Effect of the wall structure on nanochannel gas flow: A molecular dynamics study

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Abstract
Nonequilibrium molecular dynamics simulations are performed for force-driven argon gas nanochannel flow to investigate the effect of the nanoscopic wall structure on the gas flow characteristics. The monoatomic molecule argon is first used for both the fluid and wall molecules. A face-centered cubic wall structure is first investigated. It is confirmed that the fcc (111) surface structure induces the fastest flow, followed by the fcc (100) and (110) surface structures. Unlike liquid flow in a nanochannel, the density of the monolayer adsorbed on the wall surface greatly depends on the wall configuration. A lattice wall configuration that allows stronger adsorption of molecules induces higher velocity flow. From simulations with different wall molecule bond lengths, the gas flow is affected more by the surface roughness than adsorption of gas molecules to the wall. Because the density close to the wall surface is affected by the surface configuration, the relationship between gas molecule density and the velocity profile is analytically investigated in the early transition regime. The results suggest that the magnitude of the adsorbed monolayer density partially causes a kink in the velocity profile. Other wall molecule configurations are also investigated, such as silicon, diamond, and graphite. It is found that the diamond structure can induce a much larger density peak than silicon owing to the high wall density. This strong adsorption to the wall disrupts the motion of fluid molecules near the wall, which results in less slippage and lower bulk velocity. The graphite structure is comparable to the diamond structure. Finally, the wall–fluid interaction of the graphite wall and argon gas is considered using different interatomic potentials for the wall and the gas. Adsorption becomes weaker and the slippage velocity is significant because the wall surface roughness becomes the dominant factor affecting the flow.

Key words: Nanochannel gas flow, Wall structure, Molecular transport, Microelectromechanical systems, Nanoelectromechanical systems

1. Introduction

Because of the development of microelectromechanical systems, investigation of gas flow at the micro/nanoscale is important. Micro/nanoscale gas fluidics are classified into continuum, slip flow, transition, and free molecular regimes, which are characterized by the Knudsen number Kn.

Gas flow in microfluidic devices such as hard disk drives, microneedles, and micro-gyrosopes operates in the slip flow or early transition regime (Beskok, 2001; Karniadakis and Beskok, 2002; Karniadakis et al., 2005). In such flow regimes, the mean free path (MFP) becomes significant relative to the characteristic length and continuity of the Navier–Stokes is not fully satisfied, especially in the nonequilibrium Knudsen layer (Dongari et al., 2009; Watari, 2010). Thus, velocity slip is induced at the wall–fluid boundary. Since the Maxwell slip model was proposed for flat and smooth wall surfaces, many slip models have been reported, such as wall-function models, higher-order continuum models, and power-law models.

In micro/nanofluidics, the wall surface roughness effect becomes significant. For gas microchannel flow, Mo and Rosenberger (1990) investigated velocity profiles for force-driven channel flow with sinusoidal and randomly rough
walls by two-dimensional molecular dynamics (MD) simulations at Kn < 0.1. Cao et al. (2006) performed MD simulations of force-driven channel flow with rectangular, triangular, sinusoidal, and randomly triangular wavy walls with Kn = 0.1. They discussed the slip length and found that the wall friction coefficient increases with decreasing Kn and increasing wall roughness height. Liu and Ni (2009) discussed the effect of fractal wall roughness for channel flow at Kn < 0.16 by the lattice Boltzmann method. Kamali and Kharazmi (2011) reported MD simulations of liquid channel flow in channels with cavitation. Although the wall surface roughness used in the above investigations was at the nanoscale, the roughness was still large relative to the size of the fluid molecule. For example, Cao et al. (2006) used a shortest pitch of the rectangular cavity of 5.544 nm, which was much larger than the fluid molecule diameter of 0.3405 nm. The wall surface is regarded as hydraulically smooth if the height of the roughness is less than the thickness of the stagnant layer (Liu and Ni, 2009).

