

Effect of roughness geometry and temperature on adsorption of argon flow in Nano-channels: A molecular dynamics approach

Arman Salehi^{1,a}, Samrand Rash-Ahmadi^{1,b}

¹Department of Mechanical Engineering, Urmia University, Urmia, Iran

^aarmansalehi95@yahoo.com, ^bs.rashahmadi@urmia.ac.ir

Corresponding author: Samrand Rash-Ahmadi, s.rashahmadi@urmia.ac.ir

ABSTRACT Nanochannels have surface roughness due to their non-ideal surfaces. These roughnesses on the surface of nanochannels have an important effect on the flow behavior of argon atoms. This study examined the argon flow in nanochannels under various roughness geometries via molecular dynamics simulation. Also, the researchers investigated the adsorption rate, density, and diffusion of argon atoms under different temperatures and height roughness in nanochannels. The results showed that nanochannels with cylindrical roughness exhibit higher levels of interaction energy (adsorption) (-149 kcal/mol) and density (144 g/cm³) compared to nanochannels with square and conical roughness. Furthermore, as the height roughness of the nanochannels is increased (11 to 20 Å), the amount of adsorption (interaction energy) and density rise as well. By comparing the MSD (mean square displacement) diagram of nanochannels, the nanochannels with the highest diffusion of argon atoms have cone roughness in contrast to square and cylinder nanochannel roughness.

KEYWORDS adsorption; diffusion coefficient; roughness geometry; argon; nanochannels.

FOR CITATION Arman Salehi, Samrand Rash-Ahmadi Effect of roughness geometry and temperature on adsorption of argon flow in Nanochannels: A molecular dynamics approach. *Nanosystems: Phys. Chem. Math.*, 2026, **17** (4), 452–461.

1. Introduction

Over the past decade, significant advancements in nanoscale science have enabled researchers to investigate the behavior of nanofluid flow in nanochannels more precisely. Investigating fluid flow behavior in nanochannels is a highly practical and compelling issue [1–8]. Roughness is always present on the surface of nanochannels due to their non-ideality, significantly affecting the flow behavior of nanoparticles in nanochannels. Also, these roughnesses directly affect the adsorption and diffusion of nanoparticles in nanochannels. As a result, it is essential to investigate nanoparticle adsorption and diffusion in nanochannels. Compared to experimental methods, nano-scale simulation methods provide a cost-effective and highly accurate alternative, eliminating environmental errors and enabling researchers to precisely investigate particle flow behaviors in nanochannels. In previous studies on nanoparticle flow behavior in nanochannels, Chen et al. [9] found that an increase in obstacles in nanochannels leads to a change in the density of argon atoms from 0.099 to 0.093 atoms/Å³. Also, Pang et al.'s study [10] on the flow of gases in nanochannels with different geometries shows that the geometry of nanochannels has a significant effect on the speed of gas flow.

In a molecular dynamics study, Motlagh and Kalteh [11] investigated the convective heat transfer of argon in nanochannels with different roughness effects. Their results show that increasing the roughness in nanochannels raises the Nusselt number (displacement heat transfer). In another molecular dynamics study, Rashidi et al. [12] indicate that the roughness and unevenness of nanochannels reduce the fluctuations in the density of argon atoms. Also, increasing the height of the roughness results in a greater impact on the flow. In addition, the findings of the study by Motlagh and Kalte [13] on the behavior of argon poise flow in copper nanochannels reveal that the roughness of the nanochannels improves the heat transfer between the argon atoms and the walls of the nanochannels. In the same vein, it was demonstrated that the presence of aluminium nanoparticle barriers in zigzag nanochannels increases the density and temperature of argon fluid [14]. Increasing the surface roughness of nanochannels reduces the length of the thermal gradient and escalates the Nusselt number [15]. In addition, raising the number of layers in nanochannels increases nanofluids (accumulation) to the nanochannel wall [16]. Reducing the surface roughness in copper nanochannels enhances the average velocity of water nanofluid [17]. Furthermore, the results of the study by Meng et al. [18] show that by raising the roughness of nanochannels, the density of atoms increases and also improves heat transfer. In another study, Akbari et al. [19] demonstrated that wall temperature and obstacles in nanochannels significantly affect the flow parameters. Obstacles reduce the range of motion fluctuations of argon atoms and improve the thermal conductivity coefficient. The results of Qin et al. [20] show that the fluid growth rate of the hot wall is 10.5% higher than that of the cold wall in nanochannels. Among the nanostructures (square and triangular), the triangular nanostructure has the least resistance and friction against the flow. Furthermore, the presence of holes in the nanochannels causes the argon atoms to absorb additional energies

from the walls of the nanochannels, which improves the heat transfer efficiency [21]. In a molecular dynamics study on copper/argon nanochannels, Akbari et al [22] show that with larger barriers in the structure of nanochannels, the attractive force is stronger compared to smooth nanochannels (increase in the density of argon atoms around 17.3%). The roughness of the surfaces in the nanochannels can prevent the reduction of the pressure drop [23]. Another study shows that the fluid viscosity and, consequently, the flow resistance in a nanochannel can be modified by changing the material of the nanochannel walls [24]. In the present study, we used molecular dynamics simulation to examine the adsorption rate, diffusion, and density of argon flow in nanochannels with different surface roughness (square, cone, smooth, cylinder) and temperatures. Given the significance of this subject and the findings of previous studies, it was imperative to investigate these parameters.

