Rarefied Gas Flow in Rough Microchannels by Molecular Dynamics Simulation *

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The molecular dynamics simulation method is applied to investigate the rarefied gas flow in a submicron channel with surface roughness which is modelled by an array of triangle modules. The boundary conditions are found to be determined not only by the Knudsen number but also the roughness, which implies that the breakdown of the Maxwell slip model under the conditions that the surface roughness is comparable to the molecular mean free path. The effects of the rarefaction and the surface roughness on the boundary conditions and the flow characteristics are strongly coupled. The flow friction increases with increasing roughness and with decreasing Knudsen number.

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Due to the rapid advancement of the micromachining technology over the past decade, it has been feasible to fabricate micron, submicron, and even some nanon devices.[1] A number of papers have shown that flows on the microscale are different from those on the macroscale. In some cases, the Navier–Stokes (NS) equations alone are incapable of modelling the occurring phenomena.[2,3] The lack of clarity of the physical mechanism of fluid flows on the microscale bottlenecks the improvement of micro-/nano-devices.

Though great efforts have been made to perform microscale flow experiments, uniform conclusions on the flow characteristics regarding microscale effects are absent as yet. Some experimental results of gas flows in microchannels are even contradictory. Discrepancies in the reported friction factors have been reviewed by Guo and Li[4] and Rostami *et al.*[5] The reported product of the Darcy friction factor times the Reynolds number, i.e. fR_e, in microflows may be greater[6,7] or less[8−10] than that of macroscale flows. For the fully developed laminar flows on the macroscale, fR_e is independent of the Reynolds number. However, many microscale flow experiments indicated that fR_e might vary with the Reynolds number.[7,8] The experimental discrepancies may be attributed to two reasons: (1) uncertainty in experimental control and measurements of surface roughness, channel dimensions, pressure and flow rate; (2) invalidity of traditional theories and boundary conditions because of the change of physical situations on the microscale. The promising solution points to particle-based models. Though various schemes have been developed for solution of the Boltzmann equation,[11,12] it is very difficult for them to consider potential interactions between particles and complicated boundary conditions. Thus, the molecular dynamics simulation is left as a unique weapon based on first principles.

In this Letter, the molecular dynamics simulation is used to investigate rarefied gas flows fully developed in a submicron channel with surface roughness modelled by an array of triangle modules. The effects of rarefaction and surface roughness on the boundary conditions and the flow characteristics are presented.

Using the method of molecular dynamics, we study the dynamics of N gaseous argon molecules enclosed between the two parallel platinum walls as shown in Fig. 1. The space between two plates is $H = 0.1\,\mu$m. A periodic boundary condition is applied along the x-direction. The surface roughness is modelled by placing an array of triangle units with size A on each channel plate. To maintain a realistic gas–solid interaction, we build atomic structure walls based on the Einstein theory that the wall atoms vibrate around the face-centred-cubic (fcc) $[1,1,1]$ lattice sites with the Einstein frequency tethered by a harmonic spring with stiffness

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

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

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

where r is the intermolecular distance, and ε and σ are the energy and molecular diameter parameters. The parameters used in this paper are $\varepsilon_{\text{Ar-Ar}} = 1.67 \times 10^{-21}\,\mathrm{J}$, $\sigma_{\text{Ar-Ar}} = 3.405 \times 10^{-10}\,\mathrm{m}$, $\varepsilon_{\text{Ar-Pt}} = 0.894 \times 10^{-21}\,\mathrm{J}$, and $\sigma_{\text{Ar-Pt}} = 3.085 \times 10^{-10}\,\mathrm{m}$. The two-dimensional (2D) Poiseuille flow in the x direction is induced by subjecting the particles to an external gravitational field g, which ranges from $10^{10}\,\mathrm{m/s^2}$ to $10^{11}\,\mathrm{m/s^2}$ producing flows with different Reynolds

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numbers. The molecules move according to Newton's second law. The equations of motion are integrated using a leapfrog-Verlet algorithm[13] with a time step of $\Delta t = 0.01\tau$, where $\tau = (m_{\mathrm{Ar}}\sigma^2_{\mathrm{Ar\text{-}Ar}}/\varepsilon_{\mathrm{Ar\text{-}Ar}})^{1/2}$. To reduce the time-consuming part of the calculation of interparticle interactions, we mainly take two measures that (a) a typical potential cutoff of $r_{\mathrm{cut}} = 2.5\sigma_{\mathrm{Ar\text{-}Ar}}$ is employed, and (b) the link-cell method is adopted.[13] The system is kept at constant temperature by a velocity rescaling method according to

$$T = \frac{m}{2Nk_B}\sum_{i=1}^{N}[(v_{ix} - v_x)^2 + v_{iz}^2], \tag{3}$$

where v_{ix} and v_{iz} are the x and z velocity components of particle i respectively, and v_x is the macroscopic velocity.