Does the nanoscale roughness really affect the bulk flow in the channel? From the results of MD simulations of channel flow of liquid argon, Soong et al. (2007) suggested that the surface lattice configuration affects the slip length and flow rate. This indicates that even for the same wall structure, such as a face-centered cubic (fcc) structure, the flow in the vicinity of the wall is different for different surface configurations. This extends to nanoscopic electrokinetic flow (Yen et al., 2011). Liu and Li (2009) regarded the wall roughness as the wall–fluid interaction for liquid argon nanochannel flow, and reported the change of the flow profile. This concept was used by Beskok’s group for confined fluids (Barisik and Beskok, 2011a) and gas flow (Barisik and Beskok, 2011b). Although the working fluid of Soong et al. (2007) and Liu and Li (2009) was liquid argon, the above results indicate that the gas flow is affected not only by the magnitude of the wall–fluid interaction but also by the nanoscopic wall roughness.

In this paper, argon gas nanochannel flow is investigated by MD simulations. The effect of the lattice configuration of the wall of the nanochannel is first investigated. Then, other wall configurations are investigated.

2. Molecular Dynamics Simulations

2.1 Lennard-Jones fluid

In the present study, nanochannel flow driven by applying a force to each fluid molecule was simulated. Truncated Lennard-Jones 6–12 pair potentials were used for the van der Waals fluid–fluid and fluid–wall interactions:

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

(1)

where \(r_{ij}\) is the interatomic distance between atoms \(i\) and \(j\). \(\varepsilon\) and \(\sigma\) are the well depth and the distance at which the interatomic potential between atoms \(i\) and \(j\) is zero, respectively. The interatomic force \(F\) is given by

$$F = -\frac{\partial \phi}{\partial r} = \frac{24\varepsilon}{r_{ij}} \left[2\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right].$$

(2)

In a system containing only L–J molecules, the classical equation of motion can be written as

$$\frac{d^2 r^*}{dt^2} = -\frac{m r^*}{\varepsilon}\frac{\partial \phi^*}{\partial r^*},$$

(3)

where \(m, r^* = m/\sigma, t^* = t/\sqrt{m \sigma^2/\varepsilon}\), and \(\phi^* = \phi/\varepsilon\) are the mass, dimensionless length, time, and energy, respectively. For an argon molecule, \(m = 6.63 \times 10^{-26}\) kg, \(\sigma = 0.3405\) nm, and \(\varepsilon = 119.8 k_b\), where \(k_b\) is the
Boltzmann constant. The nondimensional number density $n^* = n\sigma^3$ and temperature $T^* = k_B T / \varepsilon$ are used in the L–J fluid. In calculations, to reduce the computational expense of the interactions, the potentials were truncated at a cutoff distance ($r_c$). In the present study, $r_c = 3.0\sigma$ was used.

2.2 Temperature control method

Velocity scaling was used to maintain the temperature in the computational domain. The current temperature $T_i$ is defined as

$$T_i = \frac{1}{3Nk_B} \left\{ \sum mv^2 \right\},$$

where $N$ is the number of molecules. To obtain a desired temperature $T_0$, the velocity of a molecule $v'$ is corrected at each time step as

$$v' = v \sqrt{\frac{T_0}{T_i}},$$

where $v$ is the current velocity. Using this method, a constant temperature condition can be obtained. In this study, the above velocity scaling was applied to only the wall atoms to avoid over/underestimation of the fluid molecule behavior in the domain (Khare et al., 1997). Thus, the fluid molecule temperature is controlled by the wall temperature. In our simulations using the statistical regime, the standard deviation of the fluid molecule temperature was less than 0.135 in all cases.

2.3 System using different interatomic potentials for the fluid and wall

One simulation was performed for a system with argon as the fluid molecule and graphite for the wall. In this case, temperature control was achieved by the Langevin method, as explained by Blomer and Beylich (1999). The Brenner potential (Brenner, 1990) was used for the potential of the covalent bonds of carbon.

