

## Temperature dependence of the tangential momentum accommodation coefficient for gases

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The temperature dependence of the tangential momentum accommodation coefficient (TMAC) is investigated by examining gas flows in a submicron channel using molecular dynamics simulations. The results show that the TMAC decreases with the increasing temperature following an exponential decay law, and is more sensitive to lower temperatures than to higher ones. The molecular trapping-desorption behaviors near the channel surface are found to be responsible for this dependence. © 2005 American Institute of Physics. [DOI: 10.1063/1.1871363]

The tangential momentum accommodation coefficient (TMAC), which was first introduced by Maxwell and defined as the fraction of gas molecules reflected diffusively from a solid surface, is essentially used to determine the momentum transport associated with gas flows adjacent to a solid surface in rarefied gas flows<sup>1</sup> and recent microscale flows in microelectromechanical systems (MEMS).<sup>2</sup> Most of the theoretical, analytical and numerical work concerning rarefaction effects on gas flows fundamentally depends on the Maxwell gas-surface interaction law characterized by the coefficient. Therefore, the choice of the value of TMAC is a crucial challenge faced by many researchers.

Empirically, the TMAC is often taken to be unity for most of the practical engineering conditions. However, some investigations have demonstrated that the accommodation coefficient is sensitive to many gas and surface conditions. The surface materials and gas species,<sup>3-7</sup> surface roughness,<sup>4-6</sup> and contamination<sup>7</sup> were indicated to affect the TMAC significantly. For example, the measured coefficient is as low as 0.25 of rare gases over polycrystalline metal surface in Lord's work,<sup>5</sup> while it increases to about 1.0 over steel surface with roughness 0.1  $\mu\text{m}$  by Thomas.<sup>6</sup> Arkilic *et al.* recently extracted the coefficient of about 0.8 for light gases flowing in silicon microchannels prepared with MEMS technology.<sup>8</sup> These investigations indicate that one must be cautious when using a TMAC because of its strong dependence on the condition parameters. The temperature is another important factor which has been mentioned to have effects on the TMAC as well.<sup>9</sup> Unfortunately, the existing literatures presenting the TMAC were mostly at given temperatures from 293 to 300 K, and no detailed information is offered to the temperature dependence of the TMAC thus far.

Molecular dynamics (MD) simulations are employed in this letter to investigate gaseous slip flows in a submicron channel at different temperatures. Based on a two-dimensional (2D) method,<sup>10,11</sup> our simulations focus on the temperature effect on the TMAC by modeling a Couette flow system, as shown in Fig. 1, where gaseous argon undergoes shear between two platinum plates. The enclosed microflow system has a characteristic length of  $H=0.1 \mu\text{m}$  which is indeed the situation in some MEMS devices. To maintain a realistic gas-solid boundary condition, we build atomic struc-

ture walls based on the Einstein theory that the wall atoms vibrate around the face-centered-cubic lattice sites with the Einstein frequency tethered by a harmonic spring with stiffness

$$k = \frac{16\pi^4 k_B^2 m^2 \theta}{h^2}, \quad (1)$$

where  $k_B$  and  $h$  are the Boltzmann and Planck constants, respectively,  $m$  is the mass of a wall atom, and  $\theta=180 \text{ K}$  is the Einstein temperature. Particles interact with each other via a Lennard-Jones 6-12 potential in the form

$$\phi(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right], \quad (2)$$

where  $r$  is the intermolecular distance,  $\varepsilon$  and  $\sigma$  are the energy and molecular diameter parameters. The parameters used in this letter are  $\varepsilon_{\text{Ar-Ar}}=1.67 \times 10^{-21} \text{ J}$ ,  $\sigma_{\text{Ar-Ar}}=3.405 \times 10^{-10} \text{ m}$ ,  $\varepsilon_{\text{Pt-Ar}}=0.894 \times 10^{-21} \text{ J}$ , and  $\sigma_{\text{Pt-Ar}}=3.085 \times 10^{-10} \text{ m}$ .<sup>12</sup> The equations of the particle motion are integrated using a leapfrog-Verlet algorithm with a MD time step 0.01  $\tau$  ( $\tau=2.15 \text{ ps}$ ).<sup>13</sup> The wall and the gas are set at the same temperature initially. Then, during a run, the wall temperature is controlled to be constant by a typical velocity-rescaling method, and the gas is kept at constant temperature by a Langevin thermostat method in the  $z$  direction.<sup>14</sup> The motion equation of the  $i$ th molecule is

