Advances in Nano Research, *Vol. 11, No. 2 (2021) 173-181*
https://doi.org/10.12989/anr.2021.11.2.173

Molecular dynamics investigation of pull-in instability in graphene sheet under electrostatic and van der Waals forces

Farzin Sha'bani and Samrand Rash-Ahmadi*

Department of Mechanical Engineering, Urmia University, Urmia, Iran

(*Received November 15, 2020, Revised June 16, 2021, Accepted July 6, 2021*)

Abstract. This paper investigates the pull-in instability of graphene sheets. The influence of geometry parameters such as chirality of graphene and length to gap ratio is studied using molecular dynamics (MD). For molecular interactions, the AIREBO potential is used. Furthermore, by applying the electrostatic and van der Waals (vdW) forces, pull-in voltages are calculated. Size effect is estimated, with adding the fringing field effect correction factor to the electrostatic force. In MD simulations, the graphene sheets on the armchair and zigzag structure have been investigated. The results show that the closer the moving electrode to the fixed electrode, the greater the effect of van der Waals force than the electrostatic force. The results also represent that the vdW force and fringing effect on the electrostatic load increases the pull-in deflection and decrease the pull-in voltage. The numerical results of the present study show good agreement with previous analytical and experimental researches.

Keywords: electrostatic force; graphene sheet; molecular dynamics; pull-in instability; van der Waals force.

1. Introduction

Graphene sheets have great potential for designing the actuators because of their mechanical and electrical properties. Many researchers have studied the behavior of graphene under different conditions. Korobeynikov *et al*. (2018) discussed the mechanical properties of graphene. They considered geometrical parameters as the effective parameters for estimating the elastic properties (Young's modulus, poisons ratio, etc.). Also, Genoese *et al*. (2020) studied the tensile characteristics of single-layer graphene sheet using atomistic analysis. They utilized the classical molecular mechanics method for estimating the efficiency of the introduced force field on predicting the behavior of the graphene sheet.

The previous studies depicted that investigating the effect of mechanical properties on the instability of actuators is essential. There are methods such as continuum mechanics and atomistic modeling for the modeling of nanomaterials. At the nanoscale, experimental methods are costly expensive and need precise tools. Molecular dynamics have been used in many kinds of research to understand the exact behavior of nanostructures. Nazemnezhad *et al*. (2016) studied the interlayer interactions in multilayer graphene nanostructures. They assumed vdW interaction as an effective force between layers. The effective parameters in vibrational frequencies of the graphene sheet are considered, like length and the number of layers. Similarly, the role of the different force fields on the potential energy of the systems has been investigated. Also, Ansari *et al*. (2016) used molecular dynamics on the platform of the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package (Plimpton 1995). They studied the effect of size on the instability of nanostructures. Atomistic simulation of graphene she*et al*so has been performed for estimating the capability of graphene in many applications (Sutrakar *et al*. 2015, Farazinand and Mohammadimehr 2020). A Nano-actuators consists of two conductive electrodes. The first one is movable electrodes, and the second one is fixed electrodes. There is a dielectric space between these two plates. By applying a voltage to electrodes, an electrostatic force causes a deflection in movable electrodes. When the voltage reaches a critical value, the movable electrode collapses to the fixed electrode. This unstable condition is called pull-in instability. This voltage and deflection are named pull-in instability parameters and have principal roles in the design of NEMS and MEMS.

Kuang and Chen (2005) studied the pull-in instability of actuators. They used the Adomain decomposition method to solve the nonlinear equation of motion for investigating the pull-in behavior of micro-actuators. Moreover, the effect of different boundary conditions on the pull-in behavior of the actuator is studied. An essential intermolecular force like vdW force had considered in other works such as Kumar (2018), Attia and Mohamed (2019).