2. Method and simulation

The nanochannels are modeled with argon flow using Lammmps molecular dynamics simulation software [25]. The dimensions of the nanochannels are modelled as $100 \times 100 \times 240$ Angstrom. Each nanochannel contains 500 argon atoms. Also, nanochannels have different roughness geometries, including conical, square, cylindrical and smooth (without roughness). The nanochannel surface was designed as a square area of 100×100 Å and was divided into four equal sections to incorporate roughness geometries. Three different roughness shapes were modeled: a square with dimensions of 10×10 Å, a cylinder with a diameter of 10 Å, and a cone with a base diameter of 10 Å. For each geometry, roughness heights of 11, 14, 17, and 20 Å were considered. The roughness structures were arranged such that the center-to-center distance between adjacent geometries was 50 Å. Also, these roughnesses are created on both sides of the bottom and top of the nanochannel as four pieces in the nanochannels. Fig. 1 shows the graphical output of different nanochannels under different roughnesses. The simulation system is configured as an NVT ensemble with constant atom number, constant volume, and temperature. The pressure of argon inside the nanochannels was maintained at 1 atmosphere, and the simulations were conducted at a temperature of 125 K. The temperatures of the nanochannel walls and the argon fluid were assumed to remain identical throughout the simulation. Furthermore, the system energy was equilibrated using the energy minimization command. Additionally, the boundary conditions in both the X and Y directions of the nanochannels are assumed to be periodic. Also, run repetitions and the rate of time steps were considered to be 200,000 and 0.001 for all the simulations, respectively. Also, the total simulation time lasted 300 picoseconds.

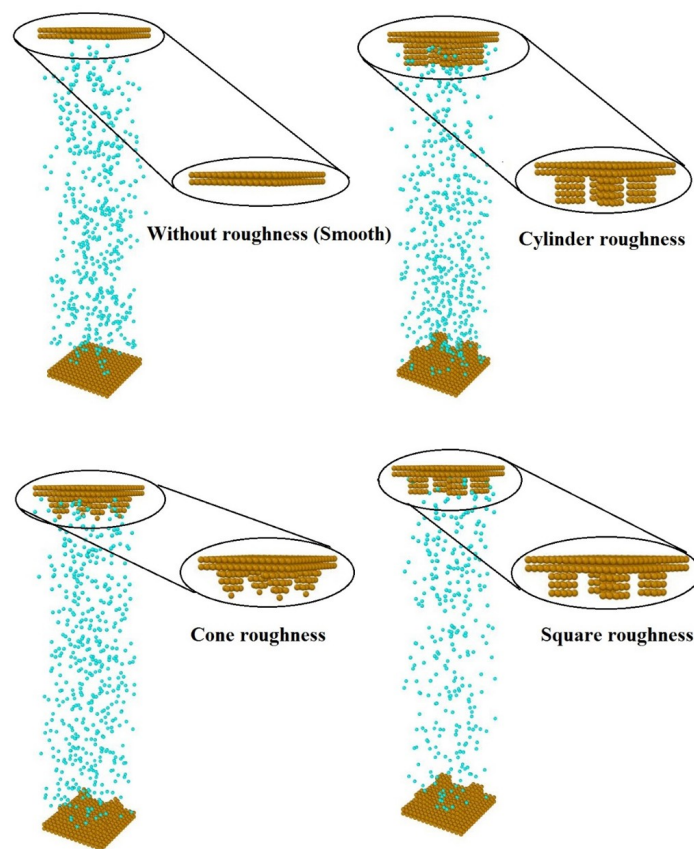


FIG. 1. The graphical output of different nanochannels under different roughnesses

2.1. Force fields

The nanochannels were composed of platinum metal (Pt) atoms, and the interaction between atoms was defined using the EAM force potential [26]. Equation 1 presents the EAM force potential.

$$E_i = F_\alpha \left(\sum_{i \neq j} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{i \neq j} \phi_{\alpha\beta}(r_{ij}). \quad (1)$$

In this equation, E_i represents the total energy. F_α is the embedded energy. r_{ij} shows the distance between two atoms of i and j . Also, the Lennard-Jones potential [27] was used to define the interaction between argon atoms and platinum atoms of nanochannels. The force potential equation of Leonard-Jones is given in Equation 2.

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

In this Equation, R_c is the cutoff radius, r is the distance between atoms, ε is the interaction strength ratio, and σ represents the diameter of the atom. Also, the cutoff radius of 4.5 Å was considered in this simulation. The Velocity-Verlet algorithm was employed to solve Newton's equations of motion [28]. This algorithm numerically integrates the trajectories of particles over successive time steps (Δt) in molecular dynamics simulations. The positions and velocities of the particles are updated through three sequential steps using Equations 3 and 4.

$$r(t + \Delta t) = r(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2, \quad (3)$$

$$v(t + \Delta t) = v(t) + \frac{1}{2}[a(t) + a(t + \Delta t)]\Delta t. \quad (4)$$

2.2. Calculation of system density (Argon density) in Z direction

Equation (5) was used to calculate the system density in the Z direction by dividing the total sampled mass within a given bin by the volume of that bin. $N_{Samples}$ is the number of sampled atoms (Argon atom) in the specific Z-slab. N_A The Avogadro constant $6.022 \times 10^{23} \text{ mol}^{-1}$ used to convert from moles to individual atoms. L_x and L_y represent the length dimensions in the X and Y directions, respectively. M denotes the mass of the Atoms (mass of the argon atom (39.95 g/mol)), N_z represents the number of available atoms.

$$\rho(z) = \frac{N_{Zi}(z)m\sigma^3 M}{N_{Sample}L_xL_y\Delta z\sigma^3 N_A}. \quad (5)$$

The number of available argon atoms (N_z), represent the total number of argon atoms within the entire simulation box, while the thickness of the sampled region corresponds to the thickness of the Z-direction slab.

2.3. Calculation of the interaction energy between argon atoms and nanochannels

Equation (6) is recruited in order to calculate the amount of interaction energy for adsorption. According to Equation (6), the interaction energy is determined by subtracting the total potential energy of the system (nanochannel with argon atoms) from the potential energy of argon atoms and the nanochannel separately. As a result, the obtained value shows the amount of surface adsorption of argon atoms to the nanochannels. As the negative value of the interaction energy increases, the surface absorption also intensifies [29].

$$E_{interaction} = E_{Pt/Ar} - (E_{Pt} + E_{Ar}). \quad (6)$$

2.4. Calculation of mean square displacement (MSD)

Equations (7) and (8) show the mean square displacement equation, which refer the diffusion of argon atoms to the surface of nanochannels by using the slope of the MSD diagram [30].

$$MSD = \frac{1}{N} \sum_{i=1}^N (R_{i(t)} - R_{0(t)})^2, \quad (7)$$

$$D = \frac{1}{6} \lim_{t \rightarrow \infty} \frac{d}{dt}(MSD). \quad (8)$$

In these equations, N denotes the number of atoms in the system and R_i represents the distance.

