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Investigating the Effect of Shape, Size and Surface Wettability of a Nanochannel on Fluid Thermal Conductivity Using Molecular Dynamics Simulation

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ABSTRACT

The main goal and innovation of this study is to analyze the effects of the configuration of the walls and their orientation (parallel or perpendicular to the flow direction) on the behavior of the thermal properties of the fluid. So, in this paper, the effects of shape, size, and surfaces wettability of nanochannel with a focus on walls configuration on the thermal conductivity of fluid are investigated. Equilibrium molecular dynamics simulation is used for this purpose. Two parallel plates, a square cross-sectional nanochannel, and a rectangular cross-sectional nanochannel are examined as three different nanochannel shapes. According to results, the shape and size of the nanochannel are a significant factor in thermal conductivity, which is caused by the effect of walls on the mobility and arrangement of fluid atoms in the nanochannel. The walls have a negative effect in terms of the mobility of atoms, but in terms of the arrangement of the atoms, they have opposite effects depending on their orientation (perpendicular or parallel to the desired direction). As a result, in a same channel height, square channels have a higher thermal conductivity than slit channels, since the side walls affect thermal conductivity positively. The results also indicate that with the increase in the wettability of the nanochannel surfaces, the thermal conductivity decreases. In this case, fluid thermal conductivity is more affected by the walls.

Nomenclature

Ar	argon atom	U	EAM potential
Cu	copper atom	V	channel volume
F_i	embedding energy of atom i	v_i	velocity of atom i
F_{ij}	force on atom i due to atom j	**Greek symbols**	
j_y	heat current in y-direction	ε	energy parameter
K_B	Boltzmann Constant	k	thermal conductivity
L	channel width	ρ	atomic electron density
m_i	atom mass of atom i	σ	length scale
r_{ij}	distance between atoms i and j	φ_{LJ}	LJ potential
T	temperature	ϕ_{ij}	pair potential interaction between atoms i and j

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INTRODUCTION

In recent decades, with the advancement of technology and the use of small equipment in many fields such as medicine and various industries, researchers have been encouraged to do studies on micro and nano scales. Investigation of fluid properties and its transport phenomena are among the fields studied in these scales. Due to the small scales in the nanoscale, the structure of the nanochannel walls can be introduced as a parameter affecting the fluid properties, which requires investigation and study. In fact, in this scale, investigating the effects of each of the nanochannel walls and analyzing the effects of their configuration and orientation (parallel or perpendicular to the flow direction) on the behavior and characteristics of fluid heat transfer is presented as an innovation and challenge.

In some studies [e.g. 1-3], experimental methods have been used to investigate the characteristics of nanofluids, however using experimental methods in micro and nano scales is difficult and costly. Therefore, numerical simulations are one of the most common study methods in these scales, which are classified based on temporal and spatial scales. The molecular dynamics method, which is based on Newton's second law and examines the location of particles at different times [4], is one of the methods used in the nanoscale. Nanoscale fluid properties and behavior have been determined using this method in many studies [e.g. 5-9].

