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Investigating the wall effect on convective heat transfer in a nanochannel by molecular dynamics simulation

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ABSTRACT

In this paper, convective heat transfer of argon in a nanochannel is investigated by molecular dynamics method. Simulations are performed by LAMMPS code and the effects of wall material, wall roughness and nanochannel size on Nusselt number are studied. To study the wall material effects on convective heat transfer, argon, copper and platinum walls are considered. Results show that convective heat transfer is affected by the wall material and the Nusselt number in the nanochannel with copper walls is higher than the other materials. Also, results illustrate that by increasing the nanochannel size, the Nusselt number increases. Finally, the presence of roughness increases the velocity and Nusselt number in the nanochannel.

1. Introduction

Heat transfer in fluids is one of the most attractive and complex phenomena in the fluid mechanics, which has always been noticeable to researchers due to its importance in industrial equipment. The investigation of fluid flow and convective heat transfer in macroscale have been well done using experimental and theoretical methods. In microscale, the use of both experimental and theoretical methods is possible, although experimental studies are expensive and difficult. Also, in this scale, the liquid can be theoretically treated either as a continuum or as a collection of particles [1]. Mala et al. [2] experimentally studied water flow in microtubes and showed that flow characteristics for microtubes with small diameters diverge from the predictions of the conventional theory. Peng et al. [3] experimentally investigated the effect of geometrical parameters on convective heat transfer of water in a microchannel. They showed that in a microchannel, heat transfer of laminar flow is complex and different from that in conventional channels. Wang et al. [4] studied forced convection of water in a microchannel. Their experimental results indicated that heat transfer characteristics of laminar flow is affected by microchannel size. Peng et al. [5] experimentally investigated forced convective heat transfer and flow characteristics of water in a microchannel. They showed that the geometric configuration (aspect ratio) of the microchannel is one of the parameters affecting heat transfer of laminar flow. Wu et al. [6] performed an experimental study on laminar convective heat transfer in the microchannel. They investigated different surface conditions and found that laminar Nusselt number depends on geometric parameters. They stated that the values of Nusselt number increase with increasing the surface roughness and surface hydrophilic property. Zhang et al. [7] investigated heat transfer of laminar flow in rough microchannels. They showed that heat transfer performance of the rough microchannels is improved compared to the smooth channels. Generally, at microscale due to the larger surface to volume ratio, surface factors have more impact on flow and heat transfer characteristics that are quite different from those of conventional scales [8]. When channel size is further reduced, empirical studies and many theoretical correlations face a great challenge. Molecular dynamics simulation is an effective method to investigate the fluid flow and transport phenomena at the nanoscale, which is based on the integration of particle motion equations [9,10].

Kumar et al. [11] used molecular dynamics simulation to study water-like molecules placed between two plates. They indicated that thermodynamic properties of water changes relative to its bulk properties. Giovambattista et al. [12] examined water molecules confined between hydrophobic and hydrophilic surfaces and illustrated that the water density near the hydrophilic surfaces is different from the hydrophobic ones. Lv et al. [13] investigated the behavior of nanofluid confined between two walls and showed that a solid-like layer of liquid atoms exists near walls. Sun et al. [14] studied the behavior of nanofluid in a nanochannel. They showed that distribution of number density has fluctuations near the walls. They stated that the reason for this phenomenon is strong Ar–Cu interactions. Kim et al. [15] investigated water flow in both rough and smooth channels. Their results showed that the density profile illustrates layering of liquid molecules near the walls.

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Nomenclature

Ar	argon atom
Cu	copper atom
F_i	embedding energy of atom i
h	heat transfer coefficient $\left(W/m^2.K\right)$
z	roughness depth (Å)
k	thermal conductivity $\left(W/m.K\right)$
l_k	thermal slip length (Å)
L	channel height (Å)
K_B	Boltzmann Constant
m_j	atom mass of atom j
n	number of bins
N	number of atoms
Nu	Nusselt number
Pt	Platinum atom
r_{ij}	distance between atoms $i$and j
T	temperature (K)
T_b	bulk temperature (K)
T_w	wall temperature (K)
U	EAM potential
v_{ave}	center-of-mass velocity $\left(m/s\right)$
v_j	velocity of atom j $\left(m/s\right)$
V_x	velocity in x direction $\left(m/s\right)$
w	roughness width (Å)

Greek symbols

ε	energy parameter (J)
ρ	atomic electron density
ρ	fluid density
σ	length scale (Å)
ϕ_{LJ}	LJ potential
φ_{ij}	pair potential interaction between atoms $i$and j

Also, they indicated that layering of liquid molecules follows the shape of the wall surface. Sofos et al. [16] investigated the effect of roughness on the argon flow in nanochannels and indicated that argon atoms are trapped inside the roughness. Noorian et al. [17] used molecular dynamics simulation to investigate the effect of roughness geometry, its height and also surface attraction energy on the fluid flow. They stated that fluid particles are trapped among the roughness elements which results in the change in density profile. Asproulis et al. [18] studied the effect of roughness on flow behavior inside micro and nanofluidic devices. They showed that the velocity profile is affected by the roughness and the surface attraction energy. Kamali et al. [19] investigated the effect of surface roughness on the fluid flow. They stated that the wall-fluid interaction and the surface roughness affect the fluid nanostructures. Also they indicated that a nanochannel containing the cavity has higher velocity than a nanochannel with bulge for the same aspect ratio. Bagheri Motlagh and Kalteh [20] used molecular dynamics simulation to investigate fluid thermal conductivity in a nanochannel. To this purpose, they examined the effect of wall material, nanochannel size and roughness on fluid thermal conductivity. Also, they studied the effect of flow on fluid thermal conductivity and stated that the existence of flow increases the amount of thermal conductivity.