2.4 Knudsen number

To compare the computational condition with that from the gas kinetic theory, Kn was estimated in each simulation using $Kn = \lambda / H$, where $\lambda$ is the MFP of the molecules and $H$ is the characteristic length of the flow domain (height of the channel). $\lambda$ is defined by the following equation with number density $n$ (Bird, 1994):

$$\lambda = \frac{1}{\sqrt{2\pi n\sigma^2}}.$$

2.5 Computational domain

The computational flow domain was a confined channel between the top and bottom walls, as shown schematically in Fig. 1. $H$ was fixed at $20\sigma$, and the length $L (X)$ and width $W (Z)$ were varied depending on the number density of fluid molecules in terms of the independence of the periodicity effects reported by Barisik et al. (2010). The details of the wall, such as the configuration and number of molecules, are given in Section 3.1. Periodic conditions were used in both $X$ and $Z$ directions. An external force was applied to every fluid molecule to drive the channel flow in the $X$ direction.

To eliminate the effect of the difference of the intermolecular force depending on the molecular species, the same monatomic molecule (argon) was used for both the fluid and the wall molecules, except for the simulation with argon fluid molecules and a graphite wall molecules. The molecule diameter is thus the same for the fluid and the wall molecules (i.e., $\sigma^f = \sigma^w$). The interaction owing to the L–J potential between the fluid and the wall molecules is also unity: $\varepsilon^f / \varepsilon^w = 1.0$. The superscripts $f, w, fw$, and $ff$ denote fluid, wall, fluid–wall, and fluid–fluid, respectively.

Statistical data of approximately $10^8$ steps were obtained after attaining steady-state flow and temperature fields (approximately $10^6$ steps). The velocity profile was obtained by averaging the fluid molecule velocity inside each bin of $0.1\sigma$, except for the nearest point from the wall surface.
3. Results and Discussion

3.1 Surface configuration of the face-centered cubic wall structure

The face-centered cubic (fcc) structure was used for the wall structure with different surface configurations: fcc (100), (110), and (111). The computational domain of the channel was as follows: 

\[ H = 20.0\sigma, \quad L \times W = 20.0\sigma \times 20.0\sigma \text{ for fcc (100),} \]
\[ 19.8\sigma \times 20.0\sigma \text{ for fcc (110),} \]
\[ 20.0\sigma \times 20.8\sigma \text{ for fcc (111)} \] 

To obtain the periodicity of the wall configuration. The numbers of fluid and wall molecules were 450 and 3200 for fcc (100), 446 and 3360 for fcc (110), and 468 and 2880 for fcc (111). Thus, the number density of fluid molecules in the computational domain was 0.0562, which corresponds to the Kn = 0.2. The dimensionless temperature of the wall was controlled at \( T = 2.0 \).

The resulting flow profile is shown in Fig. 2(a). The velocity \( U \) and distance from the wall surface \( y \) are normalized by \( \nu \sigma \) and \( \sigma \), respectively. \( \tau \) is the time step of computations. As shown in the figure, the velocity profile is affected by the wall surface configuration. An fcc (111) surface configuration results in the fastest velocity followed by the fcc (100) and (110) surface configurations. This order is the same as the liquid case reported by Soong et al. (2007).

Unlike liquid flow, gas flow has a monolayer adsorbed on the wall surface, as shown in Fig. 2(b). The magnitudes of the density peaks are in the same order as the velocities in the velocity profile. Therefore, the present simulations of gas flow suggest that a surface configuration inducing a high-density peak has a high velocity in the channel flow.