Kumar et al. [10] examined the water properties in the slit nanochannel and showed that they are different from bulk properties. They also studied the structure and mobility of water molecules and indicated that the walls change them in the nanochannel. Jioambatista et al. [11] studied the effect of wall surface type on water flow in a nanochannel. They indicated that the type of wall surface affects the fluid density near the walls. Li et al. [12] investigated the accumulation of liquid molecules at the solid-liquid interface. They showed that liquid molecules accumulate at the solid-liquid interface. Lv et al. [13] evaluated the fluid flow in a slit channel under shear flow. According to their results, a solid-like layer of fluid atoms forms around each solid surface. They also stated that this layer is the main reason for to increase in the amount of heat transfer. Noorian et al. [14] investigated the effect of the walls on fluid flow. The results showed that factors such as wall roughness and its interaction strength cause a change in fluid density in the vicinity of the wall and also a change in fluid velocity. Toghraei et al. [15] investigated the effect of the wall roughness on the fluid flow and examined temperature, velocity, and density profiles. Their results showed that density distribution is affected by the roughness. Furthermore, they showed that with increasing roughness size, the amount of flow velocity and temperature in the nanochannel increases. Ge et al. [16] simulated the fluid heat transfer in a nanochannel. They calculated the velocity and temperature distributions for the flow inside the channel and studied the effect of surface wettability. The results showed that the thermal slip length and average velocity are higher at lower wettability. Marable et al. [17] studied the effects of nanochannel size on the heat transfer rate. Their results showed that the channel height and the strength of the interaction between the fluid and the wall atoms affect the Nusselt number. Bagheri and Kalteh [18] studied the effect of the walls on the heat transfer of fluid flow in nanochannels. They showed that the size of the nanochannel and the wall material change the heat transfer properties of the fluid. In another work, Bagheri and Kalteh [19] studied the effect of nanoparticles shape, aggregation and wall roughness on the nanofluid heat transfer rate in a nanochannel. They showed that these factors change the velocity and number density of the fluid in the nanochannel. They also stated that the velocity and number density distribution of the fluid are factors affecting the phenomenon of heat transfer in the nanochannel. Yao et al. [20] investigated the role of wall-fluid interaction and wall roughness on heat and momentum exchange in the nanochannel. They showed that the roughness and the wall-fluid interaction strength has an effect on the fluid heat transfer in the nanochannel. Markvoort and Hilbers [21] investigated the strength of gas-wall interaction and its effect on heat transfer and flow behavior in a slit nanochannel. They studied the effect of surface wettability on the gas-solid interface for different gas densities. The results showed that the gas flow density profile along the surface is dependent on the wettability of the gas-solid interface. They concluded that increasing the wettability increases the heat transfer from the solid surface to the static gas and reduces the velocity of the gas flow near the wall. Cui et al. [22] investigated the fluid flow behavior in a slit nanochannel. They showed that there is a solid-like layer near the walls that affect the fluid heat transfer properties. They stated that this layer has a higher density than the base fluid and its thermal conductivity is more than the fluid bulk thermal conductivity. Sofos et al. [23] studied the effect of the wall roughness on the fluid behavior. They also used different fluid-wall interaction strengths in the simulation to evaluate the hydrophobicity or hydrophilicity of nanochannel walls. They indicated that the roughness and fluid-wall interaction strength affect thermal conductivity and velocity of the fluid in the channel. Cui et al. [24] investigated the structure of a solid-like layer at the liquid-solid interface. They found that the structure of the solid-like layer was completely different from that of the base fluid. According to their results, the structure of the solid-like layer is much more regular than the base fluid and is similar to the structure of a solid. They also stated that the microscopic behavior of atoms affects the thermal conductivity of the fluid. Li et al. [25] studied the formation of a layer of liquid molecules around nanoparticles and its effect on fluid thermal conductivity. They found that a solid-like layer forms on the interface between the liquid and the nanoparticle, which moves with the Brownian motion of the nanoparticle. They stated that this layer has a significant contribution to increasing the thermal conductivity of nanofluids. Liu et al. [26] investigated the thermal conductivity of liquid argon in a slit nanochannel. Their results showed that the nanochannel height and the strength of the solid-liquid interaction affect the thermal conductivity in such a way that the thermal conductivity of the liquid argon increases

with increasing the nanochannel height. They also showed that there is a solid-like layer at the solid-liquid interface. This layer is effective in increasing the thermal conductivity. According to their results, the number of atoms in the liquid layer near the solid surface depends on the temperature and the interaction strength between the fluid and the solid surface. Bagheri and Kalteh [27] investigated the effect of the walls on the fluid thermal conductivity in a slit nanochannel. Their results showed that the walls reduces the thermal conductivity in the direction of the height of the nanochannel. They also stated that the roughness of the walls causes a change in the number density of the fluid adjacent to the walls and affects the thermal conductivity. Sun et al. [28] calculated the thermal conductivity of nanofluid in a slit nanochannel. The simulation results showed that due to the presence of solid walls, nanoparticle vibration in the direction of the nanochannel is restrained. So, the thermal conductivity in the direction of nanochannel height (direction between two walls) is significantly less than the thermal conductivity in the other two directions. Their results also showed that the thermal conductivity in the directions perpendicular to the z direction (direction between the two walls) is significantly increased relative to its macro-scale magnitude, which is due to interatomic interactions between nanofluid atoms with wall atoms. Hyzorek and Tretiakov [29] studied the fluid thermal conductivity of liquid argon in a nanochannel. To do this, they calculated the thermal conductivity in the direction of the channel length for three nanochannel shapes: slit, square and circular. Their results showed that at the same cross sectional area, the shape of the nanochannel has an effect on the thermal conductivity in the direction of the channel length. They also stated that the density and temperature of the fluid affect the fluid thermal conductivity. Jin et al. [30] investigated the effect of solid-liquid interface on the specific heat capacity of water film. For this purpose, they investigated the water specific heat capacity for three cases: enclosed film between two parallel plates (slit channel), sessile film on the plate, and freestanding film between vacuum. Their results showed that the configuration of water affects the specific heat capacity of water. Also, Jin et al. [31] in another work investigated the effect of liquid argon film configuration on the thermal conductivity. For this purpose, they studied the thermal conductivity for three cases: confined film between two parallel plates (slit channel), sessile film on the plate, and freestanding film between vacuum. Their results showed that the thermal conductivity decreases in the direction between the walls for all three cases. They also stated that thermal conductivity increases with increasing film thickness.