Although the study of Poiseuille flow in the nanochannels, with MD, has been performed in many papers, such as [21–25], convective heat transfer has been investigated in a limited number of articles. The first study on heat transfer in nanochannels via this method was done by Markvoort et al. [26]. Unlike other studies of the Poiseuille flow, in which external force is applied to all fluid atoms, they applied the external force only to the atoms that are located in the special region at the nanochannel inlet. They also reset the temperature of the atoms across the outlet boundary to the initial temperature before re-entering the channel. Their results showed that by increasing the strength of fluid-wall interaction, the heat transfer rate increases. Ge et al. [1] modified the Markvoort's method. In the Markvoort's method, there is initially a temperature reset region, and then there is a special region to apply the external force. This will change the fluid temperature at the channel inlet relative to the desired input temperature. They achieved more accurate results by changing the place of these regions with each other. They calculated the Nusselt number for argon flow in an argon nanochannel and showed that by increasing the strength of fluid-wall interaction, the Nusselt number increases. Gu et al. [27] studied the effect of axial heat conduction on heat transfer and showed that the effect of this phenomenon on the local average temperature of fluid is less than 2%. Marable et al. [28] investigated convective heat transfer of water flow in graphene nanochannels. They obtained the Nusselt number for different channel heights and various fluid-wall interaction strengths. The results showed that by increasing the channel height and the strength of fluid-wall interaction, the Nusselt number increases. Bagheri Motlagh and Kalteh [29] studied the effect of nanoparticles and their related factors such as diameter and volume fraction on convective heat transfer of nanofluid Poiseuille flow. They stated that nanoparticles enhance convective heat transfer. For instance, their results showed that in a copper nanochannel with 40 Å width by adding spherical nanoparticles with volume fraction of 1.4%, Nusselt number increases 41%. Also, they showed that nanofluid convective heat transfer increases with increasing the volume fraction and decreasing the diameter of the nanoparticles.

According to the literature, the fluid flow and heat transfer in microchannels and nanochannels is influenced by various factors such as; fluid characteristics and surfaces properties (shape, roughness, etc.). Although, the effect of some factors such as the strength of fluid-wall interaction and nanochannel height on heat transfer has been investigated by molecular dynamics method, the effect of other effective factors, such as surfaces properties (material, roughness, etc.), has not been studied, yet. Therefore, in this paper, the effect of wall properties on heat transfer in the nanochannel is investigated. For this purpose, the Nusselt number is obtained for argon (solid atoms with argon interaction properties), copper and platinum nanochannels, and the effect of the wall material and the nanochannel height is studied. Moreover, in this study, the effect of wall roughness on heat transfer in the nanochannel is investigated using molecular dynamics method.

2. Methodology

2.1. Model and simulation details

The simulation model is a nanochannel consisting of two parallel walls that are located at a given distance from each other, called the channel height. Argon atoms are used as fluid in the space between the lower and upper walls. Argon is one of the most common fluids in molecular dynamics simulations, that allows to focus accurately on the phenomena affecting flow and heat transfer due to its simplicity of modeling and the avoidance of complexities associated with other fluids. To investigate the effect of the wall, atoms of copper, platinum and solid atoms with argon interaction properties are used separately to create the walls. The choice of materials is such that a range of fluid-wall interaction powers (more, less and equal to the fluid-fluid interaction

strength) is created to investigate and understand the phenomena that will occur during heat transfer in a nanochannel (changing in fluid atoms mobility and forming a solid-like layer). In fact, in order to make the simulation realistic, instead of changing the coefficients of the wall-fluid potential function, different materials are used for modeling the walls. The simulation box is $120 \times (L+20) \times 20\text{Å}^3$ in size. The thickness of each wall is10Å, leading to a channel height of$L$. For better application of the thermostat, each wall is modeled with two parts. The outer part of each wall, which acts as an adiabatic boundary condition, is constant. The inner part of each wall, which is considered as the "phantom atom", serves as the heat source of that wall [30]. Periodic boundary condition is imposed in the z-direction and along the y-direction the boundary condition is defined as stated above. The boundary condition in the x-direction is a quasi-periodic boundary condition which is similar to the periodic boundary condition, with the difference that before re-entering the fluid atoms into the nanochannel, they accelerate in force region and their temperature is reset to the inlet temperature [1,27,28].

Initially, wall atoms for all materials, are arranged as face centered cubic lattice (FCC), so that each of them has a lattice constant subject to its density, as shown in Table 1. Also, the argon film is modeled with face centered cubic (FCC) lattice structure based on an average density of $1200\,\frac{kg}{m^3}$[1]. The schematic model of the computational domain is shown in Fig. 1.

To investigate the effect of roughness on flow and convective heat transfer, roughness is created in the form of rectangular cavities at equal intervals along the length of the channel on the wall, as shown in Fig. 2.

To describe interactions between Ar-Ar atoms and fluid-wall atoms, the Lennard–Jones potential is used [32,33]:

$$\varphi_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{1}$$

where $\sigma$and $\varepsilon$are length and energy parameter scales, respectively and their values for interactions between various materials are shown in Table 2.r_{ij} represents the intermolecular distance between atoms $i$and j.