2.5. Radial distribution function (RDF)

Equation (9) presents the radial distribution function, which indicates the probability of finding argon atoms near platinum atoms at a distance r from each other.

In this equation, V is the total volume of the system. dr is the thickness of the spherical shell used to sample atom positions [31]. Also, the radial displacement function (RDF) was considered for argon atoms with the upper rough wall surface of the nanochannels.

$$g(r) = \frac{V}{4\pi r^2 dr} \quad (9)$$

3. Results and discussion

3.1. Investigating the effect of different roughness geometries in nanochannels

Figure 2 shows the diagram of the amount of interaction energy between argon atoms and different roughness geometries in nanochannels. According to Fig. 2, the interaction energy of the cylinder roughness geometry is higher than that of the cone and square roughness geometries over time. This means the nanochannel with cylinder roughness adsorption (-149 kcal/mol) has more argon atoms than the nanochannel with cone and square roughness. Also, the lowest amount of adsorption (interaction energy) is related to smooth nanochannels (without roughness) which adsorb the least amount of argon atoms.

In addition, Fig. 2b shows the density distribution of argon within the nanochannels. The argon density varies because the nanochannels were considered periodic condition in the X and Y directions, and the geometry of the surface roughness along the Z direction influences surface adsorption and the local argon density. As shown in Fig. 2b, the argon density is higher near the beginning and end regions of the nanochannel along the Z direction, where rough surfaces with different geometries are present. This increase in density is attributed to the stronger adsorption of argon atoms on the rough surfaces. In contrast, in the central region of the nanochannel, the argon density decreases significantly. Also, Fig. 2b shows the density along the Z-direction of different nanochannels under different roughness geometries. Based on this diagram, at the beginning and end of the nanochannel where roughnesses exist, the density in these two regions is higher than that in other regions of the Z direction. The nanochannels with cylinder roughness geometry have the highest density (144 g/cm³) of argon atoms compared to cone and square roughness geometries. This occurs due to the geometry of the cylinder roughness, the nanochannel with cylinder roughness have more adsorption of argon atoms than the other nanochannels. As a result, the nanochannel with cylinder roughness have a higher density of argon atoms than the other nanochannels. Also, it is observed that the lowest density of argon atoms belongs to smooth nanochannels (without roughness).

According to the graphs in Fig. 2, parts a and b, it can be seen that, compared to cone and square roughness geometry, nanochannels with a cylinder roughness geometry have the greatest effect on the flow of argon atoms. Therefore, this effect results in a greater adhesion of argon atoms to the surface of the nanochannels. Nanochannels with conical roughness exhibited the lowest surface adsorption and density compared to other nanochannels. Nanochannels with triangular roughness have the least effect on the flow of argon atoms due to less friction and impact on argon atoms [20].

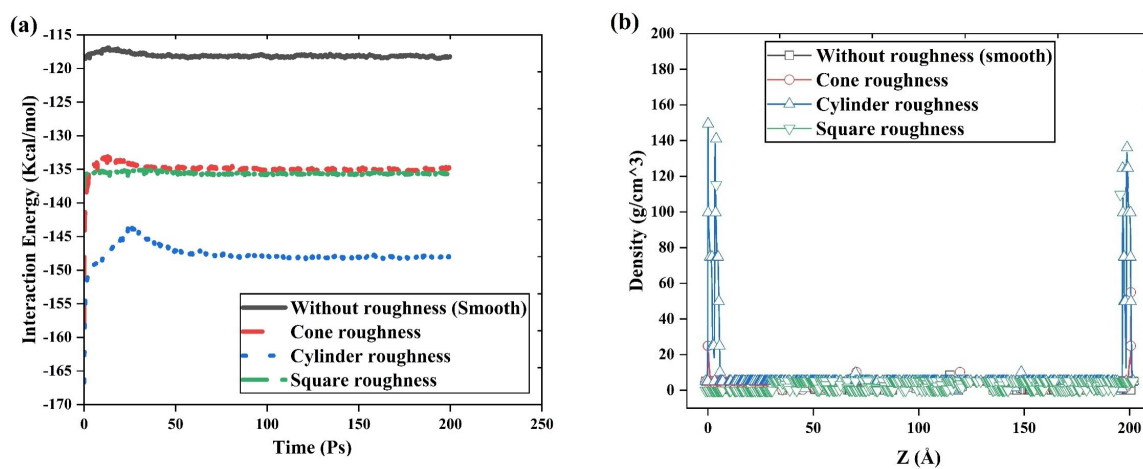


FIG. 2. Diagrams of the amount of (a) interaction energy (b) Density between argon atoms and different roughness geometries in nanochannels at a temperature of 125 K

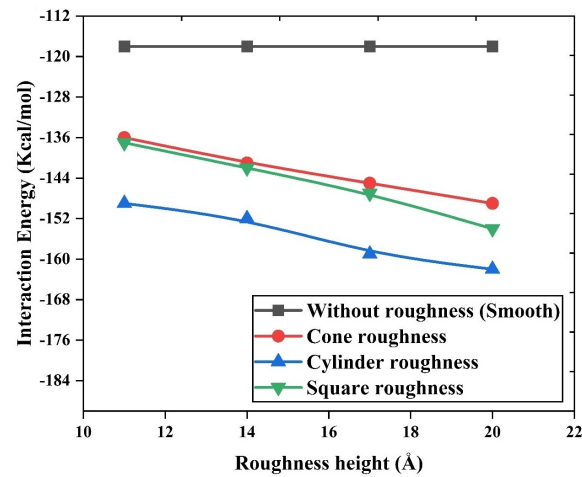


FIG. 3. The amount of interaction energy changes according to the different heights of roughness at a temperature of 125 K and at 1 atm