According to the above literature review, the walls and in general nanochannel structure affect the behavioral, structural, and transport properties of the fluid. However, in most studies on fluid thermal conductivity, the effect of nanochannel has not been observed and studies have been performed only in bulk conditions. In a few studies in which nanochannel walls have been taken into account, either the thermal conductivity in the direction of the channel length has been investigated or only nanochannels with two parallel plates (slit channels) have been considered. In this research, the effect of nanochannel shape and size on argon thermal conductivity in the direction of nanochannel width for three shapes of slit, square and rectangular nanochannels is investigated and the governing micro-mechanisms are discussed. In addition, the effects of each of the nanochannel walls based on their orientation (parallel or perpendicular to the flow direction), as well as the effects of the wetting of their surfaces on the thermal conductivity, are studied.

Model and Simulation Details

In this study, to study the effect of nanochannel shape, three types of channels including; two parallel plates (slit channel), channel with a square cross-section, and also channel with a rectangular cross-section are considered. The size of the simulation box for the slit channel is $100 \times (L + 20) \times 20A^{\circ 3}$, and for the channels with square cross-sections, it is $100 \times (L + 20) \times (L + 20)A^{\circ 3}$. The thickness of each wall is $10A^{\circ}$ and L is the distance between two parallel walls (channel width) in a certain direction. Also, for channels with rectangular cross-sections, the size of simulation box is $100 \times (L + 20) \times (2L + 20)A^{\circ 3}$. Figs. 1 and 2, respectively, show the geometric and schematic model of the channel for different nanochannel shapes.

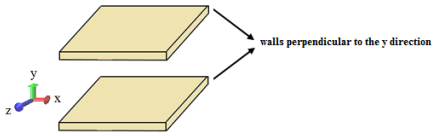
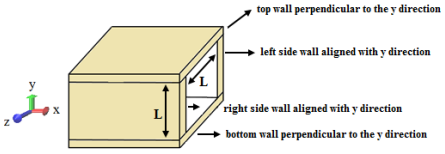
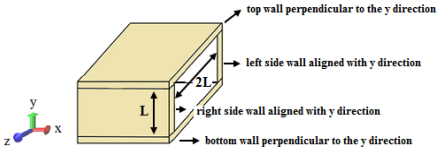
Channel type	Geometric model of the channel
Slit channel	
square channel	
rectangular channel	

Fig. 1. Geometric model of the channel for slit, square and rectangular nanochannels

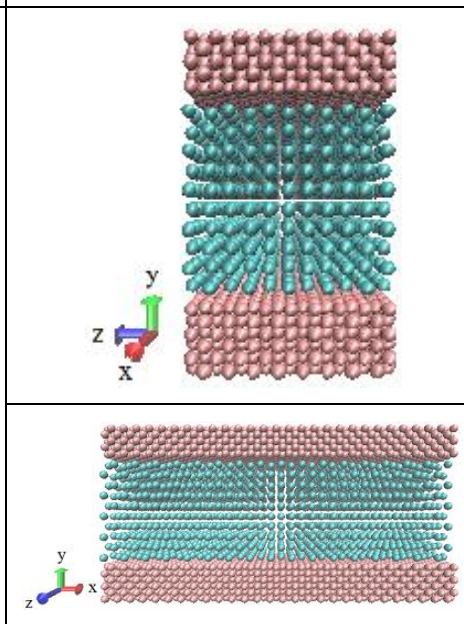
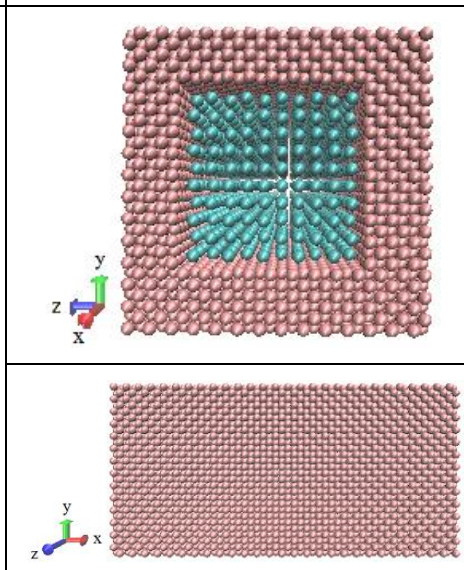
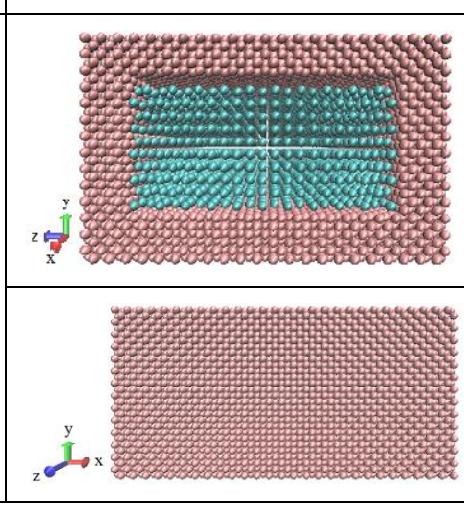
Channel type	Schematic model of the channel
Slit channel	
square channel	
rectangular channel	

Fig. 2. Schematic model of the channel for slit, square and rectangular nanochannels

Copper and argon atoms with a FCC lattice structure are used to create the walls and fluid, respectively. Their lattice constant of each is determined according to their density at the desired temperature.