Embedded atom method (EAM) potential is used to solve interactions between metal atoms [32,34]:

$$U = \sum_i F_i\left(\sum_{j\neq i}\rho_i(r_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\varphi_{ij}(r_{ij}) \tag{2}$$

where $F_i$is the embedding energy which is a function of the atomic electron density ρ, φ is a pair potential interaction, and $i$and j represent atoms $i$and$j$, respectively.

When the wall is made of argon, harmonic springs with k = 70 N/m are used to connect the atoms to the FCC network sites [1]. In this model the argon atoms vibrate around their coordinates.

2.2. Simulation procedure and flow creation

As mentioned, the initial positions of all the atoms are created by FCC lattice, so in order to achieve a state of equilibrium, the system must first be relaxed [34]. For this purpose, the system is relaxed in a micro-canonical (NVE) ensemble [1] for 1×10^6 steps with each time step of 1 fs [1]. The velocity Verlet algorithm is used to perform the simulations. After the relaxation, the flow conditions (external force and thermostat) is applied, and then the system is simulated for 3×10^6 other steps with the same time step as relaxation for sampling.

Table 1
Lattice constant for various materials of the wall.

Wall material	Lattice constant
Copper	3.61Å[30]
Platinum	2.776Å [31]
Solid argon	4Å[1]

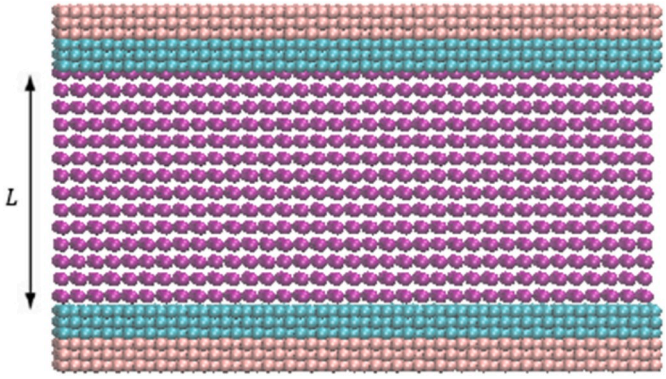


Fig. 1. The schematic model of the computational domain.

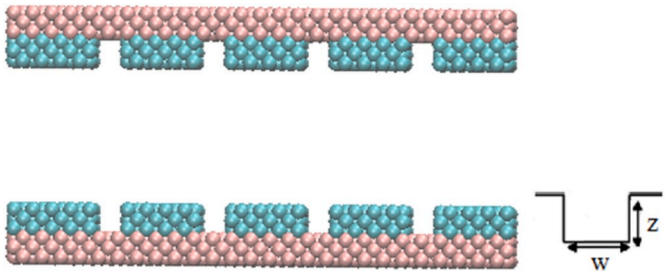


Fig. 2. Schematic view of the wall roughness.

Table 2
The parameters of Lennard–Jones potential.

Interaction	ε	σ
$Ar-Cu$[32,34]	$10.4153 \times 10^{-21}J$	2.871Å
$Ar-Pt$[31]	1.002×10^{-21}J	2.74Å
$Ar-Ar$[32,34]	$1.67 \times 10^{-21}J$	3.405Å

To create a flow and apply the quasi-periodic boundary condition, two regions are employed before the channel inlet [1,27,28]. The first is the force region in which the external force is applied, and the other is the thermostat region used to reset the fluid temperature. The length of the force region in x-direction is 10Å, which is placed at $-15\text{Å} < x < -5\text{Å}$. The external force applied to the liquid atoms in this region is set as $3.4 \times 10^{-12}N$. Also, the length of the thermostat region in x-direction is 5Å, which is located at $-5\text{Å} < x < 0\text{Å}$. The simulation domain with its three regions is illustrated in Fig. 3.

To investigate convective heat transfer, the inlet fluid temperature is set as 300 K and the temperature of both the upper and lower walls are fixed at 200 K, by Nose–Hoover thermostat baths [35]. To avoid phase transition in the process, the fluid is controlled to be in its supercritical state.

2.3. Governing equations

To obtain the density, velocity and temperature distribution in the nanochannel, the sampling region is divided into n bins. The size of each bin is $5 \times 2 \times 20\text{Å}^3$. When there is flow in the nanochannel, the velocity of each particle is the sum of the mean flow velocity and the thermal velocity. Since only thermal velocity is used to obtain the temperature,

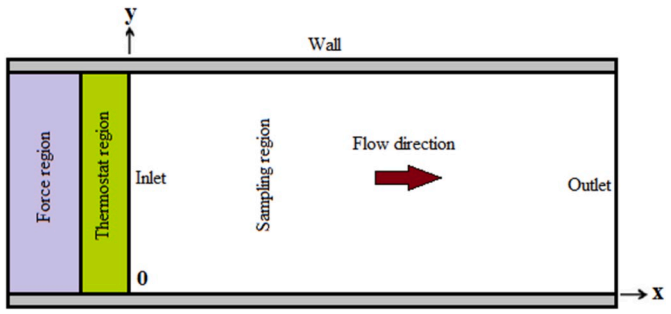


Fig. 3. The simulation domain separated into three regions; force region, thermostat region, and sampling region.

