Characteristics of Nano-Structures

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Abstract

The investigation into the behavior of the fluids in nanoscale channels, such as carbon nanotubes leads us to a new approach in the field of nanoscience. This is referred to as nano-fluidics, which can be used in nano-scale filtering and as nano-pipes for conveying fluids. The behavior of fluids in nano-fluidic devices is very different from the corresponding behavior in microscopic and macroscopic channels. In this study, we investigate the fluid flow through carbon nanotubes and graphene based nanostructures using a molecular dynamics (MD) method at a constant temperature.Three different models were created which contain single-walled carbon nanotube, graphene, and a combination of both. Liquid argon is used as fluid in the system. We employed a new approach to make a continuum flow to find out how the physical quantities such as, position, velocity, and pressure change when the fluid flow reaches the confinements of the systems. Helical pattern of the fluid flow inside the nanotube was one of the interesting points of our results which has been observed. In addition to this, the rate of changing of the flow velocity and its direction via using vector plots has been demonstrated. At last, pressure drop according to the structure of the model in the vicinity of the confinements has been reported.

Introduction

Model

A rectangular box of a $400,000\ (A^0)^3$ volume with a graphene wall at the end of it was created for all of the three models. This wall moves with a constant velocity $18\ \frac{A^0}{\mu s}$ towards the confinements of the system. Carbon nanotube, graphene wall, and a combination of both were employed as the confinements of the models. Liquid argon is used as fluid of the system. To investigate the interactions between carbon and argon atoms, a molecular dynamics simulation with 1.2×10^6 time steps was employed. Using velocity re-scaling thermostat, the temperature was kept at $85\ K$. Standard Lennard-Jones potential with cut-off radius 2.5σ is used as the inter-particle potential between a pair of atoms. Since the structures of the models are rigid, only Lennard-Jones potentials between argon atoms and between carbon and argon pairs need to be considered in the simulations.

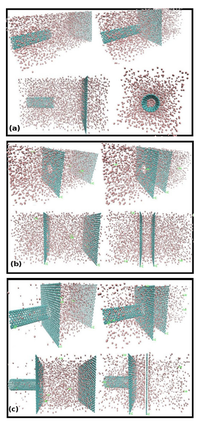
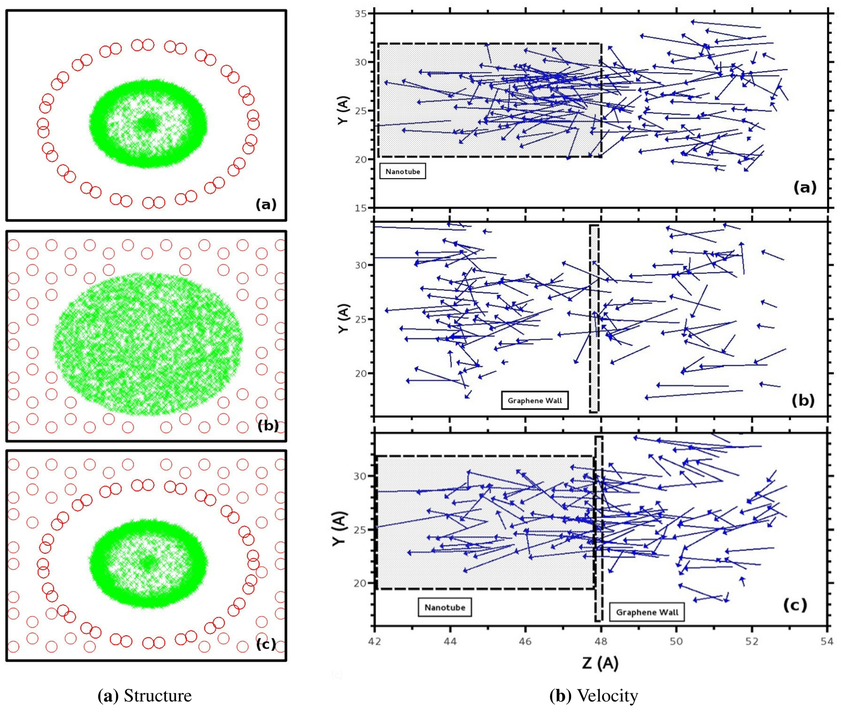


Figure 1: Snap shot of the various stages of transport of argon atoms through the confinements while graphene wall moves towards the structures. (a), (b), and (c) correspond to the Model-1, Model-2, and Model-3 respectively. Blue atoms are considered as carbon atoms, and pink atoms are presented argon atoms.

Interaction/Parameters	$\sigma[A^0]$	$\epsilon[J]$
Argon-Argon	3.8388	1.209846×10^{-21}
Argon-Carbon	3.573	1.9646×10^{-21}

Table 1: Lennard-Jones parameters for different possible interactions.

Structure & Velocity



(a) Structure **(b)** Velocity

Figure 2: Structure: Cross section area of the models during the simulations while graphene wall moves towards the structures. (a), (b), and (c) correspond to the top view of the Model-1, Model-2, and Model-3 respectively. Red atoms are considered as carbon atoms, and green atoms are represented argon atoms.
Velocity: Vector plot of the flow for models during the simulations while graphene wall moves towards the structures. (a), (b), and (c) correspond to the side view of the Model-1, Model-2, and Model-3 respectively. Blue arrows are representing argon atoms with considering the length and direction of the vector as flow speed and angle θ_{Y-Z}.