To create better conditions in the simulation, the wall was divided into two parts. The inner part is considered as the heat source [32-34]. For slit nanochannel, a periodic boundary is applied in the z- and x-directions, and there are the walls in the y-direction. For square and rectangular nanochannels, a periodic boundary is applied in the x-direction, and there are walls in the y- and z-directions.

The well-known 12–6 LJ potential (Eq. (1)) is used to model the interactions between Ar-Ar and Cu-Ar atoms [35- 37]:

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

Where σ indicates the length parameter scale and and ε indicates the energy parameter scale. In this study $\varepsilon_{\mathrm{Ar_Ar}} = 1.67 \times 10^{-21}J$, $\sigma_{\mathrm{Ar_Ar}} = 3.405A°$, $\varepsilon_{\mathrm{Cu_Ar}} = 10.4153 \times 10^{-21}J$ and $\sigma_{\mathrm{Cu_Ar}} = 2.871A°$ [15, 32, 35]. r_{ij} indicates the distance between atoms i and j. Embedded atom method potential (Eq. (2)) is used to model interactions between copper atoms [18, 35, 38].

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

where F_i indicates the embedding energy, ρ is the atomic electron density, and ϕ is a pair potential interaction.

Simulation Procedure and Governing Equations

To reach equilibrium, the simulation system is relaxed and for all atoms, temperature is kept constant at 94 K in the NVT ensemble. 2×10^5 steps are used for relaxation and the time step is considered to be 1 fs. Thereafter, a micro-canonical ensemble (NVE) is used for data collection, and the system is run for more 2×10^6 steps.

Thermal conductivity is calculated using the following equation (Eq. (3)) [29, 39, 40]:

$$\kappa_y = \frac{V}{K_B T^2}\int_0^\infty \langle j_y(0) j_y(t)\rangle\, dt \quad (3)$$

Where V is the volume of the channel and K_B is the Boltzmann constant. $\langle j_y(0) j_y(t)\rangle$ is heat current autocorrelation function (HCAF). $j_y(t)$ *and* $j_y(0)$ show the heat current in the y-direction at the time t and t_0, respectively. Also, the angular brackets represent the average over time. The microscopic heat current is given by [29, 41]:

$$j(t) = \frac{1}{V}\left(\sum_i v_i\varepsilon_i + \frac{1}{2}\sum_i\sum_{j,i\neq j} r_{ij}(v_i.F_{ij})\right) \quad (4)$$

Where v_i is the velocity of particle i, r_{ij} is the distance between particles i and j and F_{ij} indicates the force on atom i due to atom j. The microscopic site energy is calculated by [29]:

$$\varepsilon_i = \frac{1}{2}m_i|v_i|^2 + \frac{1}{2}\sum_i \phi(r_{ij}) \quad (5)$$

RESULTS AND DISCUSSIONS

Validation

For validation, first, the value of thermal conductivity for argon in the bulk state (outside the nanochannel) is obtained. Its value at the temperature of 94 K is calculated as $0.114\frac{W}{m.K}$, which is in good agreement with Lee's experimental result ($0.119\frac{W}{m.K}$) [42].

Also, the results of calculating the thermal conductivity in different widths of the slit nanochannel are compared with the results of Bagheri and Kalteh's study [27], which was done using non-equilibrium molecular dynamics simulation. As seen in Fig. 3, a good agreement exists between the results of these two studies.

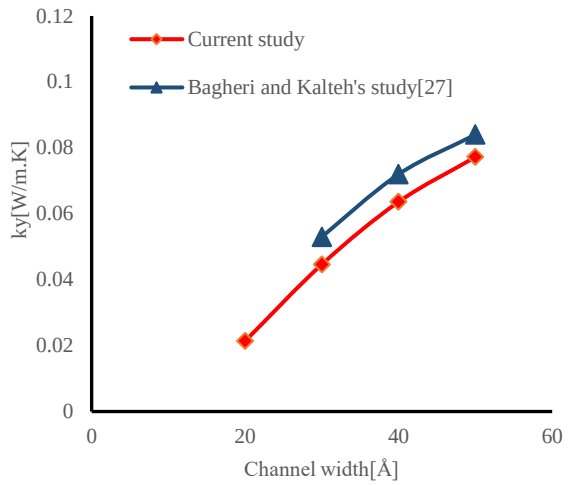


Fig. 3. Fluid thermal conductivity in slit nanochannels for various channel widths