so in each bin, the mean flow velocity of that bin must be reduced from the whole velocity of each particle to calculate its temperature. The temperature of each bin is calculated by Eq. (3) [36,37]:

$$T = \frac{1}{3NK_B}\sum_{j=1}^{N} m_j\left(v_j - v_{ave}\right)^2 \tag{3}$$

where $T$is temperature, $N$is the number of atoms,K_B is the Boltzmann Constant,m_j is the atom mass of atom j, $v_j$velocity of atom j and v_{ave}mean flow velocity of the bin. To obtain the local Nusselt number, Eq. (4) can be used in which the Nusselt number is calculated based on the heat transfer coefficient [1]:

$$Nu = \frac{hL}{k} \tag{4}$$

where L is the nanochannel height which is set as the characteristic length, $\kappa$is fluid thermal conductivity and $h$is the heat transfer coefficient obtained from the following equation [1]:

$$h = \frac{k}{T_b - T_w}\left.\frac{\partial T}{\partial y}\right|_{y=0} \tag{5}$$

where $T_w$is the wall temperature and $T_b$is the bulk temperature calculated from the following equation [1]:

$$T_b = \frac{\int_0^L \rho(y)V_x(y)T(y)dy}{\int_0^L \rho(y)V_x(y)dy} \tag{6}$$

where $\rho$is the fluid density and V_x is the velocity in $x$direction. Combining Equations (4) and (5), the Nusselt number can be calculated by Eq. (7) [1]:

$$Nu = \frac{L}{T_b - T_w}\left.\frac{\partial T}{\partial y}\right|_{y=0} \tag{7}$$

In addition, in order to better understand the phenomena affecting the fluid flow and convective heat transfer, the thermal slip at the wall, which is obtained from equation (8), is investigated [28]:

$$l_k = \frac{\Delta T(y=0)}{\left(\frac{dT}{dy}\right)_{y=0}} \tag{8}$$

3. Results and discussion

3.1. Validation

To evaluate the accuracy of the thermostat function and the temperature restoration to the initial inlet fluid temperature, the fluid temperature at the inlet boundary is calculated during the simulation and the results are shown in Fig. 4. As shown in the figure, the temperature value is well controlled at the desired value.

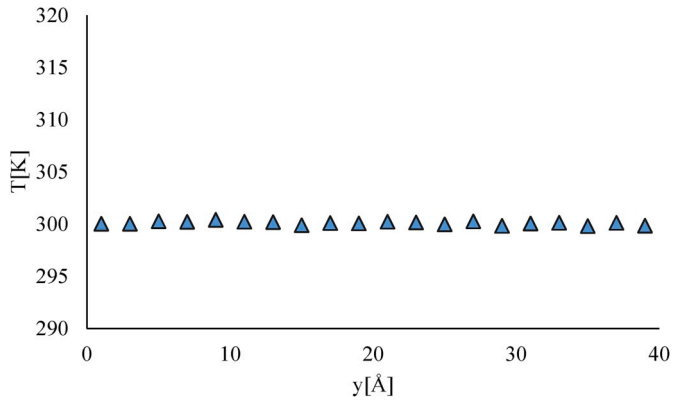


Fig. 4. Temperature of the fluid in the nanochannel inlet with 40Åheight.

To validate the results and compare them with the results of Ge [1], first the value of the Nusselt number is calculated in a nanochannel similar to that used in Ge's study, namely, the nanochannel size as 400 × 120 × 60Å^3. The nanochannel walls are made of solid atoms with FCC lattice structure. The calculated Nu number in this study for fully developed condition is 2.03, which is 3% different from the result of Ge (1.97).

3.2. Investigating the fluid flow

In order to investigate the flow inside the nanochannel and determine its type, fluid velocity and temperature are studied. The results for a nanochannel with 60Åheight are shown in Fig. 5. As shown in Fig. 5 (a), the fluid velocity along the nanochannel is almost unchanged, indicating the hydrodynamic development of the flow. Fig. 5(b) shows the temperature distribution inside the nanochannel. As the fluid moves along the channel, temperature changes are reduced. The flow is in the thermally developing condition and finally it reaches the thermal development. It should be noted that when the periodic boundary condition is used, the fluid temperature at the outlet is affected by the image of the hot atoms in the channel inlet, which is due to the unrealistic axial thermal conductivity [1,27]. To avoid the effect of axial thermal conductivity, the investigation of temperature distribution and calculation of the Nusselt number are performed only in the first half of the nanochannel.

3.3. The effect of nanochannel size

In order to determine the effect of nanochannel size on convective heat transfer, Nusselt number is calculated for different heights of copper nanochannel. The results are shown in Fig. 6. The results show that with increasing channel height, the Nusselt number increases. Due to the fact that in the nanoscale, transport phenomena (fluid properties) depend on the fluid structure and the mobility of its particles, there are two effective factors on heat transfer: the formation of a solid-like layer and the fluid particles velocity. For the first factor, when copper atoms are used to make walls, due to the stronger interaction between fluid-wall atoms relative to the interaction between fluid-fluid atoms, more atoms of argon are gathered near the wall. This leads to a lack of uniformity in the distribution of fluid atoms in the nanochannel and the formation of a layer of argon atoms in the vicinity of the walls. Although the formation of a solid-like layer improves the heat transfer from the wall to the fluid, but due to the decrease in the number of fluid atoms in the middle of the channel, the ability to transfer heat and energy in the fluid is reduced. According to Fig. 7, which shows the number density graph for copper nanochannels with 50Å and 60Å heights, when the nanochannel height increases, the wall affects a smaller fraction of the existing fluid particles. Therefore, fluid particles have more potential to