The high density near the wall is related to the wall–fluid interaction, that is, adsorption of fluid molecules to the wall surface. To confirm the surface lattice dependency on adsorption, Fig. 3 shows the time-averaged fluid density distribution in a plane at \( y/\sigma = 0.5 \) (averaged within \( y/\sigma = 0.4–0.6 \)). The circles in the figure correspond to the innermost wall molecule. In this simulation, the top surface wall molecules were initially located at \( y/\sigma = 0 \). Apparently, the distribution and range of the fluid molecule density depend on the surface configuration. Because the location where the repulsive and attractive forces work depends on the wall surface configuration, the fluid molecule density is locally low on the innermost wall molecules and high among them. The fcc (100) (Fig. 3(a)) and (111) (Fig. 3(c)) wall surfaces have high-density values, and the fcc (110) wall surface induces low density with a narrow range. This adsorption may affect the local viscosity because of collision of fluid molecules as the peak becomes large. However, in the present cases, the highest density peak case (fcc (111)) has the highest velocity. According to Soong et al. (2009), wall surface smoothness mainly affects the magnitude of the liquid velocity. In their results, the peak densities of liquid molecules for three surface configurations were almost the same. In contrast, the density peak dependency on surface orientation is remarkable for the gas cases shown in Figs. 2(b) and 3. To determine the property of the wall that mostly affects the gas flow, simulations were performed with different wall molecule densities. The imposed surface configuration was fcc (111), and the length of the unit cube (bond length (BL)) ranged from 0.8 to 1.1, which corresponds to a wall densities \( \rho_w = 1.063–2.762 \). The other conditions, such as the number of fluid molecules, size of the computational domain, and controlled temperature, were the same as those of the previous simulation.

The flow and molecule density profiles are shown in Fig. 4. The density peak increases with decreasing BL (higher density of wall molecules). This is simply because of increased adsorption of fluid molecules to the wall surface. The velocity first increases and then decreases with decreasing BL. The largest velocity is obtained for \( BL = 0.9–0.95 \). This suggests that the velocity near the wall is affected by both the wall roughness and adsorption of fluid molecules to the surface. When the BL is sufficiently large, the surface roughness significantly affects fluid flow and the motion of fluid molecules is disrupted by the rough surface. This is supported by the case of the fcc (110) wall surface in Fig. 2. For the
fcc (110) wall surface, the corrugations on the wall surface are aligned perpendicular to the flow direction, which inhibits fluid flow. As the BL decreases, the wall surface becomes denser and thus smoother. Although this also increases adsorption of fluid molecules to the wall surface, the low wall friction is more favorable for flow, and thus the bulk velocity increases. When the BL is small, adsorbed fluid molecules disrupt one another, resulting in a decrease of the flow velocity near the wall.

![Fig. 2](image)

Fig. 2 Argon gas flow in a force-driven nanochannel with fcc (100), (110), and (111) wall configurations. The common computational parameters were $\rho_f = 0.0562$, $Kn = 0.2$, $T = 2.0$, and wall-molecule bond length (BL) = 1.0.

![Fig. 3](image)

Fig. 3 Time-averaged fluid molecule density distribution at $y/\sigma = 0.5$ with innermost wall molecule locations for the fcc surface configurations. The computational conditions were the same as in Fig. 2.

![Fig. 4](image)

Fig. 4 Effect of bond length (BL) between wall molecules for the fcc (111) wall structure at $Kn = 0.2$. 

Consequently, for gas flow in a nanochannel, the dominant factor that affects the velocity profile is the wall surface roughness rather than adsorption of fluid molecules to the wall surface. Indeed, the wall number densities at the innermost layer, that is, the two-dimensional area number densities at the top wall layers, were 1.15 (fcc (111)), 1.00
(fcc (100)), and 0.707 (fcc (110)) from smooth to rough surfaces, which corresponds to the order of the velocity magnitude. For reference, the number density of the fcc structure is 1.41.

3.2 Analytical velocity profiles for the adsorbed monolayer model

The velocity depends on the surface smoothness and wall adsorption, as shown in Fig. 4. The velocity profiles in Fig. 2(a) were then normalized by each bulk velocity $U_b$, as shown in Fig. 2(c). The decrease in velocity close to the wall surface becomes remarkable as the density peak increases. It is known that this decrease can be observed in high Kn flow. However, in the present cases, the fluid molecule density is the same in the computational domain. Therefore, the effect of the adsorbed monolayer on the velocity profile was further investigated in the early transition regime. This is because the continuity of the fluid in the bulk is partially satisfied, and thus the velocity profile can be analytically derived from the Navier–Stokes equation. For simplicity, the normalized number density profile is assumed, as shown in Fig. 5. The profile is