The Effects of Nanochannel Shape and Size

As mentioned above, three types of channels including two parallel plates (slit channel), channel with a square cross-section and, also channel with a rectangular cross-section section are used to investigate the effects of nanochannel shape and size. Fig. 4 shows the fluid thermal conductivity in different nanochannel shapes for various nanochannel widths. The results show that the shape of the nanochannel change the fluid thermal conductivity. It is also found that the amount of thermal conductivity increases with the increase in the size of the nanochannel, but the rate of increase decreases with the increase of the channel width. For example, in a square channel, when the width of the nanochannel reaches from 20 angstroms to 30 angstroms, the thermal conductivity increase ratio is about 1.45, while when the nanochannel width reaches from 40 angstroms to 50 angstroms, the thermal conductivity increase ratio is about 1.07. Actually, by increasing the size, the walls affect a smaller part of the atoms.

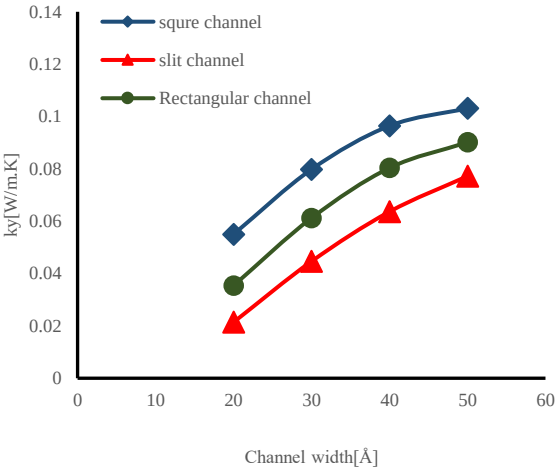


Fig.4. Fluid thermal conductivity in different nanochannel shapes for various channel widths

The walls are the main reason for thermal conductivity changes. Actually, the walls has two important effect on fluid atom behavior. They change the mobility and arrangement of fluid atoms in the nanochannel. In terms of mobility, the walls have a negative effect. Figs. 5 and 6 show the velocity graph of fluid atoms in the slit nanochannel with widths of 30Å and 50Å at iteration 1500000, respectively. As can be seen from the graphs, with the increase in the size, the mobility of atoms increases. This is due to the reduction of the effect of the wall on fluid particles. In fact, with the increase in the size of the nanochannel, the walls affect a smaller volume fraction of the fluid particles. Increasing the velocity of atoms increases the thermal conductivity of the fluid.

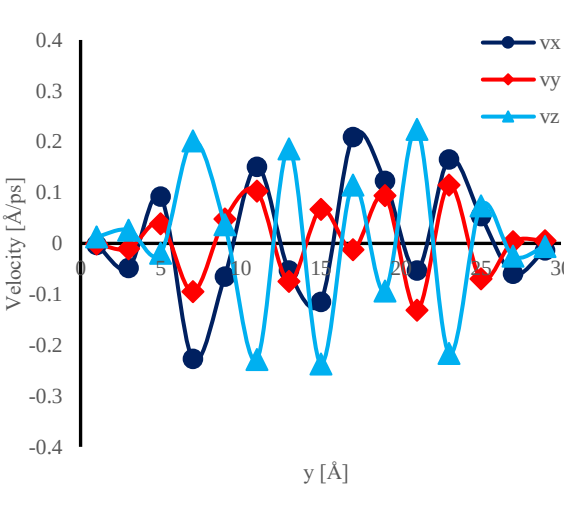


Fig. 5. Velocity graph for slit nanochannel with a width of 30Å at iteration 1500000

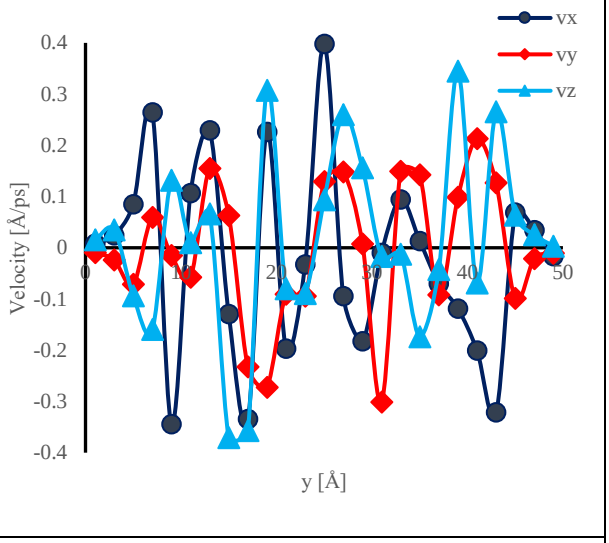


Fig. 6. Velocity graph for slit nanochannel with a width of 50Å at iteration 1500000

