

Rarefied Gas Flow Over a Solid Surface with Adsorbates

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The molecular dynamics study is applied for interaction of the gas molecule with the solid wall to analyse the flow of a rarefied gas between two walls. The wall consisting of Pt molecules is considered to be in a state of physical adsorbates. Two problems are considered : one is the flow problem and the other is the temperature problem. It is found that the tangential momentum accommodation coefficient is about 0.8 when the relative speed ratio of the two walls is unity, while it decreases with increasing Knudsen number when the relative wall speed ratio is 5.0. It is as small as about 0.6 when the Knudsen number is 10.0. It is also shown that the temperature accommodation coefficient is about 0.85 at 300K wall , 0.75 at 450 K wall , and 0.69 at 600K wall.

1. INTRODUCTION

Many studies have been made of rarefied gas flows by various analytical and numerical methods. In most cases, simplified boundary conditions at the solid surface such as the diffuse reflection, the specular reflection, the Maxwell type boundary condition, have been used. However, it is said that the simple boundary condition cannot describe the gas-wall interaction well when the solid surface is exposed to high temperature or a high speed flow, or when the gas is in an ultra vacuum. The analysis of the gas-wall interaction is interesting and important, but not easy because of its complexity. The Cercignani-Lampis model,^(1,2) and soft-cube model⁽³⁾ offer more complicated but useful boundary conditions. Recently, Matsumoto and Matsui^(4,5) studied the interaction on a clean surface of the platinum wall by the molecular dynamics method. They calculated the reflection or adsorption of an incident molecule with a given energy and direction of the molecular velocity. They also studied the gas-surface interaction with adsorbates at rather low wall temperature by a similar method⁽⁶⁾.

The incident molecule in an ordinary gas flow, however, has various energy and direction, and these varieties must change the global flow behavior. In this respect, it is interesting to

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investigate the behavior of the gas in which the interaction of the gas molecule with the solid molecule is treated by the molecular dynamics. This method may give rise to a simple and less ambiguous analysis. In the present paper, we consider the rarefied gas between two walls by the molecular dynamics method under the boundary condition in which the gas-wall interaction is analysed.

2. METHOD OF ANALYSIS

Let the distance between two walls be L , and the reference number density n_0 . We consider two problems: The one is the flow problem, that is, the upper wall have the velocity $-\frac{U}{2}$ whereas the lower wall moves with the velocity $\frac{U}{2}$. Both wall temperatures are taken to be $T_0 = 300K$ except explicitly stated. Actual calculations for the flow problem were made of the cases that the speed ratios S_L of the lower wall are 0.5 and 2.5, where $S_L = \frac{U}{2}/C_m$, $C_m = \sqrt{2kT_0/m}$ is the most probable speed, m is the mass of a gas molecule, and k the Boltzmann constant. Since the flow is symmetric with respect to the center line between the walls, we may analyse the half space of the flow field. The other one is the temperature problem, in which both wall temperatures are different. The combination of the lower (T_L) and upper (T_U) wall temperature are taken as

$$(T_L, T_U) = (300K, 600K), (450K, 600K), (600K, 300K).$$

We assume that the molecule is diffusely reflected at the upper wall.

The Monte-Carlo method⁽⁷⁾ is applied to the analysis of the flow field between two walls. The hard sphere molecule is assumed for the interaction between gas molecules in the Monte-Carlo simulation. When the molecule hits the wall surface in this simulation, we switch to the molecular dynamics at this point to trace the motion of the gas molecule interacting with the solid molecules. We used the standard molecular dynamics method for the interaction between gas and wall molecules. For this purpose, we assume that the wall consists of thin platinum layer and its surface is set on (1,1,1) plane. We take 6 and 6 Pt molecules in the direction of motion of the wall and normal to it, respectively. Four molecular layers are taken normal to the wall surface. The periodic condition is applied to the parallel direction to the surface as is usually assumed in the molecular dynamics. The Xe molecule is taken as the gas molecule to interact with the Pt wall. We take the Lennard-Jones potential,

$$\Phi(r) = 4\epsilon\left[\left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^6\right], \quad (1)$$

for Pt-Pt interaction and for Xe-Xe interaction. The Morse potential,

$$\Phi(r) = \epsilon[e^{-2\sigma(r-r_0)} - 2e^{-\sigma(r-r_0)}], \quad (2)$$

is used for Pt-Xe interaction. Here, r is the intermolecular distance, and σ , ϵ and r_0 are interaction parameters. The numerical values of these parameters are given in Table 1^(5,8).