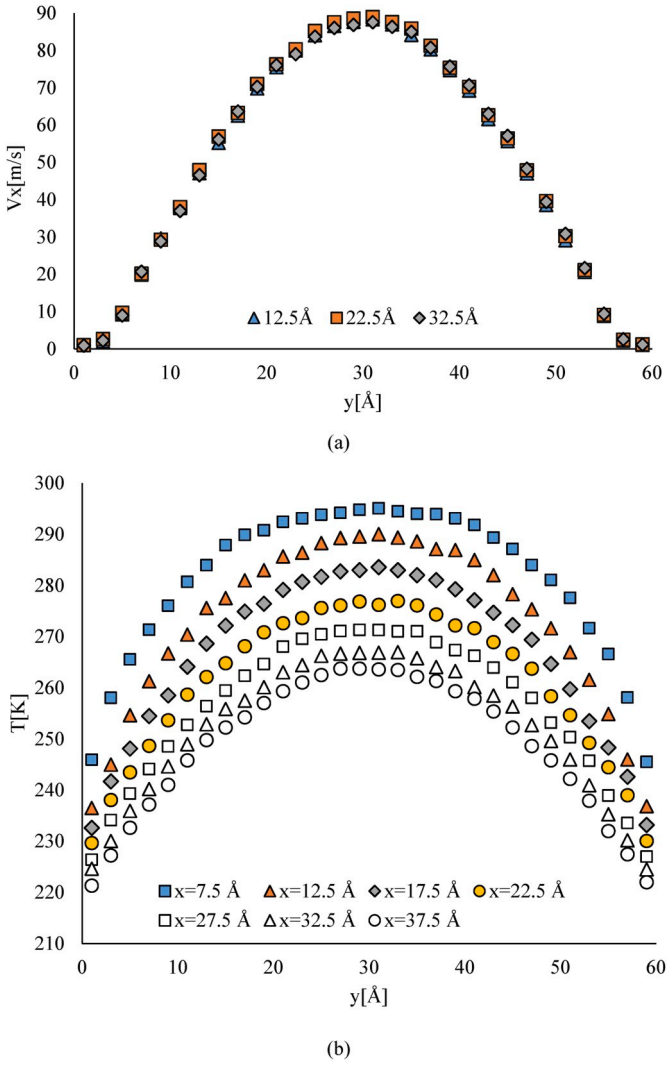


Fig. 5. The a) velocity and b) temperature profile in the nanochannel with 60Åheight.

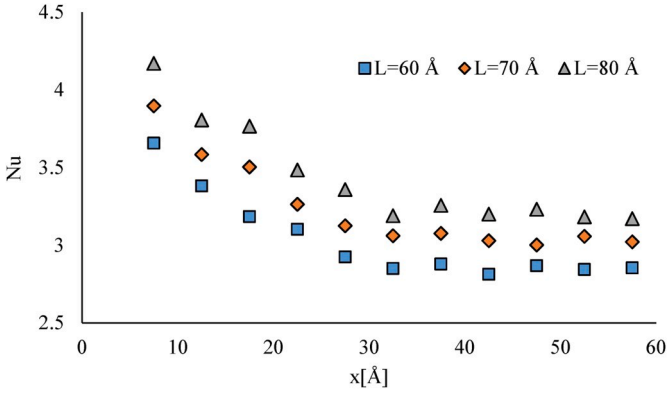


Fig. 6. The local Nusselt number along the nanochannel for nanochannels with 60, 70 *and* 80Åheights.

transfer heat and the Nusselt number increases. For the latter factor, the velocity for different nanochannel heights is calculated and shown in Fig. 8. It can be seen that as the channel height increases, the velocity increases in the nanochannel. Actually with increasing the channel height, the wall effect on the mobility of fluid particles decreases.

