisted by collisions or interactions with gas molecules as shown in Fig. 5 (case 1). The other is an evaporation of an adherent molecule without direct collisions or interactions with gas molecules as shown in Fig. 6 (case 2). In the latter case, an adherent molecule can be considered to be separated from surface by collisions or interactions with adherent molecules or surface molecules not with gas molecules. The relationships between molecular behaviors in evaporation processes and thermal conditions in macroscopic boundary conditions

$(T_g,\ T_s)$ are investigated and discussed in the next section.

5.3 Effects of gas temperature and surface temperature on molecular dynamics behaviors in evaporation processes

Figure 8 shows effects of gas temperature (T_g) and surface temperature (T_s) on molecular dynamics behaviors in evaporation processes by high temperature gas collisions. The vertical axis represents the ratio of evaporated molecules without gas molecular interactions (N_{self}) to the total evaporated molecules $(N_{col}+N_{self})$. In order to estimate the value of N_{self} and N_{col} numerically, the coordinates and velocities of all molecules during calculation time are recorded in a workstation memory for the analysis and observation of molecular behaviors. The surface at high temperature enhances the ratio of evaporated molecules without gas interactions to the total evaporated molecules. This is because adherent molecules can evaporate for themselves without any interaction with gas molecules at high surface temperature. Adhesion strength $(\varepsilon_{as}*)$ changes the ratio at the same surface temperature (T_s) but the gradients of lines in Fig. 8 are almost the same each other. In the case of $1\sim2$ adherent layers, evaporation mechanism is quite different depending on adhesion strength $(\varepsilon_{as}*)$ even at the same

(a) case 1 : with gas molecular interaction

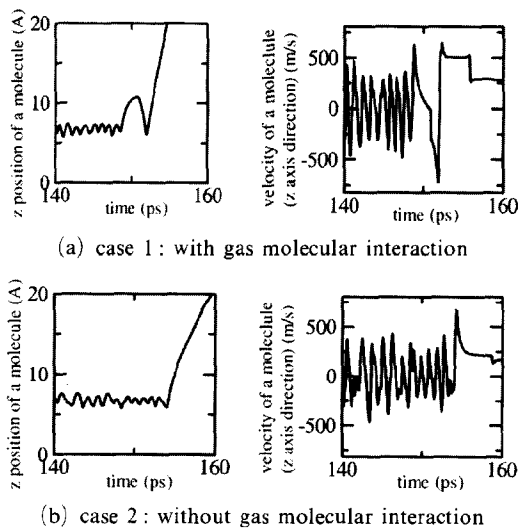(b) case 2 : without gas molecular interaction

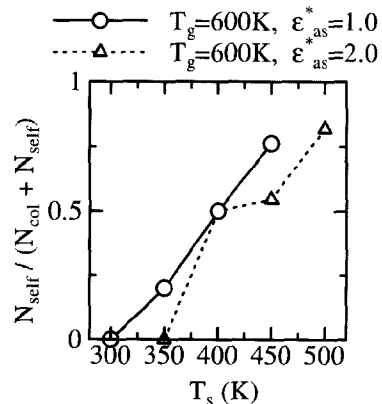**Fig. 7** Typical time histories of molecular trajectories and velocities of evaporated molecules

Fig. 8 Effects of gas temperature (T_g) and surface temparature (T_s) on molecular dynamics behaviors in evaporation processes by high temperature gas collisions

surface temperature (T_s).

Figure 9 shows the relationships between surface temperature (T_s) and the evaporation rate (dN_{col}/dt, dN_{self}/dt) in the case of $T_g = 600$ K and $\varepsilon_{as\cdot} = 1.0$. Evaporation rate ($dN/dt$) can be classified into the evaporation rate with gas molecular interactions (dN_{col}/dt) and that without gas molecular interactions (dN_{self}/dt) from a point of molecular dynamics behavior. The evaporation rate without gas molecular interactions (dN_{self}/dt) increases remarkably in accordance with the increase of surface temperature (T_s). On the other hand, the evaporation rate with gas molecular interaction (dN_{col}/dt) increases gradually with the increase of surface temperature (T_s) and saturates when surface temperature reaches above 400 K. Total evaporation rate in Fig. 4 consists of these two different evaporation rates, with gas molecular interactions and without gas interactions. Such two evaporation rates come from two different molecular dynamics behaviors, and the dependence of molecular behaviors on surface temperature is quite different each other. In the present case, gas collision interaction is dominant in evaporation processes of 1~2 adhesion layers when the surface temperature is less than 400 K. Self-evaporation processes start to play important roles above 400 K in the case of adhesion strength $\varepsilon_{as\cdot} = 1$.

The boiling point of methanal is about 340 K and alcohol molecules adhered to surface start to

evaporate spontaneously if surface temperature exceeds 350 K, as shown in Fig. 9. Therefore, the evaporation mechanism of adherent molecules (① direct collision of gas molecules ② spontaneous evaporation of adherent molecules) becomes almost same ratio when surface temperature becomes 400 K. The reversion phenomenon of evaporation mechanism of surface molecules occurs at the point of surface temperature 400 K, which is a little higher temperature than boiling point of adherent molecules due to both the boiling point of adherent molecules and the effect of adhesion strength to surface. If surface temperature exceeds 400 K, mechanism of ② becomes overwhelmingly dominant.

6. Conclusions

In order to understand thermal phenomena in evaporation processes of very thin adherent molecular layers on a surface by using high temperature gas molecular collisions, a molecular dynamics simulation was conducted in the present study. A calculation system was composed of a gas region, an adherent molecular region and a surface molecular region. Temperatures at upper part of gas region and at lower part of surface molecular region were controlled and kept at T_gK and T_sK, respectively. Evaporation rates of adherent molecules were measured for various gas boundary temperature (T_g), surface boundary temperature (T_s), adhesion strength ($\varepsilon_{as\cdot}$) and adhesion thickness (L_a) by the molecular dynamics method. The obtained conclusions are as follows.

(1) The evaporation rate of a polyatomic molecular model was higher than that of a monoatomic molecular model in the case of CH_3OH adhesion. This is due to differences of both adherent strength and an adherent molecular state to the surface from molecular scale point of view.

(2) In the case of an evaporation process of very thin adherent molecular layers, the evaporation rate consisted of that with gas molecular interactions and that without gas molecular interactions. These two different evaporation rates
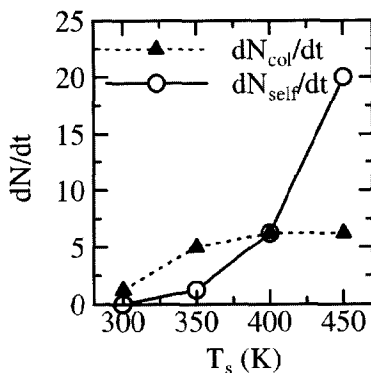

Fig. 9   Relationships between surface temperature (T_s) and evaporation rates ($T_g = 600$ K, $\varepsilon_{as\cdot} = 1$)

show different dependence on a surface temperature.

(3) Gas interaction mechanism was dominant in evaporation processes in the case of lower surface temperature and evaporation processes without gas molecular interactions became dominant with the increase of surface temperature in the case of evaporation of very thin adherent molecular layers.

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