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Molecular dynamics simulation of mechanical and oscillating characteristics of graphene nanosheets with zigzag and armchair edges

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ABSTRACT

An oscillator is a circuit that can produce a continuous, repetitive, and alternating waveform without any input. However, the oscillations caused by the conversion between the two forms of energy cannot last forever. As a result, the amplitude decreases until it becomes zero, thus causing their nature to decrease. After discovering graphene nanosheets, their use in nanoelectricity science was much considered. Due to the amazing properties of graphene nanosheets, they can be used to establish permanent oscillations. The results show that graphene nanosheets ' mechanical properties and electrical properties depend on their structure and shape. Therefore, this study investigates the effect of graphene nanosheets type, size, and temperature on the simulated nanostructure's mechanical properties and oscillating behavior with Molecular Dynamics simulation. The results show that the graphene nanosheets with zig-zag edges has higher mechanical strength than armchair edges. Young's modulus and Ultimate strength of graphene nanosheets with zig-zag edges are numerically 1079 and 115 GPa, respectively. On the other hand, the resistance in graphene nanosheets can be expressed by reducing the oscillation amplitude and increasing the oscillation frequency. The results show that by changing the armchair edges to zigzag, the oscillation amplitude of graphene nanosheets decreases from 10.36 to 9.82 Å. Also, by enhancing the length of graphene nanosheets from 30 to 100, the oscillation amplitude of graphene nanosheets increases from 7.59 to 12.12 Å. This increase is due to the increases in the contact surface of the atomic structures. Consequently, the interactions between the carbon particles and mechanical resistance decrease. According to the results of this project, the findings improve the dynamics of nanoscale oscillators and cause a significant improvement in the performance of various devices.

Introduction

Graphene is a two-dimensional single sheet of carbon atoms with a

Abbreviations: GNSs, Graphene nanosheets; MP, Mechanical properties; MD, Molecular Dynamics; YM, Young's modulus; US, Ultimate strength; LJ, Lennard-Jones; LAMMPS, large-scale atomic/molecular massively parallel simulation.

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structure similar to individual layers of graphite, whose lattice structure is hexagonal. In these plates, carbon atoms are connected by SP^2 bonds. In graphene, each carbon atom is connected to three other carbon atoms,

Nomenclature

σ_{ij}	Potential well's depth
ε_{ij}	Finite distance at which the potential becomes zero
r_{ij}	Atomic distance between i and j particles
r_c	Cut-off radius
T	Temperature
k_B	Boltzmann constant
t	MD simulation time
ns	Nanosecond

and these three bonds are in the same plane, and the angle between them is 120°[1]. The carbon–carbon bond length in graphene is about 142 nm. In recent years, graphene has attracted a lot of attention in the field of materials science due to its unique properties such as electrical, optical, and thermal properties and its extraordinary speed in transferring electrons. More precisely, this material is of special interest due to its use in the design of suitable tools in the nanoelectronics industry, such as sensors and energy conversion tools[2].

Therefore, significant research has been done on the mechanical behavior of graphene nanosheets (GNSs) in one or more layers. Due to the unique properties of GNSs, research on their use in nanoelectricity is very extensive. By reviewing the previous articles, it can be concluded that the effect of zigzag and armchair edges on the mechanical and oscillating properties of GNSs was done[3]. For example, Nazarloo et al. [4], Eftekhari et al. [5], Jafari et al. [6], Wu et al. [7] investigated the mechanical properties (MP) of GNSs with zigzag and armchair edges. They investigated the elastic modulus and strain stress diagrams and Young's modulus (YM) to investigate the MP and the effect of the structure. Research has been done on the oscillating properties of GNSs, all of which investigated the effect of the frequency of external force on the oscillating properties of GNSs [8–11].

The results show that GNs have relatively good mechanical properties. Based on similarity measurement with miniature devices that are based on carbon nanotubes, the possibility of designing a GHz oscillator based on the telescopic oscillation of GNSs, based on the telescopic movement of GNSs, and a nano resonator based on relatively small vibrations of GNSs is proposed [12,13]. These wide applications of GNSs require a comprehensive investigation of the mechanical behavior of GNSs under different loadings [14]. Also, from another point of view, among different mechanical behaviors, investigating the structure's response to synchronous oscillation conditions has been one of the basic issues in the field of designing structural components such as sheets [15]. Although considerable progress has been made in the research of nanomaterials by conducting laboratory work, many researchers have come to the use of nanomechanics calculation methods to analyze the mechanical behavior of nanomaterials because computer simulation based on reasonable physical models not only highlights the molecular properties of nanomaterials for theorists, but it can also provide guidance and interpretation for experimenters [16]. Koukaras et al. [17], the phonon and vibration behavior of ideal and flawless GNSs in large dimensions were simulated. This study shows that the Tersoff potential is suitable for studying carbon nanotube structures' mechanical and vibrational behavior. Fang et al. [18] used the Molecular Dynamics (MD) method to simulate the graphene nanofibers. After balancing this structure at ambient temperature, they stretched this sample in one direction. Thus, atomic oscillating and phonon properties were investigated by preparing nanographene strips under stress.

Dadrasi et al. [19] examined the effect of crack size and temperature on the fracture behavior of 2D carbon nanostructures. The results revealed that the MP of carbon nanostructure decreases with an increase in temperature and crack length. Bagheri et al. [20] examined the effect of grain number and atomic defects on the MP of carbon nanosheets. The results revealed that the MP of carbon nanostructure decreases with an increase in grain boundaries and crack length. Dehghani et al. [21] examined the effect of the number of grains and atomic defects on the MP of polycrystalline nanosheets. The results revealed that atomic defects decrease mechanical strength. By reviewing past articles, it can be seen that MD simulation has not affected the effect of the influencing parameters in oscillators, including the type of nanosheets, temperature, size of nanosheets, and flow velocity using MD simulation. As a result, this issue has been investigated in this research. Applying the MD method, Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software is used [22,23]. In the first step of this study, the effect of nanosheet type on the oscillating behavior of the simulated structure is investigated. Then, the effect of nanosheet size on the oscillating behavior of the sample and the stability of GNSs as a function of fluid velocity are investigated.