$$
n_0/n = n_0 + \left(\frac{n_m - n_0}{a}\right)y^* , \quad 0 \leq y^* \leq a ,$$

$$
n_m/n = n_m - \left(\frac{n_m - n_0}{b-a}\right)(y^* - a) , \quad a \leq y^* \leq b ,$$

$$
n_m/n = n_m , \quad b \leq y^* ,$$

where $n_0$, $n_m$, and $n_\infty$ are the normalized number densities in the vicinity of the wall, at the peak of the layer, and far away from the wall, respectively. They have a relation such as

$$
n_m = \frac{(2h - an_0 - bn_m)/[2h - (a + b)]}{n_\infty} ,$$

where $h$ is the center height of the channel.

![Modeled profile of the fluid molecule density.](image)

For fully developed steady state laminar flow, the momentum equation is

$$
0 = \frac{\mu}{\rho^* n/n^*} \frac{\partial^2 u}{\partial y^*^2} + \frac{F_i(y^*)}{\rho^* n/n^*} ,
$$

where $\mu$ is the viscosity constant, $\rho^*$ is the average density, and $F_i(y^*)$ is the force acting on each fluid molecule. Because the external force term in Eq. (8) is normalized by the local fluid molecule number density, the second term can be regarded constant ($F_0$).

The boundary conditions are as follows. At the channel center ($y^* = h$), the velocity gradient is zero. The velocity and shear stress profiles are continuous. The slip velocity is given by $u_s$. By integrating the momentum equation, the velocity profile is obtained as follows:
\[ u = -F_0 \left\{ \frac{n_m - n_0}{6a} \right\} y^* + \frac{n_0}{2} y^* + u_s, \quad 0 \leq y^* \leq a, \]

\[ u = F_0 \left\{ \frac{n_m - n_0}{6(b-a)} y^* + \frac{b n_m - a n_0}{2(b-a)} y^* \right\} + C_1 y^* + u_s', \quad a \leq y^* \leq b, \]

\[ u = -F_0 \frac{a^2}{2} y^* + C_1 y^* + C_2'' + u_s', \quad b \leq y^*, \]

where

\[ C_1 = -F_0 \left\{ \frac{a + b - 2h}{2} n_m - b n_m - a n_0 \right\}, \]

\[ C_1' = -F_0 \left\{ \frac{a^2 - 2(b-a) n_m - b^2 n_m}{2(b-a)} \right\}, \]

\[ C_2 = -F_0 \left\{ \frac{1}{6(b-a)} \left[ a^2 (a+b) n_m + b(a+b) n_m - a^2 n_0 \right] + u_s \right\}, \]

\[ C_2'' = -F_0 \left\{ \frac{a^2 + ab + b^2}{6} n_m - b(a+b) n_m - a^2 n_0 \right\} + u_s . \]

For the slip velocity, the second-order slip model for rarefied gases is

\[ u_s = A \lambda \frac{\partial u}{\partial y} \bigg|_{y=0} - A \lambda^2 \frac{\partial^2 u}{\partial y^2} \bigg|_{y=0} . \]

Because \( \lambda = 2h^* \sigma Kn \),

\[ u_s = A \frac{2h Kn}{h^*} \frac{\partial u}{\partial y} \bigg|_{y=0} - 4A \frac{h^2 Kn^2}{h^*} \frac{\partial^2 u}{\partial y^2} \bigg|_{y=0} = F_0 \left( A h Kn \frac{2n_m + n_0 + 4n_h h - 3n_m}{2} + 4A h^* n_h Kn^2 \right), \]

\[ = F_0 \left( 2A h^* Kn + 4A h^* n_h Kn^2 \right) \]