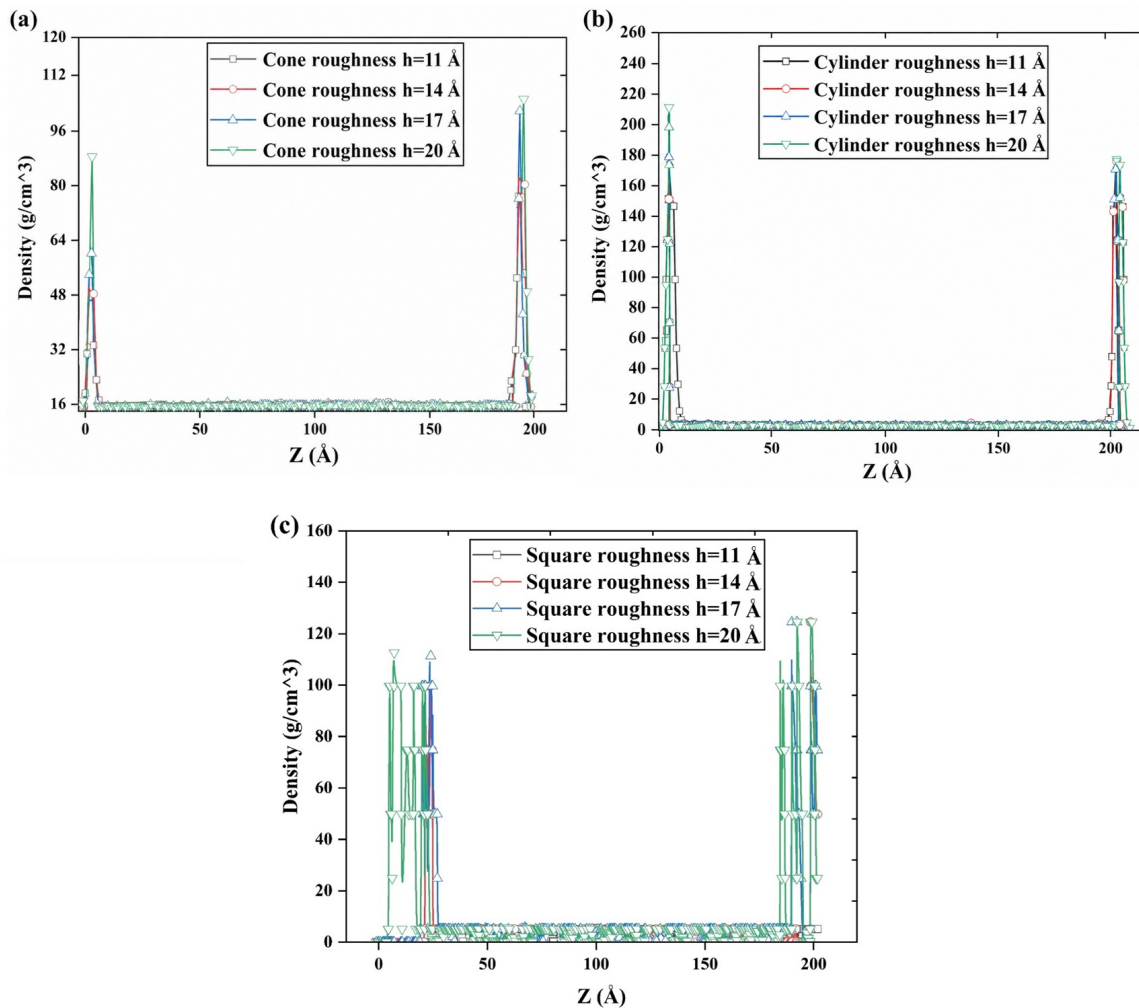


FIG. 4. The density with the increase of height roughness of the nanochannels in the Z direction (a) Cone roughness (b) Cylinder roughness (c) Square roughness at a temperature of 125 K