Computational method

MD method

MD is one of the computational branches of modern science. This method simulates interactions between particles at intervals by computer-based physics laws. MD methods describe particles' evolution based on Lagrange or Hamiltonian equations and a term derived directly from Newtonian equations of motion. The MD simulation is based on Newton's second law or equation of motion [24–27]. In MD simulation, the velocity-Verlet algorithm integrates the equations of motion [28]. In general, the results of MD simulation are obtained using the definition of potential functions. The potential function defines the interaction energy between particles. The present research uses the Tersoff and Dreiding potential functions to describe the interaction of atomic structures [29–31].

On the other hand, this potential function is one of the best approximations for simulating idea gases [32]. In Dreiding potential, the non-bonding interaction is expressed by the Lennard-Jones potential. The LJ potential function approximates interactions among the atoms and molecules. It is defined in Eq. (1)[33]:

$$U_{LJ} = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right] \quad (1)$$

Table 1 shows the values σij and ε_{ij} of the atoms.

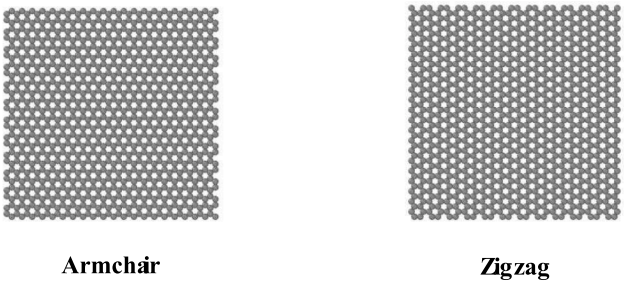
The present simulation details

This study investigates the mechanical and oscillating characteristics of GNSs with zigzag and armchair edges using LAMMPS software. The following simulation describes the oscillatory behavior of GNSs near oxygen fluid. Generally, it is possible to establish a connection between atomic oscillations and phonons by using MD simulation. This type of generalization can be implemented in the structures with equilibrium behavior and without the presence of external factors such as fluid flow in vicinity of the target sample. But in our computational research, the non-equilibrium phase of graphene in the final step of simulations, it is impossible to make a reliable connection between the oscillating

Table 1
The values of Lennard-Jones potential constant coefficients [32].

Atom type	ε_{ij} (kcal/mol)	σ_{ij} (Å)
C	0.3050	4.18
O	0.415	3.71

behavior of graphene and phonons. This simulation has been investigated in an atomic duct with carbon walls. The carbon walls show the fluid flux duct, limiting the fluid flux in a specified route. First, the initial atomic structure consisting of carbon walls, oxygen fluid, and GNSs. The simulation box's dimensions were considered 400 Å. Also, periodic boundary conditions are implemented in the X and Y directions, and fixed one is used in the Z direction. Choosing too small of a timestep leads to an unrealistic simulation time, whereas too big of a timestep leads to the system not being represented correctly (or, in the case of an algorithm like SHAKE, a SHAKE failure). The kind of structural interactions we are interested in studying, such as H-bonding, confrontational change, binding interactions, etc., each of which has a distinct



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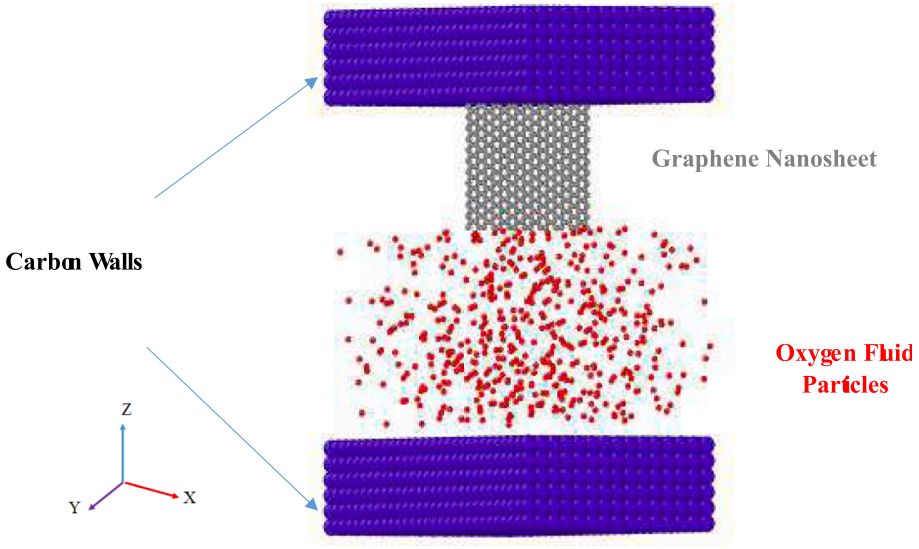

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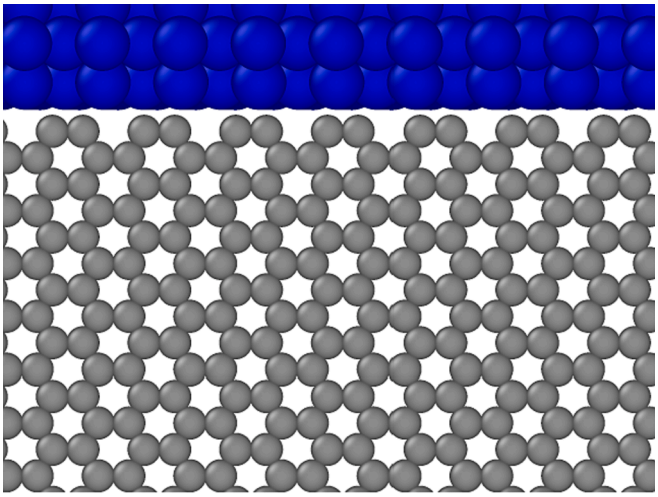