Table 1 Interaction parameters

	ϵ [eV]	σ [1/Å]	r_0 [Å]
Xe-Pt	0.0275	1.05	3.20
Pt-Pt	0.325		2.523
Xe-Xe	0.0138		4.10

When a gas molecule hits on the wall in the Monte-Carlo simulation, we put the Xe molecule at a distance of $4\sigma_{pt}$ above the most upper Pt molecule, where σ_{pt} is the distance to the zero in Pt potential. The initial velocity of this molecule has been calculated by the Monte-Carlo simulation. Newton's equation of motion of Xe molecule is integrated with Verlet's method. The time step of integration is taken to be $4.54 \times 10^{-15} s$. We could consider the clean surface of Pt wall. However, while the gas molecule hits on the clean surface successively, some of them, which have low energy, may be physically adsorbed on the surface. We should take the Pt wall on which some Xe molecules are adsorbed, and consider the interaction of the impinging Xe molecule with the solid surface as well as the adsorbates. Actually, we found that nine Xe molecules are physically adsorbed on the surface of 6×6 Pt molecules of temperature $300 K$, five Xe molecules at $450 K$, and one Xe molecule at $600 K$. They are moving around on the surface.

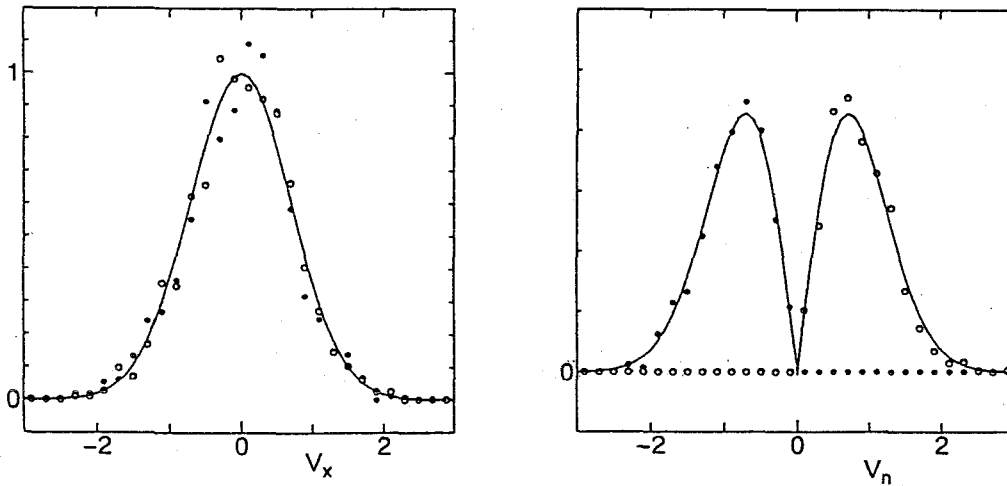


Fig. 1 Molecular velocity distributions of impinging (\bullet) and reflecting molecules (\circ) at $T_L = 300K$.

Before going to the analysis of the flow, we examined the present wall characteristics. For this purpose, we ejected to the wall the gas molecule of the Maxwellian distribution having the same temperature as the wall, and check its velocity distribution after reflection from wall surface. We impinged one thousand molecules. The velocity distribution of the molecule is shown in Fig.1. Here, the filled circle means the incident molecule and the open circle stands for the reflected molecule. The solid line is drawn from the Maxwellian distribution. It will be seen that the distributions before and after the reflection are the same Maxwellian distributions. We here only show the case of $300 K$, but the other cases are almost the same. These results indicate that our present wall is not skewed, but suitable for the analysis of the gas-wall interaction.

3. RESULT OF THE FLOW

We give here some of the results obtained. The Knudsen number K_n are taken to be 0.05,

0.1, 0.5, 1.0, 5.0 and 10.0, where $K_n = l/L$, and l is the mean free path of the molecule.

3.1 Flow velocity

Fig. 2 shows the flow velocity $\frac{Q_x}{C_m}$ at $S_L=0.5$. The flow velocity when the diffuse reflection is assumed on both walls is shown in Fig. 3 for comparison. The difference between two velocity distributions is seen near the wall surface. The velocity distributions in case of $S_L = 2.5$ are shown in Fig. 4. Those of the diffuse reflection are illustrated in Fig. 5. The difference between two distributions is more clearly seen, especially, at large Knudsen numbers. The incident molecules to the wall have large relative velocity at high Knudsen numbers, and large relative velocity results in the large slip to the wall surface.