Pressure

For the local hydrostatic pressure we have:

$$P = \frac{Nk_BT}{V} + \frac{1}{3}\frac{\sum_i^N \overrightarrow{r}_{ij}.\overrightarrow{F}_{ij}}{V} \tag{1}$$

Where $\overrightarrow{F}_{ij}$ is the inter-particle conservative force due to the Lennard-Jones potential.

$$\overrightarrow{F}_{ij} = -\left(\frac{dU(r_{ij})}{dr_{ij}}\right) \tag{2}$$

Where r_{ij} is the distance between the atoms i and j and $U(r_{ij})$ is the Lennard-Jones potential between the atoms i and j.

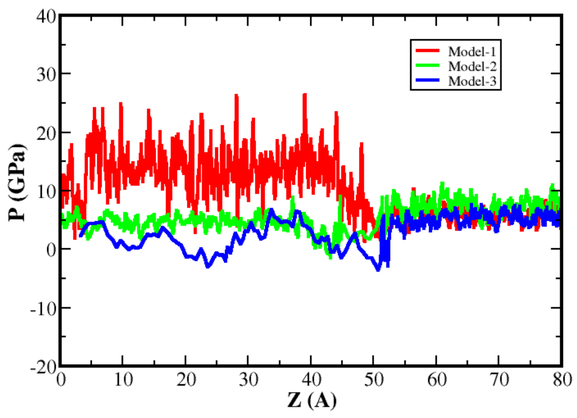
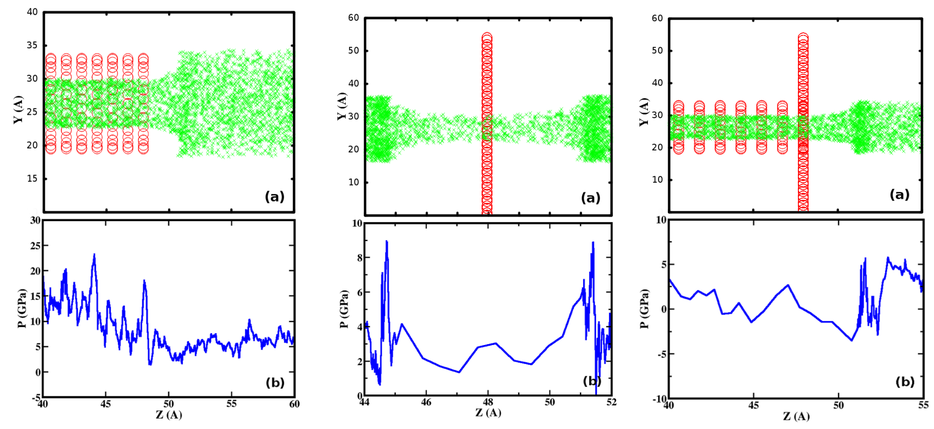


Figure 3: The variation of the pressure as a function of displacements (Z). Red line corresponds to Model-1, green line is related to Model-2, and Model-3 has been shown via blue line. Pressure measurements are in GPa unit and positions are in angstrom unit.



(a) Model-1 **(b)** Model-2 **(c)** Model-3

Figure 4: Model-1: (a) demonstrates that flow has like been sucked into the nanotube while (b) shows that the pressure corresponding to the aforementioned flow is increasing after an instant drop at the mouth of the nanotube.
Model-2: (a) demonstrates that flow has an inclination to pass through the whole on the greaphene sheet while (b) shows that the pressure corresponding to the aforementioned flow has been dropped as it is getting closer to the hole and then increased. At two critical points, $\pm 4A^0$ about the graphene sheet, there are two spikes which report $9GPa$ for the pressure.
Model-3: (a) demonstrates that flow has an inclination to pass through the whole on the greaphene sheet and nanotube while (b) shows that the pressure corresponding to the aforementioned flow has been dropped as it is getting closer to the hole and then increased while it is passing through the nanotube. At the critical points, $4A^0$ about the graphene sheet, there is a spike which reports $5GPa$ for the pressure.

Conclusions

We presented computational investigations on pressure, structure, and velocity of the fluid flow passing through models contain SWNT and graphene. In particular, we found that (i) during the MD time steps system has reached a thermodynamical equilibrium. (ii) Argon atoms passing through the confinement contains SWNT are inclined to take some ring patterns. On the contrary, for graphene based model, they just covered the whole cross section area. (iii) Moreover, using the side view of the trajectories, we have seen the argon atoms start getting narrower to pass through the confinements and made an empty area $\pm 2A^0$ about the mouth of the confinements. (iv) By observing the vector plots of the velocities of the argon flow which have shown us they have been sucked into the confinement about this area. With no doubt, the fluid flow starts getting slower when reached the confinements, but they move faster inside the nanotube. (v) The pressure of the flow and the correlation with position has been investigated. (vi) The pressure of the flow is increased by factor 4 inside the nanotube while dropping by factor 4 for graphene hole has been reported. (vii) Two spikes for pressure about $\pm 4A^0$ of the graphene sheet and one spike about $4A^0$ of the graphene sheet for model contains the comibination of the graphene and nanotube have been observed.

References

[1] Amirhessam Tahmassebi. Fluid flow through carbon nanotubes and graphene based nanostructures. 2015.

[2] Amirhessam Tahmassebi and Alper Buldum. Fluid flow calculations of graphene composites. 2015.

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