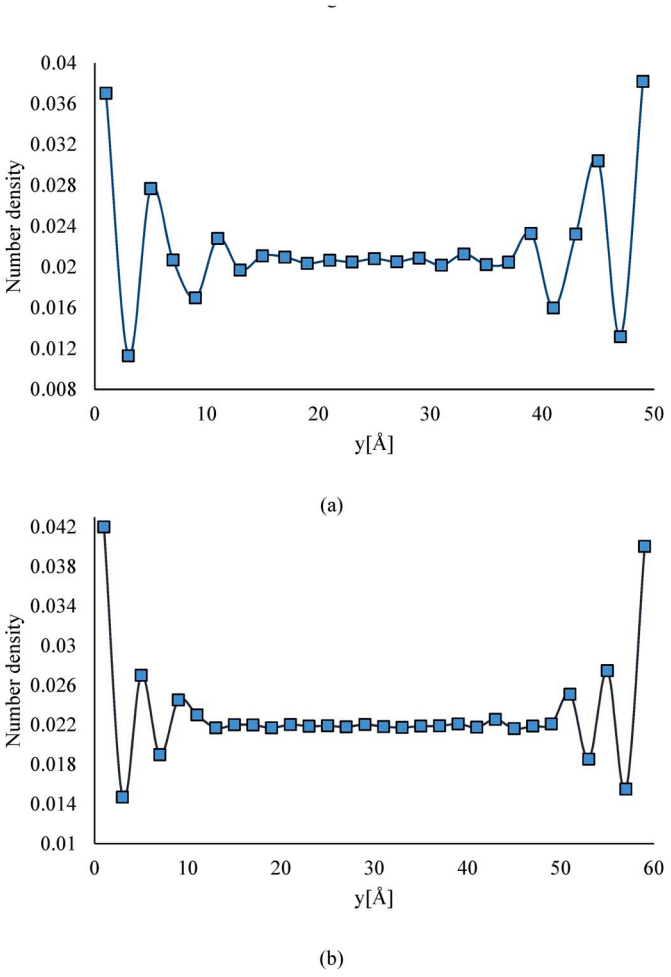


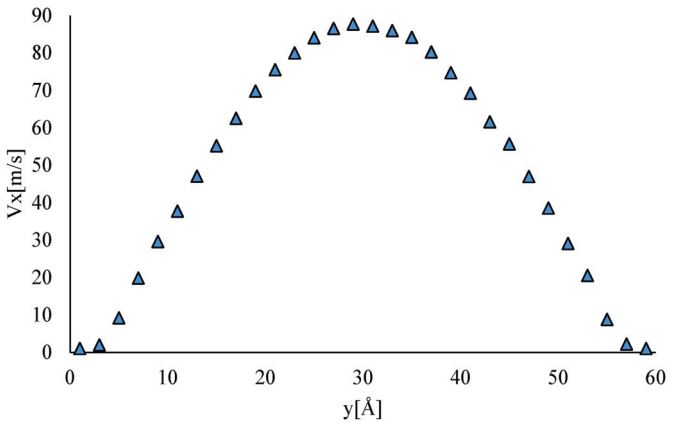
Fig. 7. Number density graph for copper nanochannels with a) 50Å and b) 60Å height.

As shown in Table 3, the results also indicate that the increase rate in Nusselt number decreases with increasing the channel height and it is greater for smaller heights of the nanochannel. For example, when the nanochannel height increases from 40Å to 50Å, the increase rate for Nusselt number is 0.22while if the nanochannel height increases from 70Åto 80Å, the increase rate is 0.15.

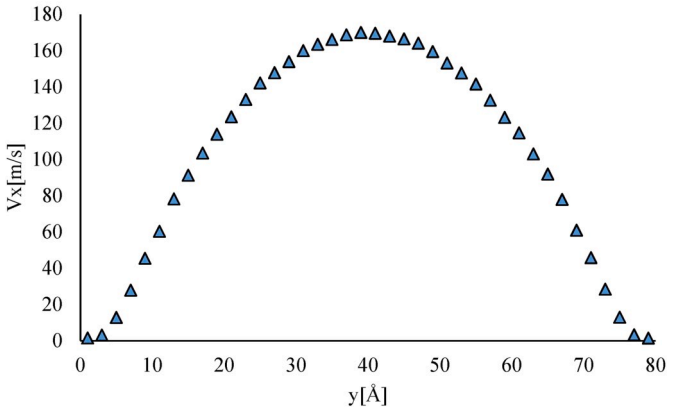
To study the liquid state in the vicinity of the walls, the thermal slip length for nanochannels with 60Å and 80Å heights is studied. The results are shown in Fig. 9. The results indicate that thermal slip length does not change significantly along the nanochannel, which is consistent with the previous studies [1,29]. It is also found that the thermal slip length is affected by the nanochannel size and decreases with increasing the nanochannel height. This observation is consistent with a previous report [28].

3.4. The effect of wall material

To investigate the effect of wall material on convective heat transfer, Nusselt number is calculated for copper, argon, and platinum nanochannels at a constant channel height (60Å). These materials are common materials in molecular dynamic simulations, and as mentioned earlier, they are used to create a range of different interaction powers between the wall and the fluid in order to study the effects of the wall. The results, shown in Fig. 10, indicate that the Nusselt number for fluid in the copper nanochannel is larger than the others. Fig. 11 shows the number density graphs in copper and platinum nanochannels and Fig. 12 illustrates the velocity profile in platinum nanochannel.



(a)



(b)

Fig. 8. Velocity profile in the nanochannel for nanochannels with *a*) 60 *and b*) 80Å height at $x = 22.5$ Å

Table 3
Nusselt number in fully developed condition for various nanochannel heights.

Nanochannel height	Nu_∞ (Nusselt number in fully developed condition)	Increase rate
40A	2.44	
50Å	2.66	$Nu_{\infty,50} - Nu_{\infty,40} = 0.22$
60Å	2.85	$Nu_{\infty,60} - Nu_{\infty,50} = 0.19$
70A	3.02	$Nu_{\infty,70} - Nu_{\infty,60} = 0.17$
80Å	3.17	$Nu_{\infty,80} - Nu_{\infty,70} = 0.15$

Investigating Figs. 12 and 8(a), it can be seen that the amount of velocity in platinum nanochannel is different from that in the copper nanochannel. In the copper nanochannel, due to the strong interaction between the fluid and the wall, the velocity in the vicinity of the walls is very low. However, in the platinum nanochannel, the velocity near the wall is noticeable which is due to the lack of proper formation of the solid-like layer. The velocity slip length is about 3.27Å for the platinum wall and the boundary is almost non-slip for copper walls. Therefore, based on the number density graphs and velocity profiles (Figs. 8, 11 and 12(a)), it can be concluded that at a constant channel height although with increasing the strength of wall-fluid interaction the fluid velocity decreases, more fluid atoms are gathered near the wall. This reduces the velocity slip length and also thermal slip length and then improves the