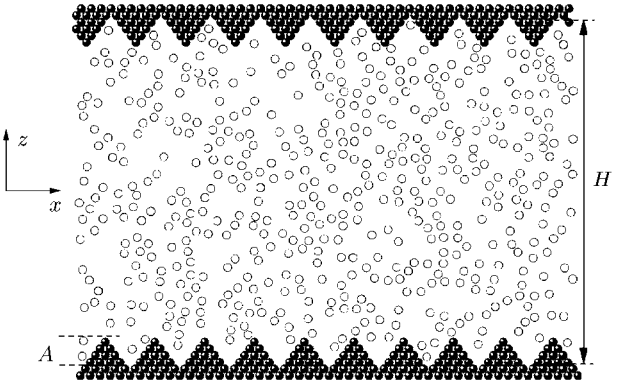

Fig. 1. Schematic snapshot of the flow system.

For the 2D Poiseuille flow, the NS equations can be solved exactly giving a quadratic velocity profile across the channel as

$$u_x = \frac{\rho g}{2\mu}(h^2 - z^2) + u_s, \tag{4}$$

in which ρ is the gas density, μ is the viscosity, $h = 0.5\,\mathrm{H}$, and u_s is the slip velocity. Our simulations, as shown in Fig. 2 of the velocity profiles in the x-direction, indicate that it indeed falls into the slip flow regime. The simulations also obey the continuum mechanics. Only if corresponding boundary conditions are adopted, are the NS equations valid for slip flows at the submicron scale.

In Fig. 2, the velocity is reduced by $U = 78.5\,\mathrm{m/s}$. The Knudsen number $K_n = \lambda/H$ characterizes the rarefaction degree of the flows by the ratio of the molecular mean free path (MFP) and the characteristic length of the flow system. A value of 0.05 signifies flows in the slip regime by the normal kinetic theory. Though large slip appears at the smooth gas–solid interface, the slip reduces significantly with increasing roughness. Even for flows with larger roughness (e.g. $A = 12.9\,\mathrm{nm}$), the slip velocity is negative according to an imaginary extrapolating of the NS profile in the middle of the channel. As a result, the slip is defined as a negative one, which has also been introduced in some previous papers[14,15]. So, the boundary conditions of velocity slip, including slip, no-slip and even negative-slip, are determined not only by the Knudsen number but also by the roughness. The roughness effect can be characterized by the ratio of the roughness scale and the MFP (A/λ). For $A/\lambda \approx 1$, the dimensionless slip length of the gas flow is nearly zero, which indicates that the no-slip boundary condition arises when the molecular MFP is comparable with the roughness. This agrees well with Mo's results[16]. For $A/\lambda < 1$, the slip boundary condition due to rarefaction effect takes places. For $A/\lambda > 1$, the slip becomes negative.

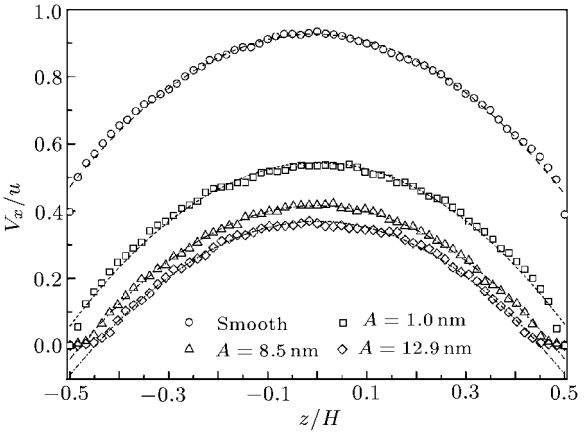

Fig. 2. Velocity profiles for various roughness with $K_n = 0.05$.

The friction factor is simultaneously affected by the Reynolds number, the roughness and the Knudsen number. We define a normalized friction constant

$$C^* = \frac{(fR_e)_{\mathrm{simulation}}}{(fR_e)_{\mathrm{theoretical}}}, \tag{5}$$

which is the ratio of the product of the Darcy friction factor times Reynolds number between our simulations and the theoretical prediction by NS equations. The theoretical value of fR_e for the fully developed laminar flow is 96 for a conventional 2D channel flow. Figure 3 shows the normalized friction constant as a function of the Reynolds number. However, we find that the constant is independent of the Reynolds number, which is different from some experiments.[7,8] This might result from the inevitable effects of compressibility and entrance/outlet effects on the experimental conditions.