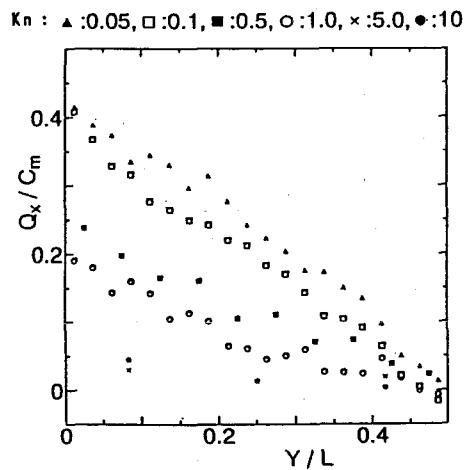


Fig. 2 Velocity distributions at $S_L = 0.5$.

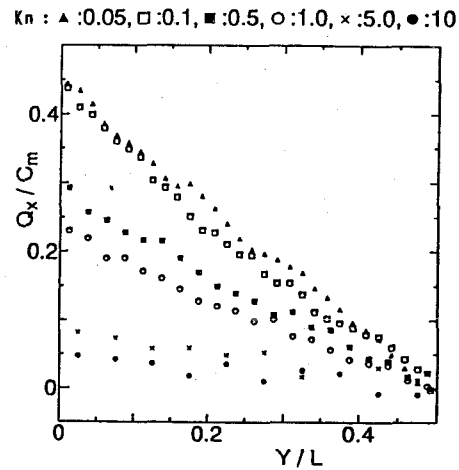


Fig. 3 Velocity distributions (diffuse reflection) at $S_L = 0.5$.

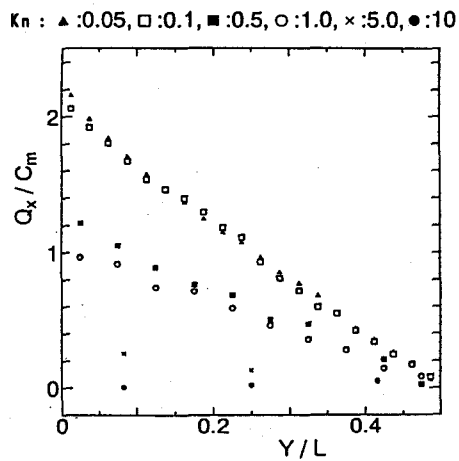


Fig. 4 Velocity distributions at $S_L = 2.5$.

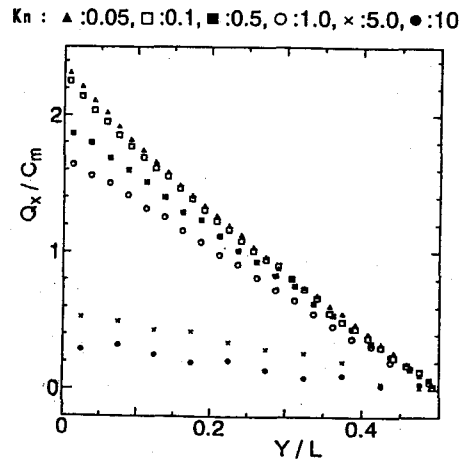


Fig. 5 Velocity distributions (diffuse reflection) at $S_L = 2.5$.

3.2 Shear stress and tangential momentum accommodation coefficient

The shear stress and the tangential momentum accommodation coefficient are calculated by the velocities of the impinging and reflecting molecules. The non-dimensional shear stress τ acting on the wall is defined by

$$\tau = \frac{\text{shear stress}}{2p_0}, \quad p_0 = kn_0T_0 \quad (3)$$

where p_0 is the reference pressure. The result is shown in Fig.6 for $S_L=0.5$ and in Fig.7 for $S_L=2.5$. The shear stress in case of diffuse reflection is also shown as filled circles in the same figure. The reduction of the stress due to the velocity slip is clearly seen.