Similarly, the effect of the vdW force in nano-electrostatic actuators is studied (Lin and Zhao 2003). Continuum models had introduced to investigate the size-dependent effect on pull-in instability of nano-switches in some works like (Taghavi and Nahvi 2013, Ansari *et al*. 2012). Mousavi *et al*. (2013) have employed the Nonlocal theory of elasticity to investigate the pull-in behavior of nonlinear nano-sensors. The emphasis was on the effect of

*Corresponding author, Ph.D.,
E-mail: s.rashahmadi@urmia.ac.ir

ISSN: 2287-237X (Print), 2287-2388 (Online)

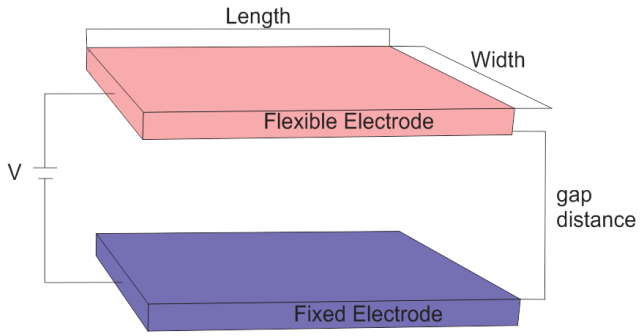


Fig. 1 Graphene sheet under voltage

fringing field effect and vdW attractions in the dynamic governing equation of motion. The dynamic pull-in had investigated by determining the influence of applied voltage and intermolecular forces (Sedighi *et al*. 2014). The vdW forces effect in the pull-in behavior of micro-switches had studied in Ref. (Batra *et al*. 2008); In addition, Ke *et al*. (2005) studied the influence of vdW force on the pull-in instability of NEMS switches.

Guo and Zhao (2004) studied the influences of the vdW force on the critical pull-in gap and pull-in voltage of nano-electromechanical switches. As depicted in their paper, the effect of the vdW force is considerable when the distance between two electrodes is less than 20 nm. Duquesne *et al*. (2002) investigate the pull-in behavior of carbon nanotube as used in Nano-actuators. In their work, a continuum model is proposed and compared with the results of the molecular dynamics model. The results were in good agreement with the continuum model.

Abdi *et al*. (2011) studied the effect of size on the pull-in behavior of nano-cantilever. The modified couple stress theory is used as an analytical method to analyze the nonlinear instability of nano-cantilevers. They find that the size effect can increase the pull-in parameters of the nano-actuators. Rotkin (2002) estimated the effect of the vdW force on the pull-in gap and obtained analytical expressions for the pull-in gap and voltage.

Ramezani *et al*. (2007) studied the pull-in instability of nano-switches under the intermolecular and electrostatic forces. Their model was nonlinear due to the essential nonlinearity of the intermolecular and electrostatic forces. Most of the continuum theories, on a small scale, cannot correctly predict the mechanical properties of nanostructures. Most of them didn't perceive the size effect. Other methods, such as the molecular dynamics, considered size effects in the nanoscale analysis and have shown significantly more exact results (Lu *et al*. 2007).

Lin *et al*. (2019) investigated the pull-in instability of nano-actuators. They employed a nonlocal Euler-Bernoulli beam model. The small-scale effect is determined using Eringen's nonlocal theory. Also, they observed the dependencies of the pull-in voltage on the length-gap ratio. In Ref. (Gupta 1997), the authors used the perturbation method for estimating the pull-in instability of carbon nanotubes. They discussed the effect of different geometries and boundary conditions in pull-in parameters. Their analysis includes nonlinear equations solved by numerical and semi-analytical methods. Fakhrabadi *et al*. (2013) used a molecular dynamics method for investigating the pull-in instability of carbon nanotubes (CNTs) with the presence of defects.

They realized that stiffer CNTs had a higher pull-in characteristic. The pull-in charges can increase, considering the factors that caused stiffening. On the pull-in instability, other studies were based on the classical continuum mechanics model and did not consider the small-scale effect (Yang *et al*. 2008). Many researchers used an analytical model for calculating the pull-in voltage (Rokni and Lu 2013). They investigated the effect of sheet layers on the pull-in voltages of the electrostatic micro-actuators. In that studies, the movable electrode had considered as an elastic beam.

Most of the researchers on the pull-in instability used continuum models (Lin *et al*. 2019, Rokni and Lu 2013, Duquesne *et al*. 2002, Abdi *et al*. 2011). They used a Bernoulli Euler beam or a thin plate to study the behavior of graphene sheets. Since the models were far from the actual structure of graphene, their results are not guaranteed. As mentioned, much research has been done to investigate the electromechanical behavior of graphene sheets. But more studies are needed to understand the electromechanical behavior of graphene.