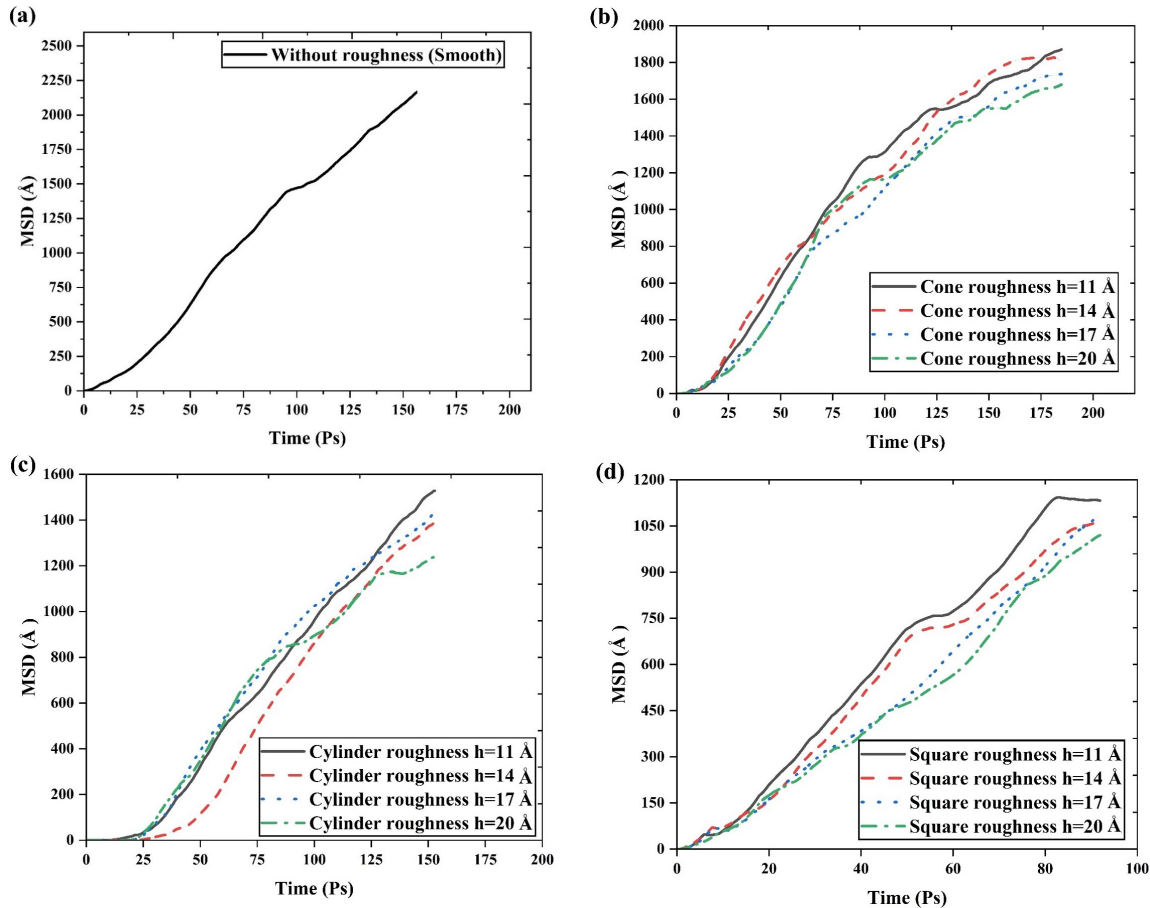


FIG. 5. The Mean Square Displacement (MSD) diagram based on different height roughness. (a) Without roughness (b) Cone roughness (c) Cylinder roughness (d) Square roughness at a temperature of 125 K

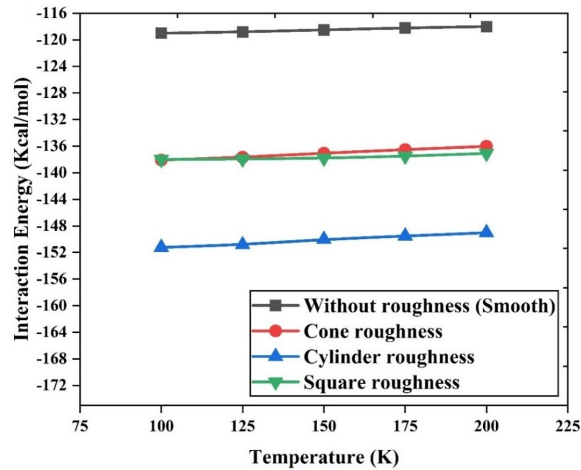


FIG. 6. The amount of interaction energy in terms of different temperatures in nanochannels

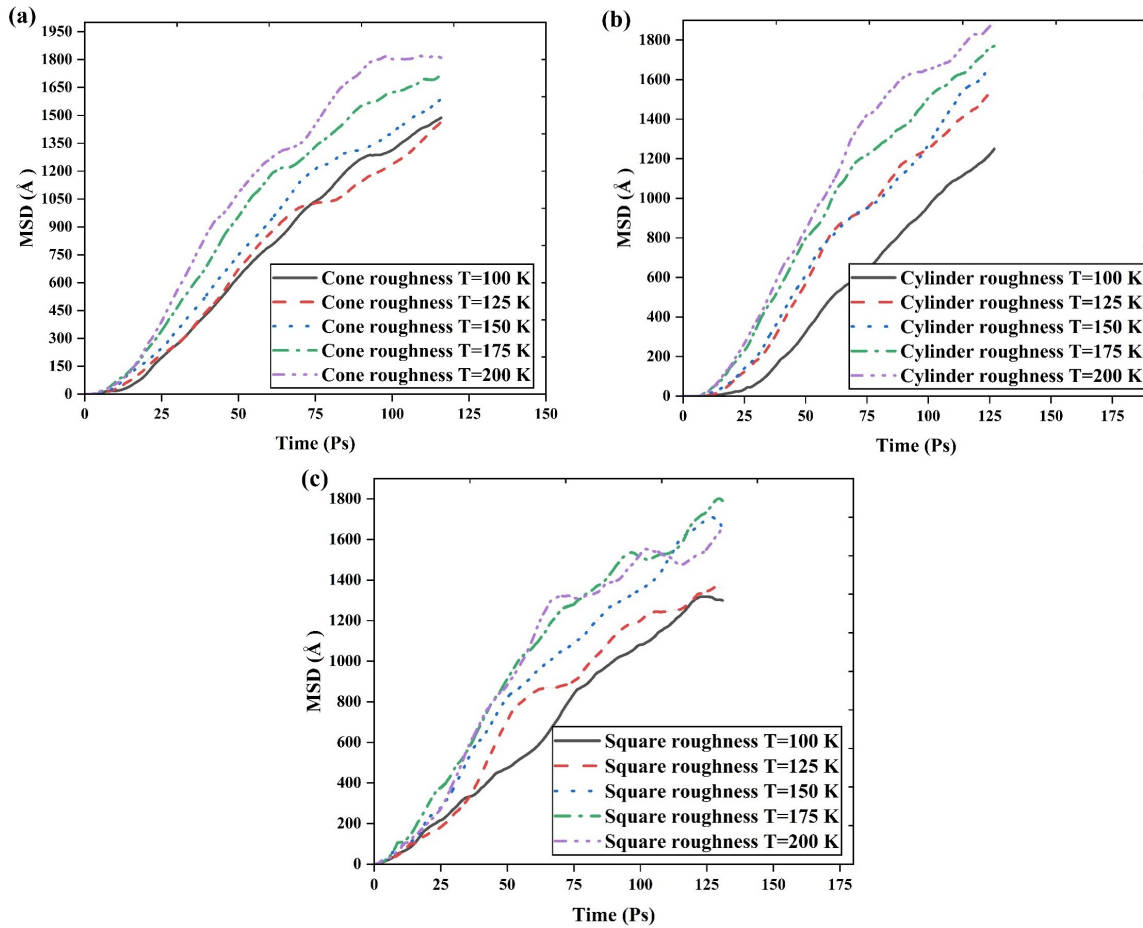


FIG. 7. The Mean Square Displacement (MSD) diagram of argon atoms in nanochannels under different temperatures