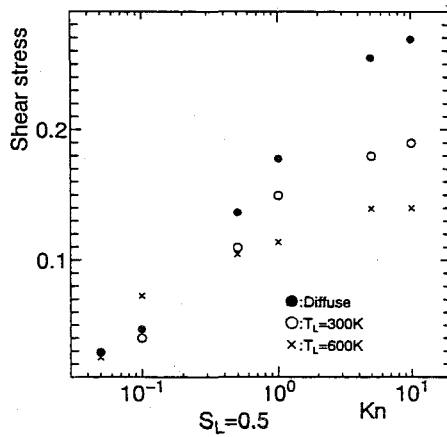


Fig. 6 Shear stress at $S_L = 0.5$.

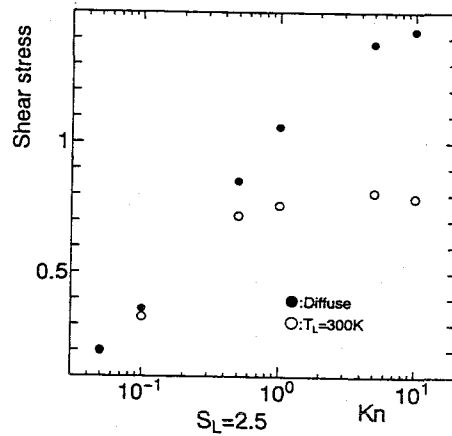


Fig. 7 Shear stress at $S_L = 2.5$.

Figure 8 shows the tangential momentum accommodation coefficient, which is defined by

$$\alpha_M = (\tau^i - \tau^r) / \tau^i, \quad (4)$$

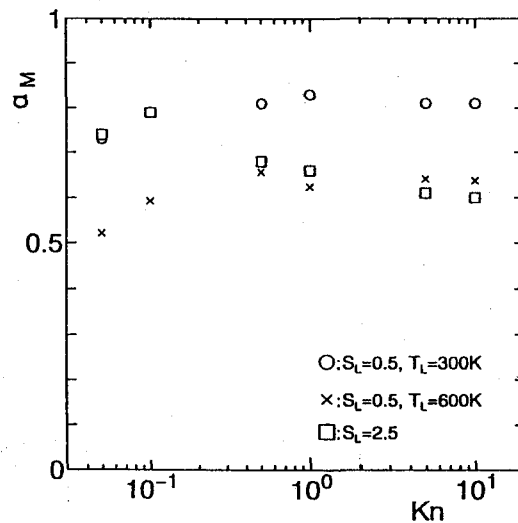


Fig. 8 Momentum accommodation coefficient.

where τ^i and τ^r are the shear stresses of the impinging and reflecting molecules, respectively. The momentum accommodation coefficient is seen to be about 0.8 for all Knudsen number when $S_L = 0.5$, and it decreases with increasing Knudsen number when $S_L = 2.5$ at 300K.

4. RESULT OF THE TEMPERATURE

We give here some of the results obtained for the temperature problem. The Knudsen number K_n are taken to be 0.05, 0.1, 0.5, 1.0, 5.0 and 10.0.

4.1 Temperature distribution

Figure 9 shows the temperature distribution $\frac{T}{T_L}$ when $T_L = 300K$. The distributions are scattered because of small numbers of sampling. The temperature distribution when the diffuse reflection is assumed on both walls is shown in Fig. 10 for comparison. The difference between two distributions is seen near the wall surface.

Kn: \blacktriangle :0.05, \square :0.1, \blacksquare :0.5, \circ :1, \times :5, \bullet :10

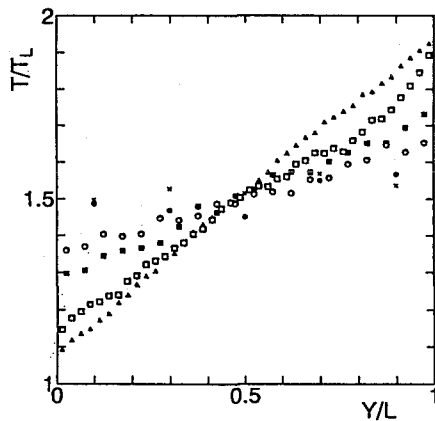


Fig. 9 Temperature distributions at $T_L = 300K$.