But in terms of the arrangement of the atoms, walls have two opposite effects depending on their orientation (perpendicular or parallel to the desired direction). This causes the thermal conductivity in the square nanochannel to be higher than that of the slit and rectangular nanochannels (see Fig. 4). Due to the strong interaction between the fluid atoms and the wall, the walls create a non-uniform distribution of fluid atoms in the nanochannel and fluid atoms accumulate near the walls. In the slit nanochannel, there are two walls perpendicular to the y direction (nanochannel width direction). The accumulation of fluid atoms near these walls causes an increase in the number of atoms in the upper and lower parts of the channel in the y direction and a decrease in their number in the middle of the channel. This reduces the heat flux transport power in the middle of the channel and the amount of thermal conductivity decreases. But in the square nanochannel, in addition to the two walls perpendicular to the y direction (nanochannel width direction), there are two other walls in the y direction. The existence of these two walls in the y direction causes an improvement in the distribution of atoms. This consequently improves the heat flux transport power in the middle of the channel and increases the thermal conductivity. In fact, it can be concluded that the presence of side walls (aligned with the desired direction) improves the distribution of atoms and subsequently improves thermal conductivity. In addition, it is concluded that the higher the ratio of the length of the side walls to the upper and lower walls, the higher the amount of thermal conductivity. So, its value for the rectangular nanochannel is higher than that of the slit nanochannel and lower than that of the square nanochannel. Fig. 7 shows the two-dimensional schematic of the distribution of atoms in the square channel.

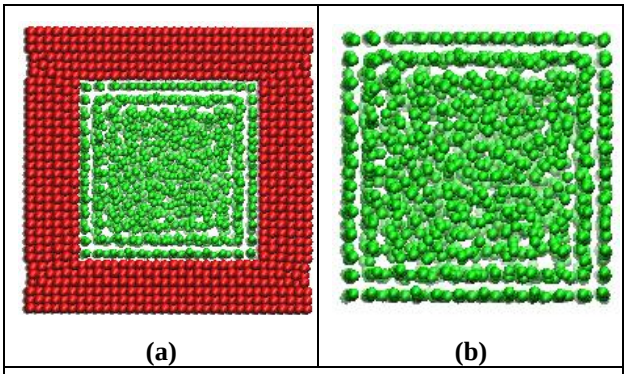


Fig. 7. Two-dimensional schematic of the distribution of atoms in the square channel. a) with walls b) without walls

Fig. 8 and Fig. 9 show the distribution of atoms in the slit and square nanochannel, respectively. As it is clear from Figs. 8 and 9, by increasing the width of the channel, the value of the number density increases in the middle of the channel and decreases near walls. Also, by comparing the channels with the same width, it is clear that in the square nanochannel, due to the side walls, the value of the number density in the middle of the channel is higher and lower in the vicinity of the walls.

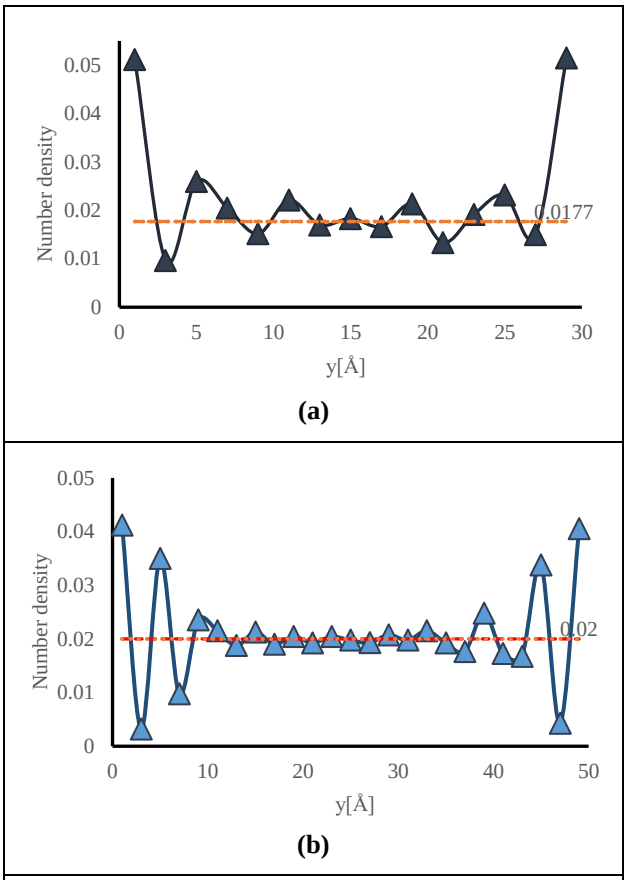


Fig. 8. Number density profile in the slit nanochannel with a width of a) 30Å b) 50Å