(c)

Fig. 1. a) GNS with zig-zag and armchair directions in presence of 1008 atoms. b) A view of the simulated atomic structure in the present study. c) The GNS and carbon wall arrangement inside computational box.

time scale, affects the choice of time step[34]. It is not heavily dependent on the system's size (box size). However, the size of the molecule is dependent on the study of the conformational changes (the time scale for such a process may vary from less than a ns to a few seconds)[35]. The findings of the study indicated that a time step of 1,000,000 fs was appropriate for GNSs[36,37]. The initial length of the GNS is considered 50 Å. This nanosheet is considered to be one end involved (fixed) in investigating the oscillatory behavior of GNSs. The used GNS with armchairs and zigzag edges is depicted in Fig. 1a. These structures have 1008 atoms, and their results can be compared with each other. Technically, for fluid and GNS modeling, the Avogadro and VMD packages are used [38,39]. After initial atomic structure modeling, these samples are packed with Packmol software[40]. The schematic of the simulated atomic structure in this study is shown in Fig 1b. Structurally, the 1.5 Å distance between GNS and carbon walls is defined to stabilize the modeled sample (see Fig. 1c). Next, the conjugate gradient method is implemented to minimize energy in the defined structure.

The initial pressure and initial temperature are considered 0 bar and 300 K, respectively, using the Berendsen barostat. In the first step, the thermodynamic stability of the simulated structure is investigated after 1 ns to ensure the simulation process's correctness. The Nose-Hoover thermostat is used to create thermal equilibrium in simulated atomic structures. Next, by changing the NVT ensemble to NVE, the mechanical and oscillating characteristics of simulated carbon nanosheets are examined. The effect of carbon nanosheet length (30–100 Å) and temperature (250 K–350 K) on the oscillating behavior of GNSs are investigated. Finally, the atomic stability of GNSs as a function of fluid velocity (0.003–0.010 Å/fs) is investigated. In Table 2, the MD simulation settings for pristine samples are reported.

Results and discussion

Thermodynamic stability of simulated atomic structures

At this research stage, the thermodynamic stability of the simulated carbon nanosheet structure with a zig-zag edge and armchair edge with a length of 5 nm is examined. The simulated structures' physical quantities, such as temperature and total energy, are reported in this regard. Fig. 2 shows the simulated structure's temperature changes with a zig-zag and armchair edges at 300 K and 0 bar during 1,000,000 time steps. Considering the changes in temperature, it can be said that the atomic oscillations in the simulated structures decrease over simulation time. The results show that temperature in zig-zag and armchair edges converged to a constant value. This convergence showed that 1 ns was enough to reach the equilibrium in simulated nanostructures. After 1 ns, the temperature in the simulated structure reaches 300 K (the initial temperature), which shows that the simulated structure was physically stable.

Fig. 3 shows the total energy changes with zig-zag and armchair edges after 1 ns. The sum of kinetic energy and potential energy equals

Table 2
The computational details in current computational research for pristine atomic systems.

Computational Parameters	Value/Setting
MD Box Length	400 × 400 × 400 Å^3
Number of Atoms in Pristine GNS with armchair/zigzag edge	1008
Boundary Condition	P-P-F
Initial Temperature and Pressure	300 K and 0 bar
Thermostat/Barostat	Nosé–Hoover/ Berendsen
Computational Algorithms	NVT-NVE
Minimization Method	Conjugate Gradient
Integration Method	Velocity Verlet
Simulation time	1 ns
Number of Time Steps	1,000,000 fs

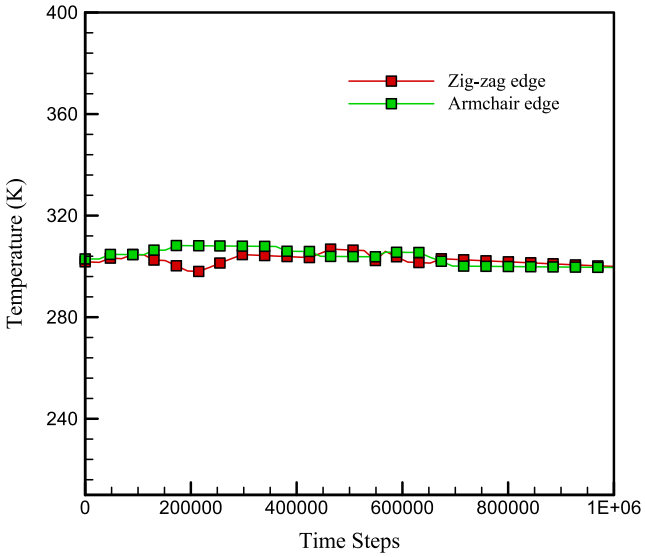

Fig. 2. Temperature changes with a zigzag and armchair edge at 300 K and 0 bar after 1 ns.

the total energy. The total energy is obtained from Eq. (2):

$$E = \sum_i \frac{1}{2} m_i v_i^2 + \sum_{ij} u_{ij} \tag{2}$$

The concept of convergence in MD simulations is based on the Ergodic Hypothesis, which states that the long-time average is equal to the ensemble average [41]. However, the definition of convergence depends on the specific quantity being examined, such as potential energy, kinetic energy, total energy, temperature, etc. The negativity of the total energy indicates that the potential energy is greater than the kinetic energy in the studied structure. Also, the more negative the studied structure's energy is, the greater the structure's stability. The value of this quantity converges at the end of the equilibration process of atomic structures and does not show much fluctuation. From a numerical point of view, the total energy in the simulated atomic structures with zig-zag and armchair edges converge to −275.91 eV and −237.92 eV in the final step of equilibrium phase simulation. This convergence shows that the atoms' position in the simulated structure was proportional to the applied force field.