Kn: \blacktriangle :0.05, \square :0.1, \blacksquare :0.5, \circ :1, \times :5, \bullet :10

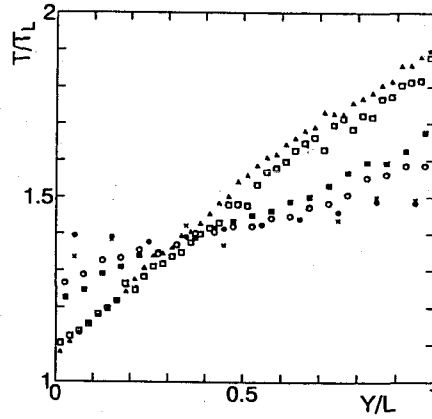


Fig. 10 Temperature distributions (diffuse reflection) at $T_L = 300$.

Kn: \blacktriangle :0.05, \square :0.1, \blacksquare :0.5, \circ :1, \times :5, \bullet :10

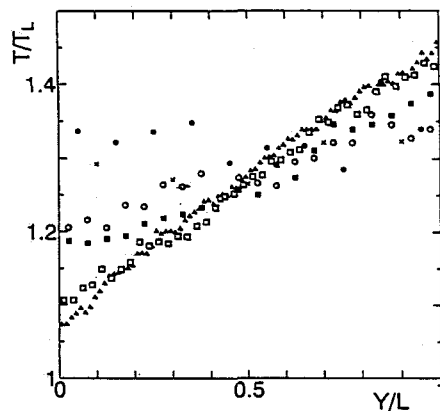


Fig. 11 Temperature distributions at $T_L = 450K$.

Kn: \blacktriangle :0.05, \square :0.1, \blacksquare :0.5, \circ :1, \times :5, \bullet :10

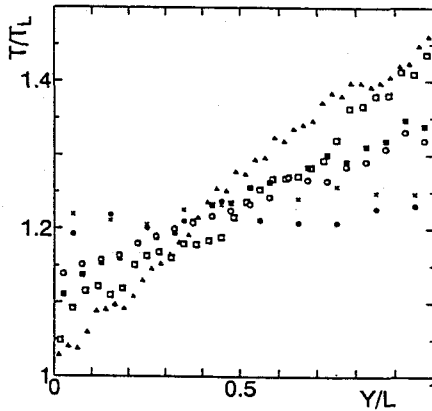


Fig. 12 Temperature distributions (diffuse reflection) at $T_L = 450$.

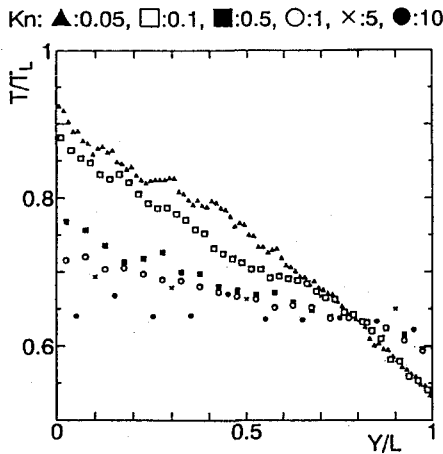


Fig. 13 Temperature distributions at $T_L = 600K$.

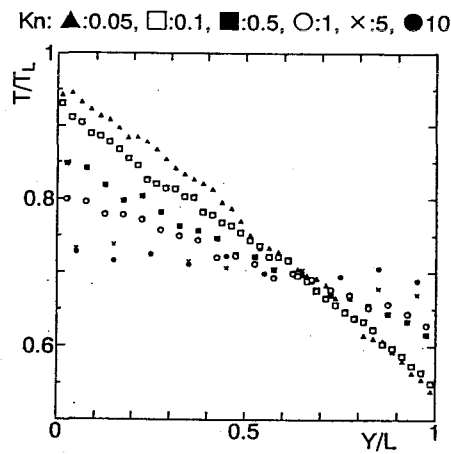


Fig. 14 Temperature distributions (diffuse reflection) at $T_L = 600$.

The distributions of the temperature in cases of $T_L = 450K$ and $600K$ are shown in Figs. 11 and 13, respectively and the corresponding distributions of the diffuse reflection are shown in Figs. 12 and 14, respectively.

4.2 Energy flux and temperature accommodation coefficient

The energy flux is shown in Fig.15. Here, the non-dimensional energy flux EF is defined by

$$EF = \frac{\text{energy flux}}{C_m^3 n_0 m} \quad (5)$$

It will be seen that the energy flux based on the present wall is rather low compared with that of the diffuse reflection at large Knudsen numbers.