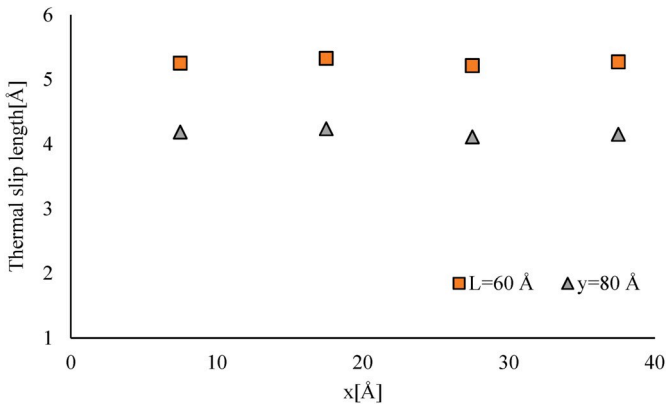


Fig. 9. The thermal slip length along the nanochannel for nanochannels with 60 *and* 80Å heights.

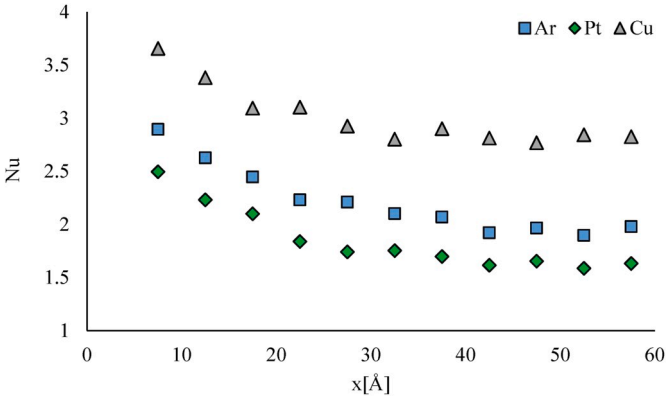


Fig. 10. Local Nusselt number along the nanochannel for various wall materials at a constant channel height (60Å).

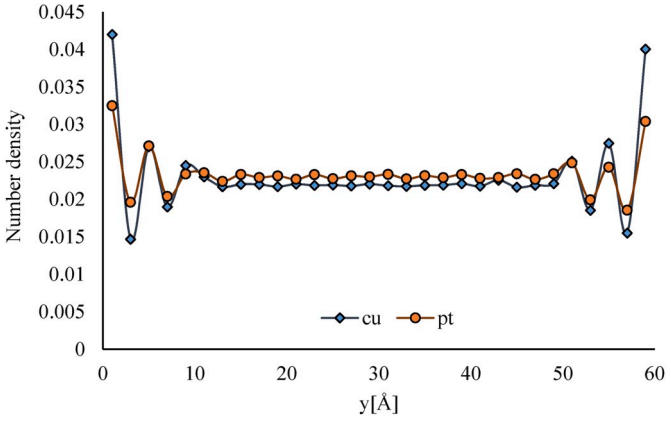


Fig. 11. Number density graph for copper and platinum nanochannels with 60Å height.

heat transfer from the walls to the fluid. Actually, the investigation of the effective factors (the velocity and number density) shows that at a constant channel height, the solid-like layer has a greater effect on the heat transfer than the velocity.

3.5. *The effect of wall roughness*

To investigate the effect of wall roughness on the flow and convective heat transfer, roughness is created in the form of rectangular

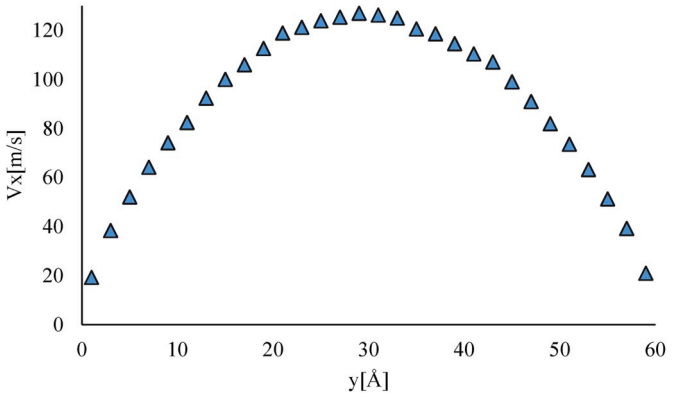


Fig. 12. Velocity profile in the nanochannel for platinum nanochannels with 60Å height at $x = 22.5$Å

cavities at equal intervals along the length of the nanochannel. The simulation is performed for two roughness sizes, as described in Table 4, and the results, as shown in Fig. 13, are compared with the results of our previous work for the smooth nanochannel [29]. In these simulations, walls are made of copper. According to the figure, increasing the roughness depth increases the Nusselt number. The results also demonstrate that the thermal slip length, as shown in Table 5, decreases with increasing the roughness size. To study the effective factors, the fluid velocity and its number density are investigated. Figs. 14 and 15, respectively, show the comparison of the velocity profiles and the number density graphs in nanochannels with 40Å height in smooth [29] and Rouhness2 cases. As shown in Fig. 14, the velocity in a rough nanochannel is more than that of a smooth nanochannel. This increases the atoms mobility and their ability to transfer heat in the nanochannel. It is worth noting that the velocity in the nanochannel depends on the type of the roughness used. In fact, on nanoscale, wall materials, nanochannel size, and the shape of roughness are the factors affecting the fluid velocity. When using roughness, if the roughness is in the form of a cavity, namely it creates more space between the two walls, the velocity increases in the nanochannel. But if the roughness is in the form of a bump, namely it creates less space between the two walls, the velocity decreases in the nanochannel [19]. According to Fig. 15, the results show that the density fluctuations in the rough channel are larger than the smooth channel and these fluctuations in the rough channel penetrates more distances from the wall. Furthermore, the graph illustrates that in rough channel more fluid atoms accumulate near the walls and this increases the heat transfer from wall to the fluid.