The MP of GNSs

In this study, YM and US of simulated carbon nanosheets with both armchairs and zigzag edges have been investigated to investigate the MP of carbon nanosheets. Computationally, the stress–strain curve is calculated in this section. For this purpose, the stress of each atom is calculated below the equation,

$$S_{ab} = -mv_a v_b - W_{ab} \tag{3}$$

Here, the first term is a kinetic energy contribution for each atom. The second term is the virial contribution due to intra and intermolecular interactions. The MD results show YM and US for carbon nanosheets with armature edges equal to 1054 and 104 GPa. Also, these quantities for a zig-zag edge are equal to 1079 and 115 GPa. So, it can be concluded that the zig-zag edge of the graphene structure has higher mechanical strength than the armchair edge. This issue is due to the unique shape of zig-zag and armature GNSs. In the zig-zag edge, there is a kind of symmetry in the hexagonal structure between the carbons, which makes the tensile force and the compressive force equal in this model, and YM is higher in this model [42]. Carbon atoms in zig-zag GNSs are more condensed than armchair type, and due to Van der Waals interaction

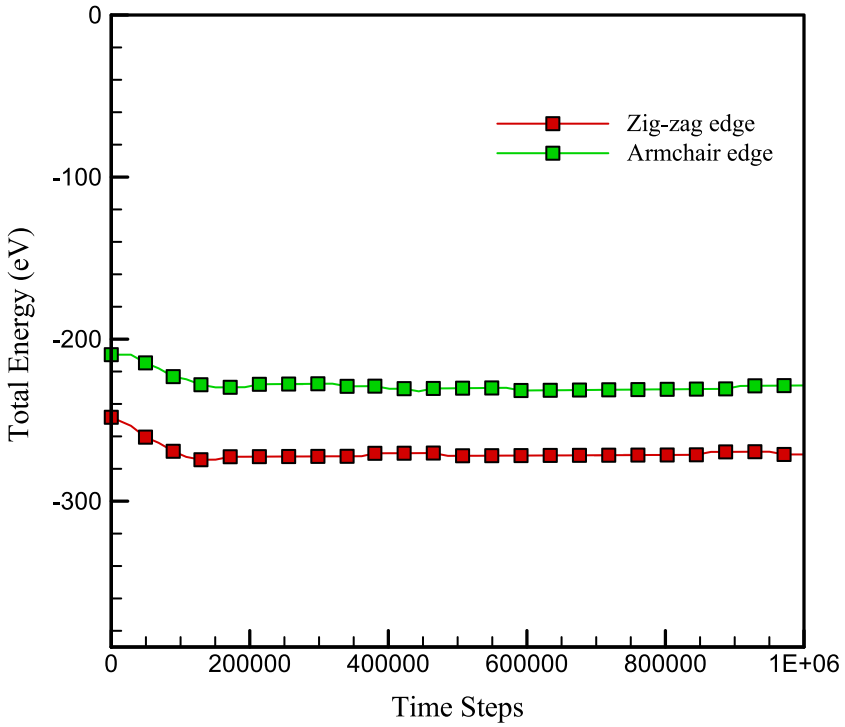

Fig. 3. Total energy changes with a zig-zag and armchair edge at 300 K and 0 bar after 1 ns.

between atoms in adjacent tubes, they tend to keep their constant distance from each other; thus, nested tubes of zig-zag DWCNT have better adjusting and aligning effects on each other [43]. The present results are in good agreement with previous studies. Li et al. [44] provided almost similar results for carbon nanosheets. Numerical results are reported in Table 3. In another study, Zhan et al. [45] showed that the YM of GNSs with various edges and thickness changes from 0.75 TPa to 1.07 TPa.

The effect of simulated nanosheet type on the oscillating behavior

The results show that the zigzag edge of the graphene structure has higher mechanical strength than the armchair edge. The researchers' results have shown that the mechanical resistance decreases with the increase in the oscillation amplitude of the atoms and the decrease in the bond energy and van der Waals energy between the carbon atoms [10,47]. According to the results of the previous part, the zigzag edge had the highest mechanical resistance, and it is expected that it has the lowest amplitude of fluctuations. Also, according to the relationship between the amplitude and frequency of oscillations, which are the opposite [48], the zig-zag edge is expected to have the highest frequency value as the amplitude of oscillations decreases. As a result, it can be expected that graphene with a zig-zag edge has a higher resistance to external factors. This higher resistance can be expressed by reducing the oscillation amplitude and increasing the oscillation frequency in the simulated graphene sample. In this part of the research, the oscillating behavior of the carbon sample using the oscillation amplitude and frequency calculation is expressed for a GNS with a 50 Å dimension. This GNS is located near an oxygen fluid with a velocity of 0.001 Å/fs at 300 K. The results show that by changing the armchair edges to zigzag ones, the oscillation amplitude of GNSs decreases from 10.36 to 9.82 Å. These behaviors arise from effective interaction between GNSs and fluid particles. MD outputs predicted the interatomic force in the armchair GNSs-fluid system is larger than zigzag GNSs-fluid. So, atomic acceleration in armchair GNSs converged to a larger value between simulated samples. This described atomic evolution caused the effective oscillation detected in armchair GNSs, which should be expected in actual applications.

Also, the oscillation frequency of GNSs increases from 2.37 to 3.45 fs^{-1} by changing the armchair edges to zigzag ones. This part of the simulations shows more resistance of zigzag than armchair samples in the vicinity of the simulated fluid flow. Physically, the mechanical strength of zig-zag GNSs is more than that of armchair types, and this mechanical behavior caused the inertia of the nanosheet to increase in response to the external factor. So, the oscillation frequency of zig-zag GNSs converged to larger values. Numerical results are shown in Table 4. The results are consistent with those of Li et al. [49]. They investigated the MP of CNT, and their results show that, with increasing temperature, the mechanical resistance increases, and as a result, the amplitude of oscillation decreases. Also, with the decrease in amplitude of oscillations, the frequency of oscillation increases.

The effect of simulated nanosheet size on the oscillating behavior

Since, in the previous section, simulated GNSs with a zigzag edge

Table 3
YM and US of graphene sample with a length of 50 Å.