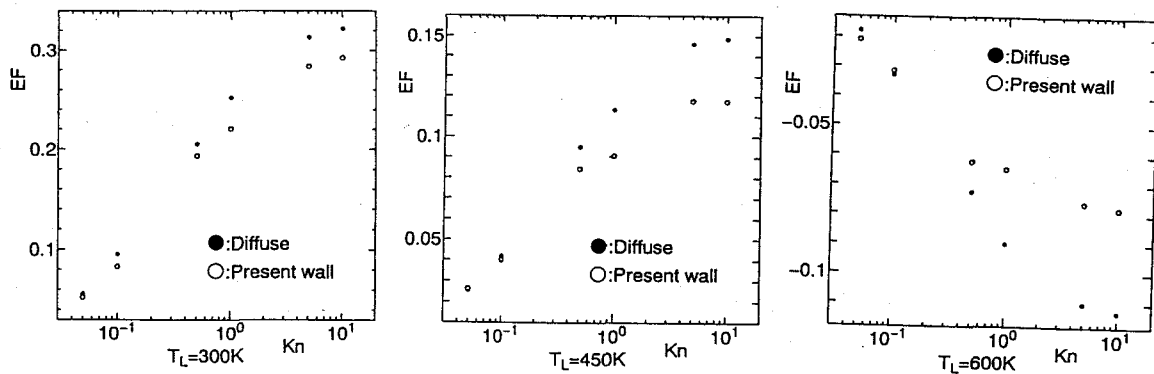


Fig.15 Energy flux.

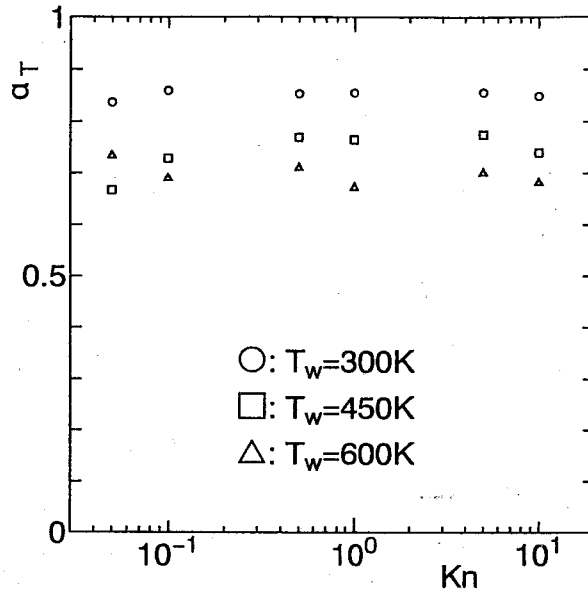


Fig.16 Temperature accommodation coefficient.

Figure 16 shows the temperature accommodation coefficient, which is defined by

$$\alpha_T = (E_i - E_r)/(E_i - E_M), \quad (6)$$

where E_i and E_r are the energy fluxes of the impinging and reflecting molecules, respectively, and E_M is the energy flux of the molecule having the Maxwellian distribution with the wall temperature. It will be seen that the temperature accommodation coefficient is temperature dependent and its value is about 0.85 at $T_L = 300K$, 0.76 at $T_L = 450K$, and 0.70 at $T_L = 600K$.

5. CONCLUSION

We have analysed the rarefied gas flow between two walls. The molecular dynamics method was applied for the interaction between gas molecule (Xe) and the wall surface (Pt). We obtained the following conclusions :

(1) The gas molecule is physically adsorbed on the wall surface ; nine gas molecules are adsorbed at 300K of the wall temperature, five molecules at 450K, and one molecule at 600K on the 6x6 wall molecular surface.

(2) The tangential momentum accommodation coefficient of the 300K wall temperature is about 0.8 when the lower wall speed ratio $S_L = 0.5$. It is about 0.7 when $S_L = 2.5$ and decreases with increasing Knudsen number.

(3) The shear stress acting on the wall is fairly small compared with the case of diffuse reflection when the Knudsen number is larger than about unity.

(4) The temperature accommodation coefficient depends on the wall temperature. Its value is about 0.85 when the wall temperature is 300K, 0.76 at 450K and 0.70 at 600K.

(5) The energy flux to the wall surface is fairly small compared with the case of diffuse reflection when the Knudsen number is larger than about unity.

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