$$m\ddot{z}_i = \sum_{j \neq i} \frac{\partial \phi_{\text{LJ}}}{\partial z_i} - m\Gamma \dot{z}_i + \eta_i, \quad (3)$$

where  $\Gamma$  is a friction constant determining the rate of heat exchange between the simulation system and the heat reser-

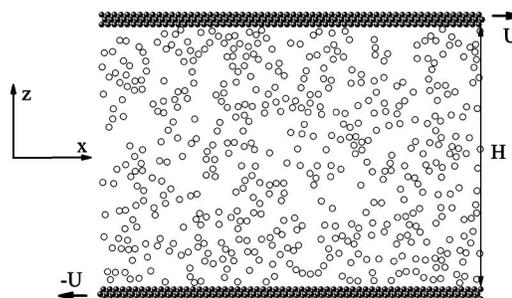


FIG. 1. Schematic of the Couette flow system. A periodic boundary condition is applied along the  $x$  direction.

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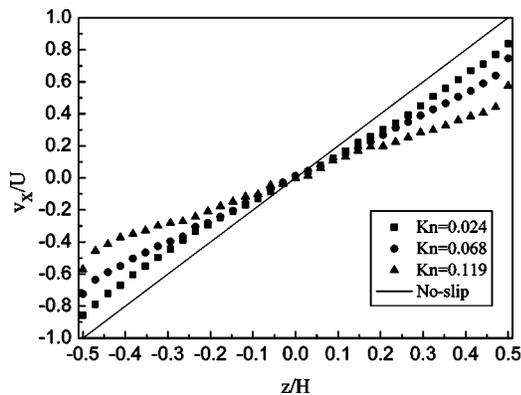


FIG. 2. Steady-state velocity profiles of Couette microflows for various Knudsen numbers at 119.8 K.

voir, and  $\eta_i$  is a Gaussian distributed random force. Thus, the system temperature distribution is kept homogeneous, and it enables us to simulate flow systems at different temperatures from 83.9 to 388.2 K.

The flows are induced by translating the walls with velocities of  $U=0.5\sigma_{Ar}/\tau$  in the plus and minus  $x$  directions, respectively. The shear rate  $\dot{\gamma}=\sigma_{Ar}/(\tau H)$  is much smaller than the critical value  $\dot{\gamma}_c\sim(m\sigma_{PtAr}^2/\varepsilon_{PtAr})^{-1/2}$ , and thus the boundary slips should be independent of the wall velocities in our simulations.<sup>15,16</sup> After an equilibrium of about 1 500 000 steps, the wall shear stress and the velocity profiles can be collected. The shear stress  $P_x$  is calculated as the net change of momentum of gas molecules at the wall per unit area and time. The steady-state velocity profiles are obtained by running average in divided  $x$ -oriented bins covering the whole channel as shown in Fig. 2. It shows that the velocity profiles are linear in the middle of the channel, and velocity slips due to the rarefaction effect that appears in the region adjacent to the wall, which agrees with the predictions of kinetic theory. Then the slip length  $L$  can be computed as  $L=U/(dv_x/dz)-H/2$ . Based on a dimensionless slip length definition  $\ell=L/H$ , Maxwell theory predicts the slip length for slip flows as<sup>17</sup>

$$\ell = \frac{2-f}{f}Kn, \tag{4}$$

in which  $f$  is the TMAC, and  $Kn=\lambda/H$  is the Knudsen number defined by the ratio of the mean free path of gas molecules and the characteristic length of the flow system. In terms of the effective viscosity  $\mu$  calculated by  $P_x=\mu(dv_x/dz)$ , the mean free path is precisely defined as  $\lambda=\mu/\rho[(\pi m/2k_B T)]^{1/2}$ . Based on Eq. (4), we are able to calculate the TMAC through examining gas microflows at different temperatures.