4. Conclusion

In this work, the effect of the wall on convective heat transfer and Nusselt number in the nanochannels is investigated. For this purpose, the effect of nanochannel size, walls material and wall roughness on Nusselt number are examined. The results show that the Nusselt number is affected by the channel dimensions and with increasing the channel height, the Nusselt number increases. The reason for this difference is that in the nanoscale the mobility of each particle is affected by its interaction with other particles, so when there is wall, due to the stronger interaction between fluid-wall atoms relative to fluid-fluid atoms, a fraction of the argon atoms are gathered near the wall. When

Table 4
Roughness dimensions used in the simulation.

Case	z(Roughness depth)	w(Roughness width)
Roughness1	2.5Å	5Å
Roughness2	5Å	5Å

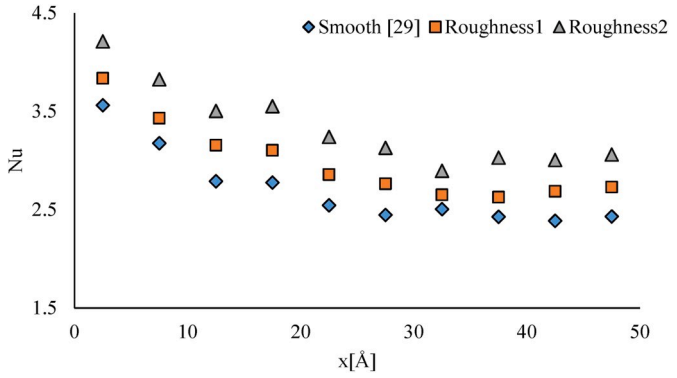


Fig. 13. Local Nusselt number along the nanochannel for various roughnesses and smooth walls at a constant channel height (40Å).

Table 5
Thermal slip length in fully developed condition for various roughnesses and smooth walls at a constant channel height ($40A^{\circ}$).

Case	Thermal slip length
Smooth [29]	6.39Å
Roughness1	5.24Å
Roughness2	4.11Å

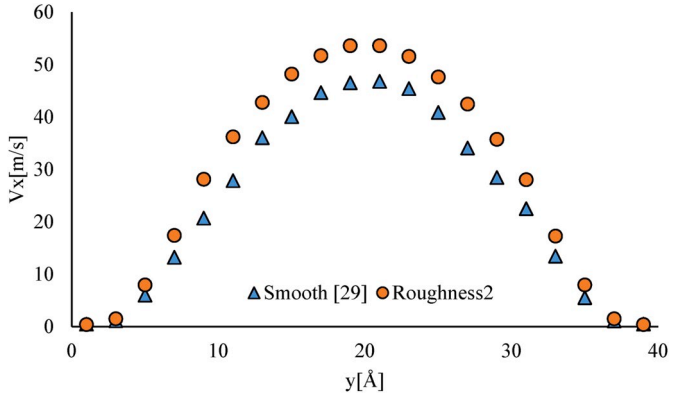


Fig. 14. The velocity profile in the nanochannel for nanochannels with 40Å height in smooth and Rouhness2 cases at $x = 22.5$Å

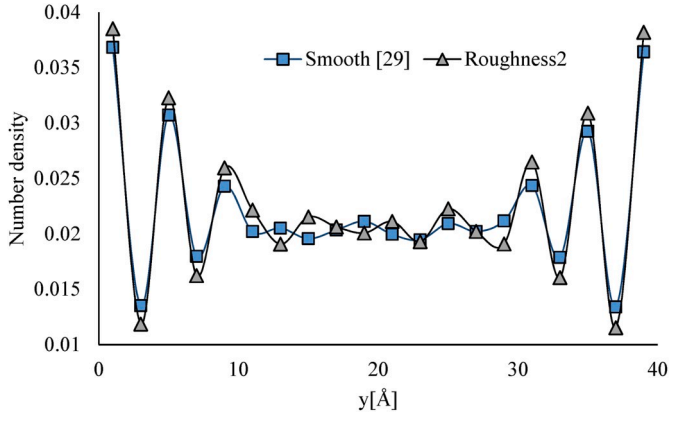


Fig. 15. Number density graph for nanochannels with 40Å height in smooth and Rouhness2 cases.

the nanochannel height increases, the wall affects a smaller fraction of the existing particles. Therefore, fluid particles have more potential to transfer heat and the Nusselt number increases. Also, the results show that thermal slip and the increase rate in Nusselt number decrease with increasing channel height. The results also show that the Nusselt number is affected by the wall material and its value for fluid in the copper nanochannel is larger than it in the platinum and argon nanochannels.

The results also show that surface roughness is effective on Nusselt number and with increasing the roughness depth, the Nusselt number increases. As well as the results illustrate that thermal slip decreases with increasing the roughness size. It is also found that the velocity and the density fluctuations in the rough channel are larger than the smooth channel.

Declaration of competing interest

We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

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