Finally, the analytical velocity profile was obtained, as shown in Fig. 6. The parameters were \( a = 0.5, b = 1.7, F_0 = 1.0, h = 10 \sigma, Kn = 0.2, n_0 = 0, \) and \( n_m = 7 \) or 10. \( A_1 = 1.11 \) and \( A_2 = 0.61 \) were obtained from Hadjiconstantinou (2003). As shown in Fig. 6, velocity bend depends on the density of the adsorbed monolayer. A high-density peak induces a remarkable velocity bend at \( y^* \approx 1.0 \), as shown in Fig. 6(b). The profiles in Figs. 6(a) and 6(b) are qualitatively similar to those of fcc (100) and (111) wall surfaces. The location of the bend is closer to the wall in the MD simulation results because only the density profile influences the analytical solution. In Eq. (12), the slip velocity depends on the channel height \( h \) and the number density in the vicinity of the wall \( n_0 \). This suggests that the slip velocity is not affected by the density peak. Note that \( U_0 \) differs in each case, so \( U/U_0 \) near the wall becomes different in Fig. 6. This is different from the MD results where the density peak influences the velocity profile depending on the surface smoothness. This is because the analytical model uses a flat wall, whereas the MD tracks the motion of each fluid molecule considering the wall surface roughness.
3.3 Effect of number density of fluid molecules in the computational domain on the velocity

We have confirmed that the velocity profile in nanochannel gas flow is affected by the configuration of the wall surface and the wall molecule density. Another factor that affects the flow profile is the fluid molecule density $\rho_n$, which is investigated in this section. In these simulations, the channel height was $20\sigma$, the number density of fluid molecule was $n = 5.63 \times 10^{-3}$, and the estimated $Kn = 2.0$. The channel length ($X$) and width ($Z$) were $46.0\sigma \times 46.0\sigma$ for fcc (100), $42.4\sigma \times 44.0\sigma$ for fcc (110), and $44.0\sigma \times 43.3\sigma$ for fcc (111).

The results are summarized in Fig. 7. The trends of the magnitude of the density peak and the velocity are same as those for $Kn = 0.2$ (Fig. 2). The densities of the adsorbed monolayers are slightly higher than the corresponding cases with $Kn = 0.2$. The fluid molecule density profile is nondimensionalized by the bulk number density. Therefore, the velocity near the wall indicates that the wall surface smoothness dominates over wall adsorption. Indeed, the velocities near the wall are almost the same as the respective cases with $Kn = 0.2$ with the same acting force on the fluid molecules. In contrast, the velocity bend is remarkable and the velocity profile is flat in the bulk region, which is more pronounced in the velocity profile normalized by bulk velocity $U_b$ (Fig. 7(c)).

3.4 Diamond, silicon, and graphite wall structures

The wall structure and its density are crucial for surface smoothness and fluid molecule density layering, which affect the velocity profile of nanochannel gas flow. Other wall structures were investigated: diamond, silicon, and graphite. Diamond and silicon have the same structure but different interatomic distances. The number density of wall atoms of diamond is 7.00, and that of silicon is 1.97. The minimum interatomic distances are $0.4527\sigma$ for the diamond structure and $0.6905\sigma$ for silicon. Schematics of the structures of diamond and graphite are shown in Fig. 8.
To investigate the effect of the atomic configuration of the wall and its density, argon molecules were also used for both the fluid and wall molecules in this section. For the silicon wall configuration, the channel size was $15.79\sigma \times 20.00\sigma \times 15.62\sigma$ with 2688 wall atoms and 278 fluid atoms. The diamond wall configuration had almost the same channel size ($14.79\sigma \times 20\sigma \times 15.37\sigma$) with 9600 wall molecules and 256 fluid molecules. Therefore, $Kn = 0.2$ for all systems and the temperature was controlled at 2.0.

The resulting velocity and density profiles for the diamond and silicon wall structures are shown in Fig. 9(a) and (b), respectively, and a comparison of the velocity profiles is shown in Fig. 9(c). The diamond wall structure induces a much higher density peak. This is because of the denser diamond wall structure ($\rho_w = 7.00$) compared with that of the silicon wall structure ($\rho_w = 1.97$). The two-dimensional area wall number density at the innermost layer was 2.11 for the diamond structure and 0.91 for the silicon structure. This suggests that the surface of the silicon structure is comparable to the fcc (100) wall structure, and the diamond structure has very high adsorption ability. Therefore, the slippage velocity of the diamond structure becomes negligible. The velocity in the bulk region of the diamond structure also becomes smaller than that of the silicon structure.