Nanosheet type	YM (GPa)	US (GPa)
Armchair	1054 [Present Research] 1075 [44] 1100 [46]	104 [Present Research] 108 [44] 100 [46]
Zigzag	1079 [Present Research] 1097 [44]	115 [Present Research] 119 [44]

Table 4
Amplitude and oscillation frequency in simulated graphene sample with the length of 50 Å.

Nanosheet type	Oscillation amplitude (Å)	Oscillation frequency (fs^{-1})
Armchair	10.36	2.37
Zigzag	9.82	3.45

have the maximum mechanical resistance to fluid flow, in the continuation of this study, the sample with a zig-zag edge is used to investigate the effect of simulated nanosheet size on the oscillating behavior of the sample. These atomic structures with dimensions of 30, 40, 50, 75, and 100 Å are simulated to investigate the effect of simulated GNS size. Fig. 4 represents the change in oscillation amplitude with increasing the length of GNS. The oscillation amplitude/frequency was calculated from XYZ outputs of the current MD simulation. By using this output, the position of various atoms inside the computational box in various time steps can be calculated. Technically, by using the XYZ file and VMD package, MD outputs, which are represented in Figs. 4 and 5, can be estimated. According to Fig. 4, it can be said that increasing the simulated GNS's dimensions increases the value of oscillation amplitude. By increasing the length of the simulated graphene sample from 30 to 100 Å, the oscillation amplitude in atomic structures increases from 7.59 Å to 12.12 Å.

Due to the increase in the length of GNSs, the distance and bond length between carbon atoms increases. With the increase of molecular distance, according to Lennard-Jones potential theory, the potential energy between molecules reaches zero, and the attraction force is weak. So, atoms become unstable [50]. As a result, the MP decreases with the increase in the length of the nanotube. Miyashiro et al. [51] investigated the effect of the length of CNT on their MP and vibration behavior. The results show that the MP decreases with the increase in length of CNT. Therefore, it can be said that with increasing the oscillation amplitude in the structure, mechanical strength in the CNT decreases. The numerical results are reported in Table 5.

Fig. 5 represents the change in oscillation frequency values with increasing the length of carbon nanosheets. Generally, as the simulated samples' oscillation amplitude increases, the oscillation frequency is expected to decrease. To be more precise, with increasing oscillation amplitude in the simulated samples, each atomic oscillation is visible for a longer period. Physically, the frequency in the present study reveals the number of occurrences of GNS oscillation per unit of simulation time. With increasing length (dimensions) in simulated nanostructures from 30 Å to 100 Å, the oscillation frequency in the simulated carbon structure decreases from 5.21 to 2.58 fs^{-1}. The numerical results are shown in Table 5. From these results, we concluded the net force implemented to GNSs enlarged with the increase in nanosheet length. This procedure arises from the effective collision number increasing inside the GNS-fluid system, which improved the oscillate evolution of modeled nanosheets. This change in the oscillating behavior of GNSs can be considered in the industrial applications of this promising sample.

The frequency also decreases by reducing the MP, as explained in the previous section. The results are consistent with the results of Miyashiro et al.[51] and Bedi et al.[52].

The effect of simulated nanosheet temperature on the oscillating behavior

In this part of the study, the effect of simulated samples' temperature on the oscillating behavior of carbon nanosheets is investigated. To investigate the effect of this parameter, the temperature is set to 250, 275, 300, 325, and 350 K. Similar to examining the model of electromagnetic waves in a closed box, where the final limit was taken for the photon frequency, Debye assumed to explain the specific heat of material that there is an upper limit for the vibrational frequencies of the atoms of matter, which is called the Debye temperature. Or, in simple words, if we consider states possible for atoms to vibrate in the crystal lattice, a temperature called Debye temperature is defined as the highest possible state (which has the most energy)[53]. The Debye temperature for graphene is equal to 1813 K [54]. Khalkhali and Khoeini [55] investigated the quantum temperature and phonon spectrum of Si nanowires by MD simulation. In the presented research, the temperature difference in the Si nanowires is considered. This temperature difference causes atomic vibration in the structure. The results showed that, by increasing the mean temperature of the system, the thermal conductivity decreases. This is resulted from suppressing the excited high energy phonons and increasing phonon–phonon scattering. Also, the Debye temperature and properties of GNSs have been carried out by MD simulation[56–58]. In this research, the specific heat for the nanoplates is considered constant and at a certain time, the entire length of the GNSs is placed at the same temperature. The authors suggest to

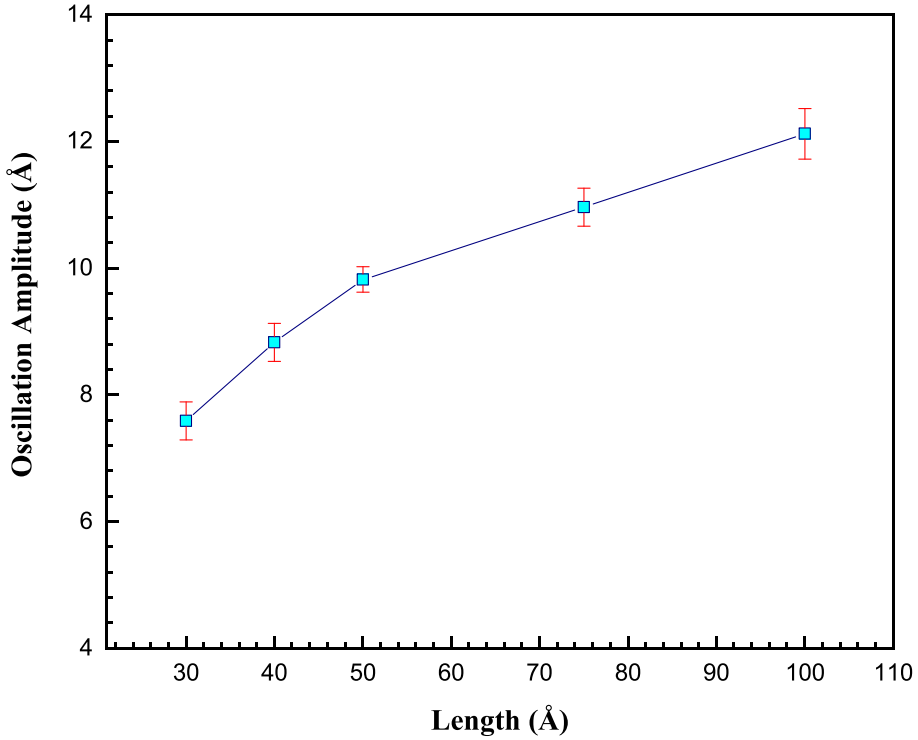

Fig. 4. The oscillation amplitude change in the simulated graphene with increasing the carbon nanosheet lengths.