In Fig. 3 we present the variation of the dimensionless slip length with the Knudsen number at different temperatures in our simulations. The Knudsen number is 0.01–0.12, which implies apparent slips at the gas-wall interface. For a given temperature, the dimensionless slip length appears proportional to Knudsen number as predicted by Maxwell theory. Thus, the TMAC could precisely be extracted by fitting the slope of the  $\ell-Kn$  curve. For different temperatures, it is very clear that the dimensionless slip lengths are different at the same Knudsen number. In other words, the  $\ell-Kn$  curves have different slopes, which indicates that the

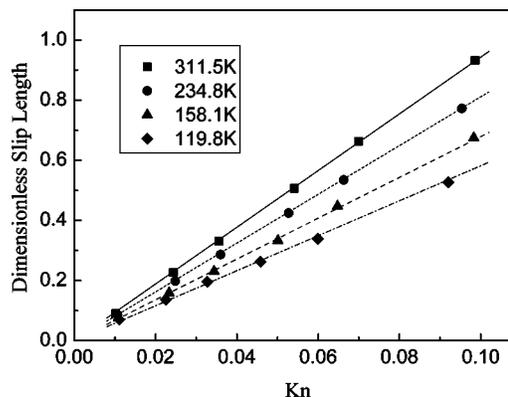


FIG. 3. Dimensionless slip length vs Knudsen number at different temperatures. The lines are obtained by linear fits using the least-squares method, in which we assume there would be no slip as the Knudsen number goes to zero.

accommodation coefficients differ at different temperatures as well.

Figure 4 shows the variation of the TMAC with temperatures obtained from our simulations. At 388.2 K, the TMAC calculated in our three-dimensional (3D) simulations turns out to be 0.19, which is quite close to the 2D simulation result of 0.18. Quite similarly, the coefficient in the 3D method at 311.5 K is 0.21, while it is 0.19 in the 2D one. The TMAC in 3DMD is 0.27 at 158.1 K while 0.25 in 2DMD. Meanwhile, the TMAC by a 3D method in Ref. 18 is also 0.19 at 300 K. They could validate our simulation results. It should be noted that the computation burden in the 3DMD simulations may be thousands of times of that of the 2DMD for the TMAC calculation,<sup>11</sup> which makes the calculation for flows on the submicron scale and at a series of Knudsen numbers almost impossible. However, the accommodation coefficient clearly varies with the temperature. The coefficient is 0.28 at 119.8 K, and is 0.18 at 349.5 K. It indicates that the temperature has significant effects on the TMAC and even the surface conditions and intermolecular interactions remain unchanged. A higher temperature will lead to a smaller TMAC. It also means that an experimentally determined value of TMAC may not be applicable to other different temperatures. On the basis of current simulations, the TMAC-temperature relationship can be well described by an exponential function of  $f=f_0+f_1 \exp(-\beta T)$ , which fits the simulation data with  $f_0=0.173$ ,  $f_1=0.323$ , and  $\beta=0.00871/K$  as shown in Fig. 4. It is shown that the

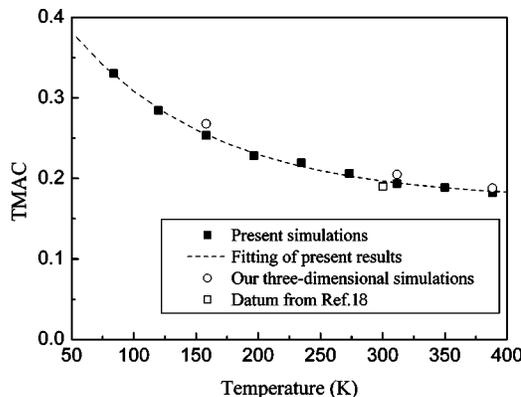


FIG. 4. Variation of the TMAC with the temperature. The dashed line represents the fitting function of  $f=f_0+f_1 \exp(-\beta T)$ .