The discrete structure of graphene in small dimensions has complex behavior, which causes a big difference in modeling results. Considering the discrete construction is closer to reality and will produce more accurate results. This assumption is the advantage of the present research for estimating the pull-in instability of graphene sheets.

Only one paper has used the molecular dynamics method to investigate the pull-in behavior in carbon nanotubes (Fakhrabadi *et al*. 2013). They studied the behavior of carbon nanotubes in the presence of an electric field. In addition, they simulated graphene as a fixed electrode. The difference between the present method and research at reference (Fakhrabadi *et al*. 2013) is that in the present study, we tried to reduce the costs of molecular dynamics modeling by removing the fixed electrode and adding the effect of the fixed electrode to the molecular dynamics modeling.

In this way, the number of atoms in the molecular dynamics model is reduced significantly, and simulations were performed with less cost and time. As nanostructure size increases, molecular dynamics simulations become more difficult. In this method, the effect of an atomic structure is considered instead of its physical presence.

Molecular dynamics calculations are limited to interatomic physical interactions. Due to the neglect of electrons in molecular dynamics simulations, it is not possible to find electron-based properties such as electrical and magnetic properties. These properties will be determined using the density functional theory. This imperfection is more evident in the study of the electric field effect caused by the size effect. As shown in the research, this edge effect has been introduced as a fringe effect, and the proposed method can evaluate the fringe effect acceptably.

So far, no satisfactory studies performed on the pull-in

behavior of graphene sheets, with attending to molecular dynamics simulation and under intermolecular and electrostatic and vdW forces. The present paper studies the pull-in instability of nano-actuators under electrostatic and intermolecular forces using molecular dynamics simulation. The influence of the fringing field effect and vdW force effect investigates the size scale effect on pull-in parameters (Fig. 1).

2. MD equilibrium

The molecular dynamics simulation was applied to estimate the behavior of the nano-actuators under pull-in instability. We used AIREBO potential to define the atomic interactions between carbon atoms in graphene. The AIREBO potential can represent by a sum over pairwise interactions, including covalent bonding (E_{ij}^{REBO}) interactions, Lennard-Jones potential (E_{ij}^{IJ}) terms, and torsion ($E_{kijl}^{TORSION}$) interactions. AIREBO potential describes as bellow (Stuart *et al*. 2000):

$$E = \frac{1}{2}\sum_{i}\sum_{j\neq i}\left[E_{ij}^{REBO} + E_{ij}^{IJ} + \sum_{k\neq i,j}\sum_{l\neq i,j,k} E_{kijl}^{TORSION}\right] \quad (1)$$

3. Pull-in Simulation

The pull-in behavior of the nano-actuator is studied using simulation results. The time step of the simulation is 0.1 fs. The temperature keeps constant using the NVT ensemble. The electrostatic and vdW force applied to each atom. Pull-in instability takes place when the atom deflection reaches near gap distance. For calculating the applied forces, the atom area is considered. For calculation of the atom area, the length and width of the relaxed graphene sheet are multiplied, then divided by the number of atoms.

4. Forces acted in nano actuator

4.1 Electrostatic force with fringing-field effect

The fringing effect will create due to the small size of the electrodes. In this phenomenon, over the edges, the electric field doesn't have parallel lines. Hence, the electrostatic force equation was corrected, with additional factors that specified the fringing field effect. Investigating the fringing field effect on the pull-in behavior of the system is performed using the capacitance-based approach. The behavior of the parallel plate capacitor is investigated under an electrostatic force due to applied constant voltage using the LAMMPS simulation.

The two edge sections are assumed to have a wedge-shaped contour, with a capacitance that is given as $C_1 = \frac{2\varepsilon_0 bL}{\pi b}\left(1 + ln\left(\frac{\pi b}{d-w}\right)\right)$. By adding the center parallel plate capacitor $C_2 = \frac{\varepsilon_0 bL}{d-w}$; The capacitance of the system, considering the fringing field effect, expressed as (Cheng *et al*. 2003):

$$C_{plate} = \frac{\varepsilon_0 bL}{d-w}\left[1 + \frac{2(d-w)}{\pi b} + \frac{2(d-w)}{\pi b} ln\left(\frac{\pi b}{d-w}\right)\right] \quad (2)$$

where, b and L are the width and length of the plate, respectively; d is the initial gap between two plates and, w is the deflection of the moveable electrode. Also, ε_0, is the free-space permittivity constant(or permittivity of gap space, $\varepsilon_0 = 8.854 \times 10^{-12}\, C^2 N^{-1} m^{-2}$). The potential energy, U, stored in each parallel-plate of the capacitor is:

$$U = \frac{C_{plate}V^2}{2} = \frac{\varepsilon_0 bLV^2}{2(d-w)}\left[1 + \frac{2(d-w)}{\pi b} + \frac{2(d-w)}{\pi b} ln\left(\frac{\pi b}{d-w}\right)\right] \quad (3)$$