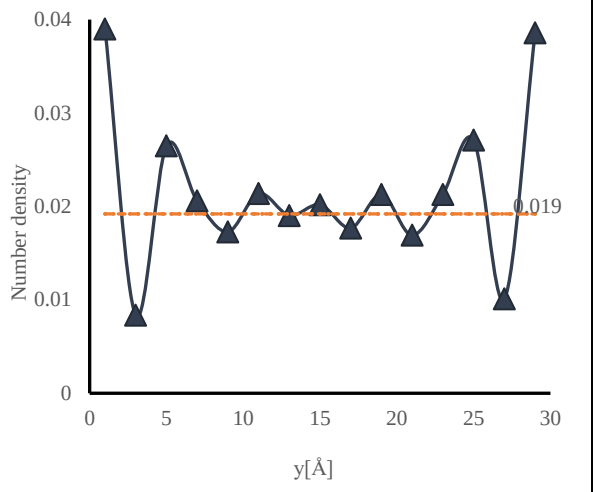


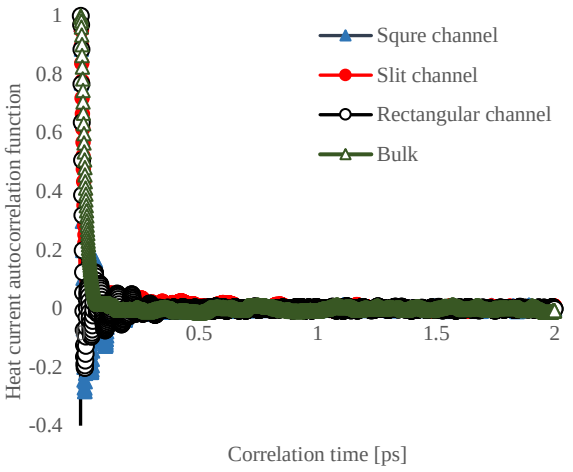
Fig. 9. Number density profile in the square nanochannel with a width of 30Å

The hydraulic diameter in a channel is obtained using $\frac{4A}{P}$, where A and P show the cross-sectional area and the perimeter of the channel, respectively. The results show that in the same hydraulic diameter, the amount of thermal conductivity in various channels is different. For example, the results of thermal conductivity for the hydraulic diameter of 40Å in slit, square and rectangular channels are shown in Table 1. As it is clear from Table 1, the thermal conductivity in the square channel is higher than in the slit and rectangular channels.

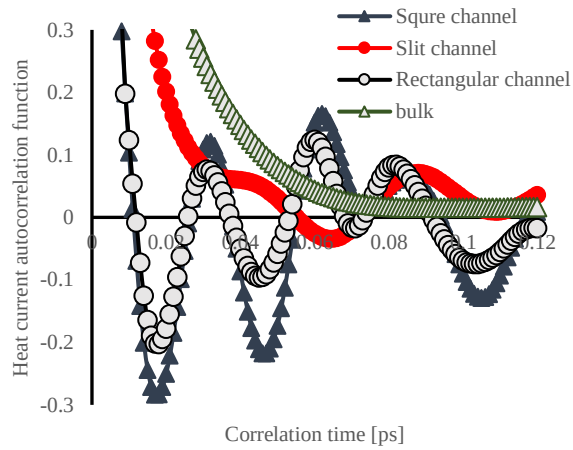
Table 1
Fluid thermal conductivity along the width for hydraulic diameter of 40Å in slit, square and rectangular channels

Type of channel	hydraulic diameter $\frac{4A}{P}$	L (channel width)	ky [W/m.K]
slit	$2L$	$2L = 40Å \rightarrow L = 20Å$	0.022
square	L	$L = 40Å$	0.096
rectangular	$\frac{4L}{3}$	$\frac{4L}{3} = 40Å \rightarrow L = 30Å$	0.061

The average the heat current over time is known as heat current autocorrelation function (HCACF) [43]. Fig. 10 shows the diagram of HCACF for the fluid in the bulk state and different nanochannels. The results show that in the bulk state, HCACF uniformly decays to zero, while it decays oscillatory to zero for the fluid in the nanochannel. Also, the results show that the HCACF remained correlated for a longer time in the square nanochannel than in the slit nanochannel. The thermal conductivity is obtained by integrating the HCACF. Therefore, in cases where fluctuations have long lifetimes and HCACF decays slowly, thermal conductivity has a higher value.



(a)



(b)

Fig. 10. a) HCACF decay with Correlation Time in different nanochannels. b) The initial part of HCACF graph for a better understanding

The effects of nanochannel surface wettability

To further evaluated the effect of the walls, the fluid-wall interaction strength is studied for three different values of energy including $\varepsilon_1 = \varepsilon_{Cu_Ar} = 10.4153 \times 10^{-21} J$, $\varepsilon_2 = \frac{1}{2}\varepsilon_{Cu_Ar}$ and $\varepsilon_3 = 2\varepsilon_{Cu_Ar}$ in a square nanochannel with a width of 30 angstroms. The results are presented in Table 2.