3.2. Investigating the effect of height roughness in nanochannels

The diagram in Fig. 3 shows the amount of interaction energy changes according to the different heights of roughness. According to Fig. 3, the interaction energy (adsorption) increases with the greater height of nanochannel roughness. As the height of roughness increases, among the nanochannels those with cylinder roughness exhibit the highest level of adsorption in comparison to cone and square roughness variations. This occurs due to the geometry of the cylinder roughness, as increasing the height roughness of nanochannels with cylinder roughness have more friction between argon atoms and nanochannels. Also, the lowest amount of adsorption (interaction energy) is related to nanochannels with cone roughness. Also, in general, the increase in interaction energy with increasing roughness height can be attributed to enhanced friction and greater contact between the rough surfaces and argon atoms. In addition, Fig. 4 diagrams a, b, and c illustrate the highest density with the increase of height roughness at the beginning and end of the nanochannels in the Z direction. By increasing the height of the roughness in nanochannels ($h = 11 \text{ Å}$ to $h = 20 \text{ Å}$), the density rises. The highest density profile occurs at the roughness height $h = 20 \text{ Å}$. On the other hand, the lowest density corresponds to $h = 11 \text{ Å}$.

3.3. Investigating the effect of roughness height on the diffusion of argon atoms

Figure 5 shows the Mean Square Displacement (MSD) diagram based on different height roughness. According to Fig. 5, the diffusion of argon atoms decreases as the nanochannel height roughness (11 Å to 20 Å) increases. By comparing the diffusion of nanochannels, smooth (without roughness) and cone-shaped nanochannels exhibit higher diffusion rates than other nanochannels. Compared to other types (square and cylinder), the higher diffusion of cone and smooth roughness is due to their peak-like geometry which results in less contact and friction with argon atoms. However, square and cylinder roughness geometry have the most friction and impact. This is because the diffusion of cone roughness geometry is higher than square and cylinder roughness. Surface roughness is directly correlated with the diffusion of nanoparticles. Diffusion increases as the diameter of the surface geometry decreases [32].

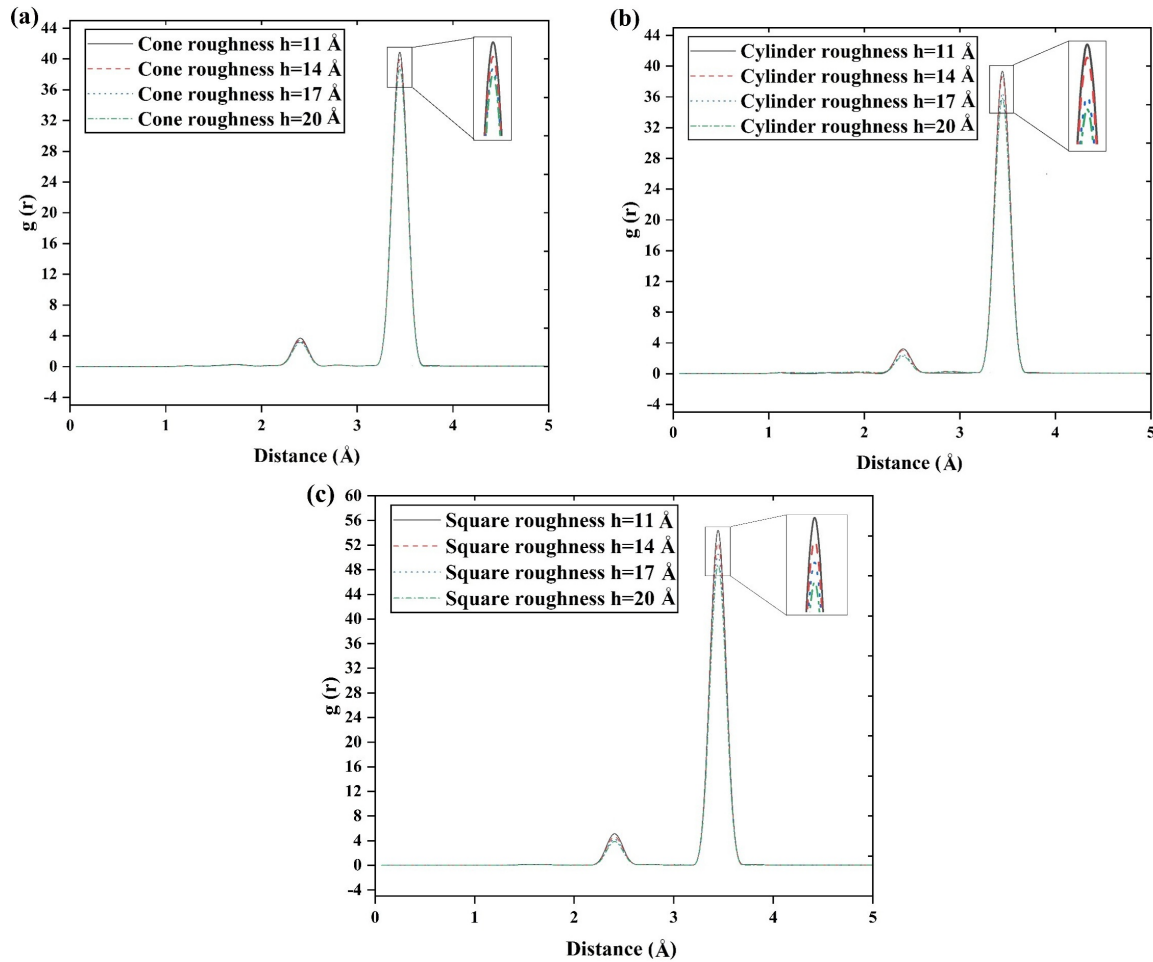


FIG. 8. The radial distribution function between the argon atom and the platinum atom under different heights of roughness