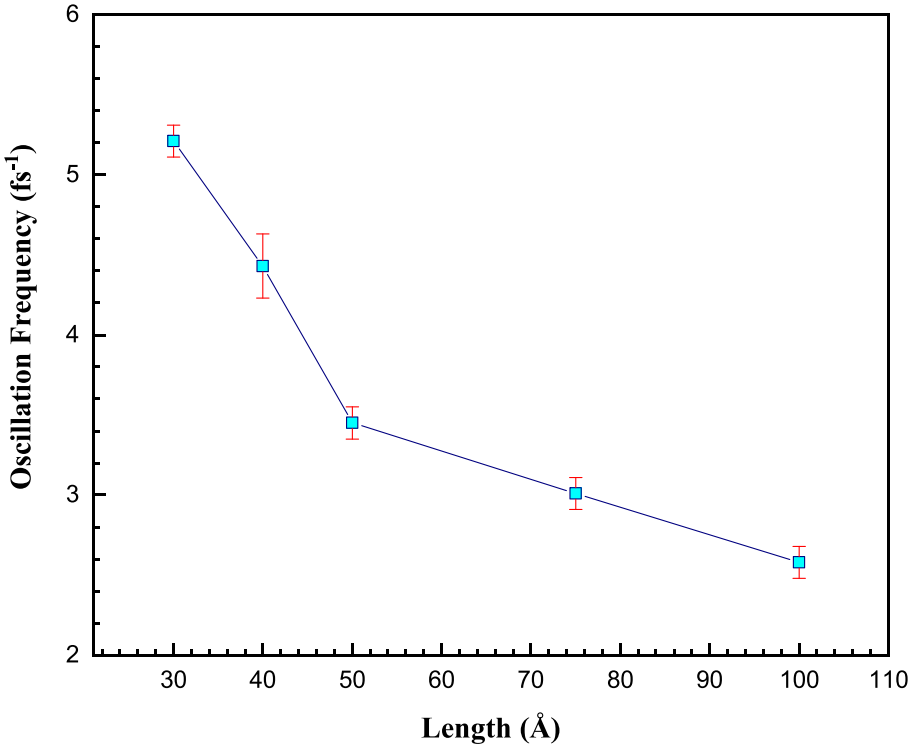

Fig. 5. The oscillation frequency change in the simulated graphene with increasing the carbon nanosheet lengths.

Table 5
Oscillation amplitude and frequency in simulated graphene samples with different lengths at 300 K and 0 bar.

Nanosheet length (Å)	Oscillation amplitude (Å)	Oscillation frequency (fs^{-1})
30	7.59	5.21
40	8.83	4.43
50	9.82	3.45
75	10.96	3.01
100	12.12	2.58

investigate and report the effect of external electromagnetic force or external heat flux on the mechanical and thermal properties of this system for future works. The temperature investigated in the research was determined based on previous research [36,59,60]. The results of these studies show that the thermal, mechanical and vibrational properties of GNSs change in this temperature range.

Fig. 6 represents the oscillation amplitude change in the simulated graphene with increasing the carbon nanosheet temperature. Generally, the temperature in simulated atomic structures directly affects their evolution. The structures' oscillation amount increases with increasing temperature. This increase reduces the interaction force between the atoms. The simulated atomic structures show less mechanical strength. As the simulated samples' mechanical strength decreases, carbon nanostructures experience greater overall fluctuations in the face of an external force. Numerically, with the increasing temperature to 350 K, the oscillation amplitude increases from 8.84 to 11.11 Å. Typically, as the initial temperature of a structure increases, the fluctuations and mobility of NPs and atoms within the sample increase, providing them with the necessary energy to move more freely. As the temperature increased, based on $Average\,Kinetic\,Energy = \frac{1}{2}mv^2 = \frac{3}{2}K_BT$ the kinetic energy increases [61]. With the increase of kinetic energy, the amplitude oscillations increase, and this increase causes a decrease in MP. By increasing the amplitude oscillations and its inverse relationship with frequency, with increasing temperature, the frequency decreases. The results of this part follow the results of Li et al.[49].

Fig.7 represents the oscillation frequency change in the simulated graphene with increasing the carbon nanosheet temperature. The results showed that the oscillation frequency in the structures decreases with increasing temperature. This decrease in oscillation frequency is due to increased oscillation amplitude in the samples, which increases the time required to complete an oscillating motion. Physically, the temperature increase caused the mobility of modeled GNS to enlarge, and this evolution increased the GNS displacement from the fluid particle collisions with C atoms. Furthermore, the increasing temperature value improved the mobility of fluid particles, and this procedure caused more net force to be inserted into C atoms inside GNS. Numerically, the corresponding oscillation frequency value changes from 4.02 to 3.05 fs^{-1} with increasing temperature from 250 to 350 K. As a result, it can be said that with increasing temperature, the MP of simulated GNSs decreases. The numerical results are reported in Table 6.