Table 2
Thermal conductivity of the fluid along the width of the square channel for the described conditions

Case study	ε_{wall_fluid}[J]	ky [W/m.K]
1	$\varepsilon_1 = \varepsilon_{Cu_Ar} = 10.4153 \times 10^{-21}$	0.079
2	$\varepsilon_2 = \frac{1}{2}\varepsilon_{Cu_Ar} = 5.2076 \times 10^{-21}$	0.103
3	$\varepsilon_3 = 2\varepsilon_{Cu_Ar} = 20.8306 \times 10^{-21}$	0.065

It is found that with increasing Cu_Ar interaction strength, the effect of the walls increases, and the thermal conductivity decreases, which is in accordance with the results obtained above. Figs. 11 and 12 show the number density and velocity graph of fluid atoms in the slit nanochannel with width of 30Å for $\varepsilon = \frac{1}{2}\varepsilon_{Cu_Ar}$. By comparing Figs. 11 and 8a (for ε_{Cu_Ar}), it is clear that with the decrease in the fluid-wall interaction strength, the amount of accumulation of fluid atoms near walls decreases, which leads to more uniformity in the distribution of fluid atoms. This causes more fluid atoms to be in the middle of the channel, which increases thermal conductivity. Also, by comparing Figs. 12 and 5, it is clear that by reducing the fluid-wall interaction strength, the effect of walls on the movement of atoms is reduced. Increasing the velocity of atoms increases the thermal conductivity.

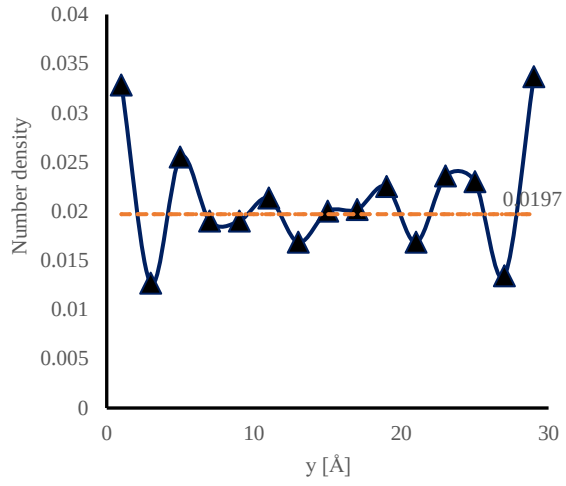


Fig. 11. Number density profile for slit nanochannel with a width of 30Å for $\boldsymbol{\varepsilon = \frac{1}{2}\varepsilon_{Cu_Ar}}$

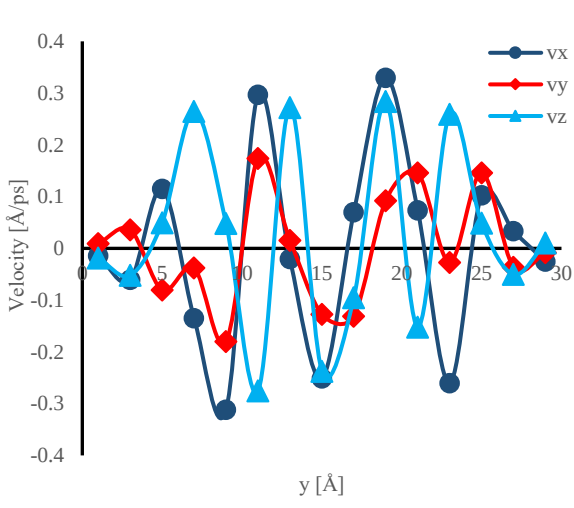


Fig. 12. Velocity graph for slit nanochannel with a width of 30Å for $\boldsymbol{\varepsilon = \frac{1}{2}\varepsilon_{Cu_Ar}}$ at iteration 1,500,000

CONCLUSION

In this study, thermal conductivity of the fluid in three nanochannel shapes, including slit, square and rectangular, is investigated, and the effect of shape, size, and surface wettability of nanochannel on its amount is studied. According to results, it is affected by the shape and size, which is caused by the effect of the walls on the mobility and arrangement of atoms in the nanochannel. The walls reduce the mobility of atoms and increase their accumulation in the vicinity of the surfaces. This is because the fluid-wall interaction is stronger than the fluid-fluid interaction. When the width of the nanochannel increases, the effect of the walls decreases. The results also show that the side walls improve the arrangement of atoms and subsequently the thermal conductivity. Therefore, its amount in the square nanochannel is higher than that of the slit nanochannel. It was also found that nanochannels with different shapes have a different thermal conductivity in the same hydraulic diameter. In addition, the results show that with the increase in the wettability of the nanochannel walls, the amount of thermal conductivity decreases, which is due to the greater effect of the walls on it. Also, the investigation of HCACF showed that its behavior is affected by the nanochannel and its shape. HCACF remained correlated for a longer time in the square nanochannel than in the slit nanochannel. Therefore, the thermal conductivity in the square nanochannel is higher than in the slit nanochannel.

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