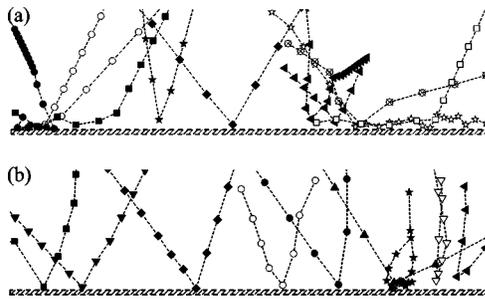


FIG. 5. Molecular trapping-desorption behaviors near a surface at temperatures of (a) 119.8 K and (b) 311.5 K.

TMAC may vary with the temperature through a decaying exponential law. It also implies that the TMAC is more sensitive to lower temperatures than to higher ones. It runs to a constant  $f_0$  as temperature becomes very high.

The TMAC is a parameter that characterizes the fundamental process of momentum exchange and equilibrium between the fluid and the solid surface. It is understandable that the momentum transport through the collisions is affected by the temperature as well, besides the species of the fluids, the surface condition of the solids, etc. In kinetic theory, the gas molecule's behaviors are often described based on a hard-sphere bounce-back assumption. However, from a molecular simulation view, molecules reaching a surface are often trapped by the potential well, undergo many collisions and may escape only after some residence time, through which momentum exchange between the fluid and the wall is accomplished. In the present simulation, tracing of the molecular trajectory shows that the collisions between the fluid molecules and the surface behave very similarly to those observed in molecular beam scattering experiments.<sup>19,20</sup> At low temperatures, the trapping-desorption behavior combining with multiple collisions make a substantial contribution to the momentum transfer between the surface and the gas molecules. At higher temperatures, the trapping-desorption of the incident molecules will gradually transit to a direct scattering with the rising of the temperature, as shown in Fig. 5. Consequently, the TMAC shows an increase with the decreasing temperature because molecules with higher energy are easier to desorb from the surface and it results in a less sufficient exchange of momentum between the fluid and the solid surface. In other words, as the trapping-desorption happens at low temperatures, a direct inelastic scattering is more possible to take place as the temperature increases. The trapping-desorption behavior also leads to layering and oscillating density profiles near the channel surface, which are also strongly related to temperatures as shown in Fig. 6.

In summary, the temperature dependence of the tangential momentum accommodation coefficient is studied through the molecular dynamics simulations of gas flows in a submicron channel. The results show that the TMAC decreases with the increasing temperature through a decaying exponential law, and is more sensitive to lower temperatures

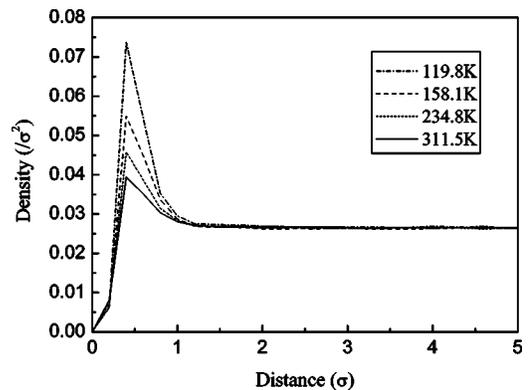


FIG. 6. The average density profiles normal to the surface. The length unit is reduced by the diameter parameter  $\sigma$  of the argon molecules.

than to higher ones. The reason for this temperature dependence of TMAC is the near-wall trapping-desorption behavior of the gas molecules. The increase of the fluid temperature will enhance the ability of the gas molecule's desorbing from the solid surface, and will decrease the residence time of the absorbed molecule and its collisions with the channel wall. The temperature sensitivity of the TMAC reminds us to be cautious when extending an experimentally determined coefficient to any other thermal situations.

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