The stability of GNSs

In the final step of our MD simulations, we estimate the atomic stability of GNSs as a function of fluid velocity. Increasing fluid velocity to 0.003 Å/fs can detect atomic destruction after t = 3.61 ns. As fluid to 0.010 Å/fs, the destruction time of the nanosheet is reported. Fig. 8 shows the change in the destruction time of GNS near atomic fluid as a function of fluid velocity.

According to the flow of fluid over the GNSs, the flow velocity is one of the influencing parameters on the properties of the GNSs. The researchers' results showed that the interaction between the fluid and the GNSs increases with the increase in the velocity. With the increase in interactions, the probability of breaking the bonds between carbon–carbon increases, and the MP decreases [10,49]. According to the mentioned points, by reducing the MP of GNSs, they are destroyed faster, and the destruction time is reduced by increasing the velocity. This procedure arises from inserting force increasing to GNS by fluid velocity enlarging. Theoretically, the amplitude of atomic fluctuations converged to larger values by net force increasing in the GNSs-fluid

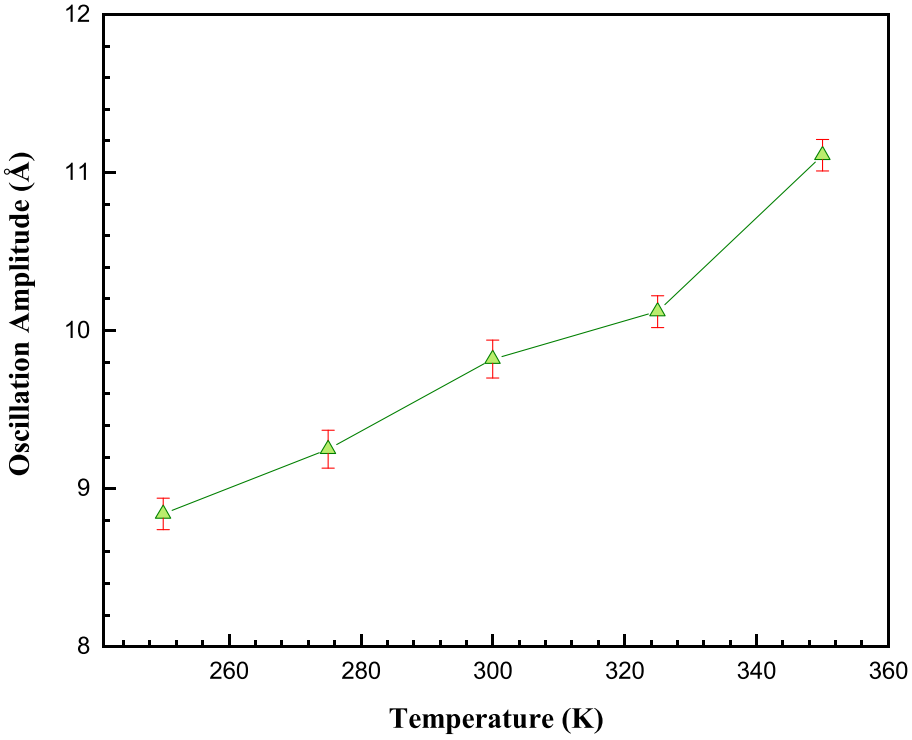

Fig. 6. The oscillation amplitude change in the simulated GNS with increasing the temperature.

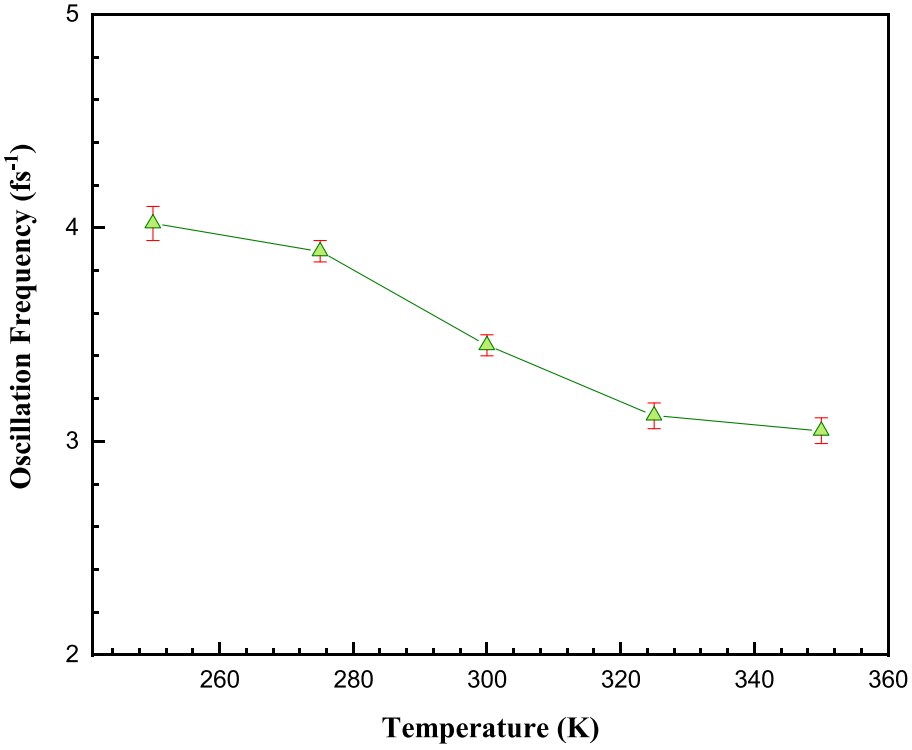

Fig. 7. The oscillation frequency change in the simulated graphene with increasing the carbon nanosheet temperature.

system. The atomic interaction inside GNSs (and other nanostructures) decreased by average interatomic distance increasing. So, the physical stability of modeled nanosheets decreased by fluid velocity converging to higher values.

The results of this section show that as velocity increases, the destruction time in simulated structures decreases. Numerically, the destruction time of the simulated nanosheet decreased to 2.88 ns by fluid velocity increasing to 0.010 Å/fs (see Table 7). The results of this part of the simulations indicated the limitation of GNSs used near nanofluid mixtures. They should be considered in the actual application of these atomic systems.