![Fig. 8 Wall structures of diamond and graphite.](image)

![Fig. 9 Results for diamond and silicon wall structures at Kn = 0.2 and T = 2.0.](image)
suggested by the density peak value. Because of similar surface adsorption, the velocity profile is also similar to that of diamond.

Finally, a simulation was performed using different interatomic potentials for the carbon atoms in the graphite wall structure and argon in the channel to explicitly investigate the effect of using different potentials for the fluid and the wall structure. The L–J potential of argon–carbon can be easily constructed using the coefficient values, that is, $\sigma = 0.3403$ nm and $\epsilon = 0.87 \times 10^{-22}$ J. The L–J potential is shown in Fig. 11(a). The well depth of argon–carbon is lower than that of argon–argon. Because the force is derived from the gradient of the potential, the wall–fluid interaction should be weak.

The resulting velocity and number density profiles are shown in Fig. 11(b). The size of the computational domain was $15.02\sigma \times 20.00\sigma \times 15.90\sigma$ and number of fluid molecules was 269, and thus Kn = 0.2. The controlled temperature was 2.0. In this case, the external force on the fluid molecules was less than the other cases (~0.1 times) because the fluid molecule is easily accelerated owing to the aforementioned weak wall–fluid interaction, and to avoid the temperature increase because of acceleration. As shown in Fig. 11(b), the peak of density layer is less than half of the argon–argon case (Fig. 10) using the L–J potential of argon–carbon. The peak magnitude is comparable to the fcc (111) wall structure at $BL=0.8$, but the velocity profile is flatter. Although the velocity cannot be directly compared with the other cases because of the small force acting on the fluid molecules, the velocity difference close to the wall and at the channel center is small. This is apparently because of the weak wall–fluid interaction and the smoothness of graphite wall. As previously mentioned, the graphite wall density at the surface is 4.42, which is higher than that of the diamond (2.11) and fcc (111) (1.15) wall structures. The wall–fluid interaction is certainly the dominant factor in the flow profile, and it is important to include both the interaction and the wall-surface roughness for discussion of gas-flow profiles.
4. Conclusion

In this study, gas flow in a nanochannel was investigated by nonequilibrium MD simulations for the early transition regime. The effect of the wall configuration on the velocity profile was investigated by using identical monoatomic molecules for both the fluid and the wall. The significant findings are as follows:

1. Gas flow in the channel is affected by the nanoscopic wall configuration, such as the surface lattice configuration. Unlike liquid flow, the adsorbed monolayer density is greatly affected by the surface configuration for gas flow. As the density peak becomes high, the velocity becomes high and velocity bend is remarkable.

2. As the wall molecule density increases, the velocity increases and then decreases. This is because of the change of dominant factor from surface roughness to wall adsorption.

3. The velocity profile was analytically investigated considering the fluid molecule density profile. As the density close to the wall surface becomes high, velocity bend is remarkable. In contrast, it has little effect on the slip velocity in the analytical solution.

4. For diamond and graphite wall structures using the argon potential for the wall atoms and the gas molecules, adsorption to the wall surface has a greater effect on the gas-flow velocity than the surface roughness because of the high wall density. Therefore, the velocity near the wall is lower than that for the fcc surface structures.

5. A system with a graphite wall and argon gas in the channel was investigated using different L–J potentials for the carbon atoms of the wall and the argon atoms in the channel. The velocity near the wall increases owing to the decrease of adsorption of argon to the wall because of the L–J potential and surface smoothness.

From the above findings, it can be concluded that the wall surface configuration affects the gas density near the wall surface, and the channel flow characteristics are affected by both adsorption to the wall and the wall surface smoothness. Therefore, an optimal wall molecule density exists for each wall molecule configuration. The L–J potential is another important factor of the wall–fluid interaction, and the actual gas flow in a nanochannel can be optimized by considering all of these factors.

References