3.4. Investigating the effect of different temperatures on the adsorption and diffusion of argon atoms in nanochannels

Figure 6 depicts the amount of interaction energy in terms of different temperatures in nanochannels. Also, the interaction energy (adsorption) between argon atoms and nanochannels decreases as the temperature increases. The decrease in adsorption and adhesion between argon atoms and nanochannels is due to the increase in kinetic energy and mobility of argon atoms in nanochannels [33]. A rise in temperature causes an increase in the kinetic energy and speed of argon atoms in nanochannels, which reduces the adhesion (adsorption) of argon atoms to the surface of nanochannels. In addition, Fig. 7 shows the diffusion of argon atoms in nanochannels under rough geometries and different temperatures. According to Fig. 7, with escalating the temperature, the diffusion of argon atoms in nanochannels increases. The results of these graphs are in agreement with the findings of liquid aluminum diffusion to the copper surface by Mao et al. [34] under different temperatures. The reason for the rise in diffusion with increasing temperature is due to that temperature escalates the kinetic energy and mobility of argon atoms, which raises the diffusion of argon to the rough surface of nanochannels.

3.5. Investigation of radial distribution function (RDF) between argon and platinum atoms

Figure 8 shows the radial distribution function between the argon atom and the platinum atom (under different heights of roughness). According to Fig. 8, parts a, b, and c, the distance between argon atoms and platinum atoms is around 3.5 Å, which agrees with the results of the RDF diagram of the distance between argon atoms and platinum atoms by Zeng et al [35]. In RDF diagrams, as the distance increases, the simulation system's $g(r)$ tends to reach equilibrium [36]. According to the diagrams in Fig. 8, the simulation system has reached equilibrium, and $g(r)$ tends to a constant number as the distance increases. Also, with the rise in the height of the roughness of the nanochannels, the proximity between argon atoms and platinum atoms decreases.

4. Conclusion

In this study, molecular dynamics simulation has been used to investigate the behavior of argon flow in nanochannels under different roughness geometries. The effect of temperature, and height roughness on diffusion and adsorption of argon atoms in nanochannels was investigated. The results indicate that the interaction energy (adsorption) in nanochannels is higher in cylinder roughness geometry compared to square and cone roughness geometries. Also, the lowest adsorption of argon atoms belongs to smooth nanochannels (without roughness). Furthermore, the highest amount of density in the nanochannels at the beginning and end of the nanochannels in the z direction was related to the nanochannels with cylinder roughness. In addition, as the roughness of the nanochannels increases, the amount of adsorption and density increases as well. Moreover, with the rise in height roughness, the diffusion of argon atoms in nanochannels decreases. By comparing nanochannels with different roughness geometries, nanochannels with cone and smooth roughness (without roughness) have more diffusion than square and cylinder roughness geometries. In addition, increasing the temperature decreases the surface adsorption between nanochannels with argon atoms. Besides, with escalating the temperature, the diffusion of argon atoms in different nanochannels increases.

References

- [1] Ghahremanian S., Abbassi A, Mansoori Z, Toghraie D. Molecular dynamics simulation of annular condensation of vapor argon through a nanochannel for different saturation conditions with focusing on the flow and heat transfer. *International Communications in Heat and Mass Transfer*, 2020, **116**, P. 104704.
- [2] De La Escosura-Muñiz, A. Merkoçi, A. Nanochannels preparation and application in biosensing. *ACS nano*. 2012, **6**(9), P. 7556–83.
- [3] Sun Q., Zhao Y., Choi K.-S., Mao X. Molecular dynamics simulation of liquid argon flow in a nanoscale channel. *International Journal of Thermal Sciences*, 2021, **170**, P. 107166.
- [4] Zhang X., Liu H., Jiang L. Wettability and applications of nanochannels. *Advanced materials*, 2019, **31**(5), P. 1804508.
- [5] Rudyak V.Y., Belkin A., Egorov V.V., Ivanov D.A. Simulation of flows in nanochannels by the molecular dynamics method. *Nanosystems: Physics, Chemistry, Mathematics*, 2025, **2**(4), P. 100-12.
- [6] Lukashenko S.Y., Gorbenko O.M., Felshtyn M.L., Sapozhnikov I.D., Pichakhchi S.V., Zhukov M.V., et al. Effect of nanoscale water media confinement on the approach curve in SICM. *Nanosystems: Physics, Chemistry, Mathematics*, 2026, **16**(6), P. 770-7.
- [7] Rudyak V.Y., Lezhnev E.V. Modeling the rarefied gas thermal conductivity in nanochannels. *Nanosystems: Physics, Chemistry, Mathematics*, 2023, **14**(2), P. 186–94.
- [8] Rudyak V.Y., Lezhnev E.V. Viscosity of gases in nanochannels. *Technical Physics Letters*, 2020, **46**(10), P. 1045-8.
- [9] Chen J., Saleh Z.M., Saadon N., Zahra M.M.A., Said M.G., Altamari U.S., et al. Molecular dynamics simulation of obstacle number effect on heat and mass transfer of argon flow inside the platinum nanochannels. *Journal of Molecular Liquids*, 2022, **363**, P. 119871.
- [10] Pang Y., Fan D., Chen S. A novel approach to predict gas flow in entire knudsen number regime through nanochannels with various geometries. *SPE Journal*, 2021, **26**(05), P. 3265-84.
- [11] Motlagh M.B., Kalteh M. Investigating the wall effect on convective heat transfer in a nanochannel by molecular dynamics simulation. *International Journal of Thermal Sciences*, 2020, **156**, P. 106472.
- [12] Rashidi M.M., Ghahremanian S., Toghraie D., Roy P. Effect of solid surface structure on the condensation flow of Argon in rough nanochannels with different roughness geometries using molecular dynamics simulation. *International Communications in Heat and Mass Transfer*, 2020, **117**, P. 104741.
- [13] Motlagh M.B., Kalteh M. Molecular dynamics simulation of nanofluid convective heat transfer in a nanochannel: Effect of nanoparticles shape, aggregation and wall roughness. *Journal of Molecular Liquids*, 2020, **318**, P. 114028.
- [14] Bantan R.A., Abu-Hamdeh N.H., Nusier O.K., Karimipour A. The molecular dynamics study of aluminum nanoparticles effect on the atomic behavior of argon atoms inside zigzag nanochannel. *Journal of Molecular Liquids*, 2021, **331**, P. 115714.
- [15] Song Z., Cui Z., Cao Q., Liu Y., Li J. Molecular dynamics study of convective heat transfer in ordered rough nanochannels. *Journal of Molecular Liquids*, 2021, **337**, P. 116052.
- [16] Shen X.-Y., Hekmatifar M., Shukor M.Y.A., Alizadeh Aa, Sun, Y.-L., Toghraie D., et al. Molecular dynamics simulation of water-based Ferro-nanofluid flow in the microchannel and nanochannel: effects of number of layers and material of walls. *Journal of Molecular Liquids*, 2021, **338**, P. 116924.
- [17] Yan S.-R., Toghraie D., Hekmatifar M., Miansari M., Rostami S. Molecular dynamics simulation of Water-Copper nanofluid flow in a three-dimensional nanochannel with different types of surface roughness geometry for energy economic management. *Journal of Molecular Liquids*, 2020, **311**, P. 113222.
- [18] Meng S., Zhang L., Ma X., Cao Q., Wang B., Gong H., et al. Heat transfer characteristics in nanochannels with rough walls based on capillary flow: A molecular dynamics study. *International Communications in Heat and Mass Transfer*, 2023, **147**, P. 106983.
- [19] Akbari O.A., Saghafian M., Shirani E. Investigating the effect of obstacle presence on argon fluid flow characteristics in rough nanochannels using molecular dynamics method. *Journal of Molecular Liquids*, 2023, **386**, P. 122462.
- [20] Qin S., Chen Z., Wang Q., Li W., Xing H. Effect of surface structure on fluid flow and heat transfer in cold and hot wall nanochannels. *International Communications in Heat and Mass Transfer*, 2024, **151**, P. 107257.
- [21] Miao S., Xia G. Molecular dynamics investigation of the effect of nanostructured surfaces on flow boiling. *Journal of Molecular Liquids*, 2024, **400**, P. 124457.
- [22] Akbari O.A., Shirani E., Saghafian M. Investigating the temperature distribution behavior and flow parameters of argon fluid in a nanochannel with changing dimensions of the obstacle using the molecular dynamics (MD) method. *Heliyon*, 2024, **10**(2).
- [23] Cao C., Chang B., Yang Z., Yong L., Li C. A transient nanoscale flow model for alkanes considering inhomogeneous flow properties and rough surfaces. *Journal of Molecular Liquids*, 2024, P. 125145.
- [24] Rudyak V., Belkin A. Molecular dynamics simulation of fluid viscosity in nanochannels. *Nanosystems: Physics, Chemistry, Mathematics*, 2018, **9**(3), P. 349-55.
- [25] Plimpton S. Fast parallel algorithms for short-range molecular dynamics. *Journal of computational physics*, 1995, **117**(1), P. 1–19.
- [26] Daw M.S., Baskes M.I. Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. *Physical review B*, 1984, **29**(12), P. 6443.