Table 6
Amplitude and oscillation frequency in simulated graphene sample with the length of 50 Å based on sample temperature at 0 bar pressure.

Atomic structure temperature (K)	Oscillation amplitude (Å)	Oscillation frequency (fs^{-1})
250	8.84	4.02
275	9.25	3.89
300	9.82	3.45
325	10.12	3.12
350	11.11	3.05

Conclusion

This study simulates an atomic structure of carbon walls, oxygen fluid, and GNS using the MD method and LAMMPS software. After studying the stability by calculating quantities such as temperature and total energy, the mechanical and oscillating quantities included oscillation amplitude, and the oscillation frequency of the GNS was studied. Also, the effect of simulated nanosheet type on its oscillating behavior and simulated nanosheet size on its oscillating behavior were investigated. The results of the simulations of this research can be expressed as follows:

- After 1,000,000-time steps in the present simulations, the simulated structure's temperature reaches 300 K, corresponding to the temperature of the simulated atomic structures.
- In the final simulation step in the equilibrium phase, the total energy in the simulated atomic structures with zigzag and armchair edges converged at −275.91 and −237.92 eV.
- The simulation results show that the sample with a zigzag edge has more resistance than the sample with an armchair edge near the oxygen fluid flow.
- As the length of the simulated graphene sample increases from 30 Å to 100 Å, the amplitude of oscillation in atomic structures increases from 7.59 Å to 12.12 Å.
- Numerically, with increasing oscillation amplitude in simulated samples, the oscillation frequency decreases. Increasing the length (dimensions) in the simulated nanostructures from 30 to 100 Å, the oscillation frequency in the simulated carbon structure reaches 5.21 to 2.58 fs^{-1}.
- As the simulated samples' temperature increases from 250 to 300 K, the oscillation amplitude increases from 8.84 to 11.11 Å, and the corresponding oscillation frequency decreases from 4.02 to 3.55 fs^{-1}. As a result, it can be said that with increasing temperature, the MP of the simulated GNS decreases.
- By increasing fluid velocity, the destruction of the GNS is observed in a shorter period. Numerically, the destruction time of GNS reaches 2.88 ns in the presence of fluid atoms with v = 0.010 Å/ps.

Using these computational results can cause actual oscillator efficiency improvement for some purposes, such as gas detector apparatuses, etc. Also, some other research can be completed in current computational work. Atomic defects such as Vacancy and Stone-Wales can affect atomic oscillator behavior. This atomic parameter influence on graphene-based oscillators isn't reported in our MD simulations. So, describing this atomic parameter behavior on graphene-based oscillators is proposed for future studies.

CRediT authorship contribution statement

Qiang Fei: Investigation, Writing – original draft. **F. Al-dolaimy:** Investigation, Formal analysis, Writing – original draft. **S. Mohammad Sajadi:** Writing – original draft. **Ahmed Hussien Alawadi:** Supervision, Writing – review & editing. **Noor Hanoon Haroon:** Methodology,

Table 7
The destruction time of simulated GNS over atomic fluid velocity.

Velocity (Å/ps)	Destruction Time (ns)
0.001	–
0.003	3.61
0.005	3.25
0.007	3.02
0.010	2.88

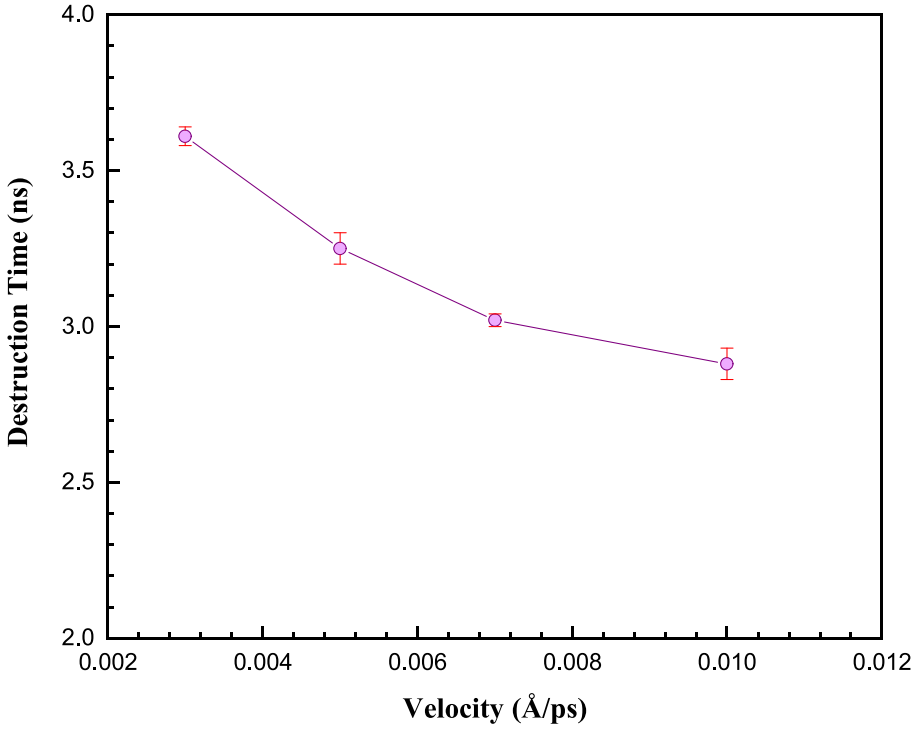

Fig. 8. The destruction time of GNS near atomic fluid over velocity.

Project administration. **Dheyaa J. Jasim:** Validation, Methodology, Conceptualization, Data curation, Formal analysis. **Soheil Salahshour:** Formal analysis, Writing – review & editing. **Ali Alsaalamy:** Conceptualization, Data curation, Formal analysis. **S. Ali Eftekhari:** Formal analysis, Writing – review & editing. **Maboud Hekmatifar:** Formal analysis, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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