Effects of roughness and rarefaction are illustrated in Fig. 4. From the diagram, it is clear that the Knudsen number and the roughness have integrative effects on the flow friction. An increasing Knudsen number reduces the friction of flow with given roughness. Meanwhile, the trend of increasing friction constant with increasing roughness is also observed for the given Knudsen number. Thus, for larger roughness

and smaller Knudsen numbers, the flow frictions both increase. It should be noted that the Knudsen number is 0.01–0.12 in our computer experiments, which indicates a significant rarefaction effect by normal theory of rarefied gas flow examined in Refs. [9,10]. Considering the rarefaction effect, the friction constant for a fully developed laminar flow can theoretically be drawn as[9]

$$C^* = \frac{1}{1 + 6\alpha K_n}, \tag{6}$$

where α is the slip coefficient. The slip coefficient is determined to be 5.0 by our simulations for the smooth surface, and it is related to the roughness for other cases. We find that Eq. (6) can predict the friction characteristics of microflows in the smooth channel very well. However, the roughness may result in a large deviation of friction from the traditional theory even for gas flow in slip regime. The effects of roughness and rarefaction are strongly coupled. Unfortunately, there is no theoretical model to depict the coupling phenomena thus far.

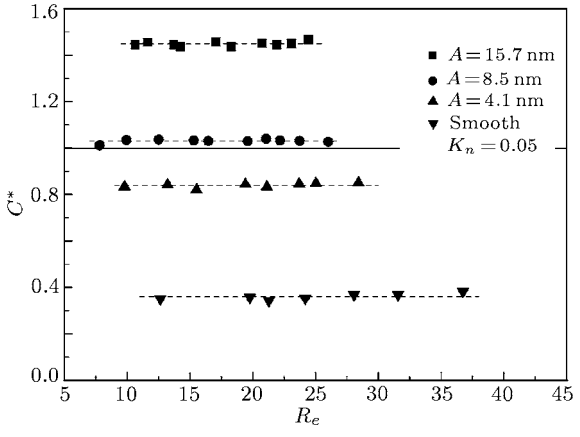

Fig. 3. Normalized friction constant vs Reynolds number.

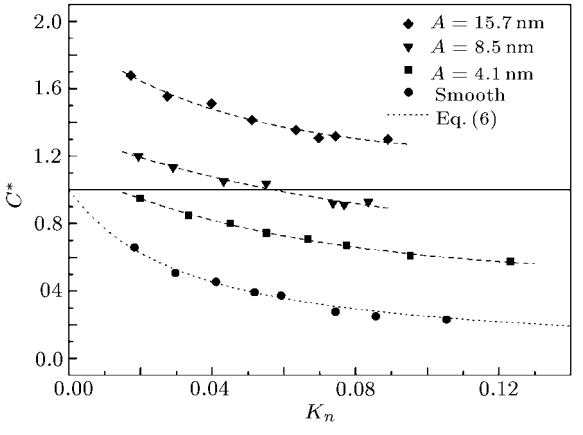

Fig. 4. Effects of roughness and Knudsen number on normalized friction constant.

From a molecular simulation view, we can tentatively probe how the coupling takes place. For macroscopic roughness in continuum mechanics, the roughness effects behave as obstructing the flow directly and affecting the streamlines.[17] However, for gas flows in micromachined channels, the molecular MFP may be comparable to roughness size. For example, the MFP of normal air, which is about 0.065 μm, is comparable to the roughness in microdevices by recent micromachining technologies.[18] The molecules near walls may undergo many collisions in the roughness diastema through which the momentum exchange is accomplished. This means that the molecules can penetrate through the wall boundary region, which is different from an imaginary mathematical surface. With different roughness, the permeability varies. Therefore, the molecular behaviours of combining collisions and permeability show a possible relation to the coupling phenomena.

In conclusion, the rarefied gas flows in a submicron channel with surface roughness is studied through molecular dynamics simulations. The simulation results show that the boundary conditions of velocity slip are determined not only by the Knudsen number but also the roughness, which implies the breakdown of the Maxwell slip model on the conditions that the surface roughness is comparable to the molecular MFP. The effects of roughness and rarefaction on the boundary conditions and the flow characteristics are strongly coupled. For larger roughness or smaller Knudsen numbers, the flow friction increases.

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