- [27] Jorgensen W.L., Chandrasekhar J., Madura J.D., Impey R.W., Klein M.L. Comparison of simple potential functions for simulating liquid water. *The Journal of chemical physics*, 1983, **79**(2), P. 926-35.
- [28] Allen M.P., Tildesley D.J. *Computer simulation of liquids*. Clarendon Press Oxford, P. 1987.
- [29] Salehi A., Rash-Ahmadi S. Effect of adsorption, hardener, and temperature on mechanical properties of epoxy nanocomposites with functionalized graphene: A molecular dynamics study. *Journal of Molecular Graphics and Modelling*, 2022, **117**, P. 108311.
- [30] Frenkel D., Smit B. *Understanding molecular simulation: from algorithms to applications*. Elsevier, 2023.
- [31] Wang Y., Yang G., Wang W., Zhu S., Guo L., Zhang Z., et al. Effects of different functional groups in graphene nanofiber on the mechanical property of polyvinyl alcohol composites by the molecular dynamic simulations. *Journal of Molecular Liquids*, 2019, **277**, P. 261-8.
- [32] Ledesma-Durán, A., Juárez-Valencia, L.H. Diffusion coefficients and MSD measurements on curved membranes and porous media. *The European Physical Journal E*, 2023, **46**(8), P. 70.
- [33] Salehi A., Rash-Ahmadi S. Effect of temperature and oxygen functional groups on interaction between epoxy resins and graphene surface. Proceedings of the Institution of Mechanical Engineers, Part C: *Journal of Mechanical Engineering Science*, 2023, **237**(4), P. 941-51.
- [34] Mao A., Zhang J., Yao S., Wang A., Wang W., Li Y., et al. The diffusion behaviors at the Cu-Al solid-liquid interface: A molecular dynamics study. *Results in Physics*, 2020, **16**, P. 102998.
- [35] Zeng K., Smaït D.A., Mohammed A.Q., Kadim A.M., AL-Khafaji R.M., Izzat S.E., et al. Numerical study of obstacle effect on atomic behavior of argon fluid flow inside a nanochannel with molecular dynamics approach. *Journal of Molecular Liquids*, 2022, **363**, P. 119954.
- [36] Salehi A., Ghaderiazar N., Rash-Ahmadi S. Investigation of thermal conductivity and mechanical properties in multi-layer of graphene and graphene oxide: a molecular dynamics study. *Molecular Simulation*, 2024, P. 1–15.

Submitted 15 May 2026; revised 24 June 2026; accepted 1 July 2026

Information about the authors:

Arman Salehi – Department of Mechanical Engineering, Urmia University, Urmia, Iran; ORCID 0000-0003-4785-0005; armansalehi95@yahoo.com

Samrand Rash-Ahmadi – Department of Mechanical Engineering, Urmia University, Urmia, Iran; ORCID 0000-0002-4719-7926; s.rashahmadi@urmia.ac.ir

Conflict of interest: the authors declare no conflict of interest.