By considering the fringing effect, the electrostatic force "per unit length" take the form (Batra *et al*. 2006):

$$F_{electrostatic} = -\frac{\mathrm{d}U}{\mathrm{d}(d-w)} = \frac{\varepsilon_0 bV^2}{2(d-w)^2}\left(1 + 0.65\frac{d-w}{b}\right) \quad (4)$$

where, the DC voltage (V) is applied.

4.2 The vdW force

As mentioned in Ref. (Fakhrabadi *et al*. 2013), the vdW force has an important rule when the gap distance between two electrodes is below 20 nm. For estimating the attractive and repulsive interactions between two separated atoms by a distance r, the Lennard-Jones potential is considered as below (Lv *et al*. 2011):

$$U(r) = 4\epsilon_0\left(\left(\frac{\sigma_0}{r}\right)^{12} - \left(\frac{\sigma_0}{r}\right)^{6}\right) \quad (5)$$

Here, σ_0 is the equilibrium distance when the interaction force is null and ϵ_0 is the corresponding energy. The $1/r^{12}$ term describes the strong repulsive interaction that in the large distances between atoms can be neglected. Then the Lennard-Jones potential is usually approximated by the $1/r^6$ part:

$$U(r) = -\frac{D}{r^6} \quad (6)$$

where, $D = 4\epsilon_0\sigma_0^6$. The values of ϵ_0 and σ_0 for Media as a fixed electrode (Cu), interacting across vacuum (air) are 65.5815×10^{-21} J and 0.2338 nm, respectively.

The vdW forces are calculated as the pairwise summation of the Lennard-Jones energies. Because of the short cut-off radius of vdW forces, the plane can be considered infinite (Maugis 2000). Let us consider an atom P, at a distance "d" from an unbounded half-crystal, having β atoms per unit volume (Fig. 2).

Using the notations of Fig. 2, the contribution of the volume is:

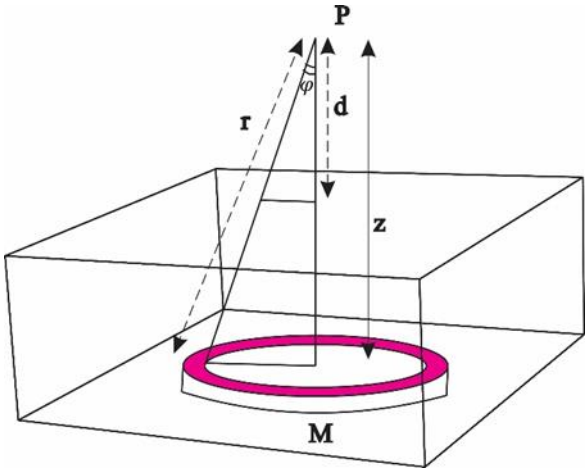


Fig. 2 Notations for attraction force between a molecule and a rigid, infinite plane

$$\mathrm{d}V = 2\pi z^2 \frac{sin\varphi}{cos^3\varphi} d\varphi dz \tag{7}$$

The adhesion energy between a single atom and a molecule M can be formulated as below:

$$\mathrm{d}U_{vdW} = -\frac{D}{r^6}.\beta.dV \tag{8}$$

Since, $r = \frac{z}{cos\varphi}$, there is:

$$\mathrm{d}U_{vdW} = \frac{2\pi\beta D}{z^4} cos^3\varphi.sin\varphi d\varphi dz \tag{9}$$

Then,

$$U_{vdW} = -2\pi\beta D \int_d^\infty \frac{dz}{z^4} \int_0^{\pi/2} cos^3\varphi.sin\varphi\, d\varphi$$
$$\rightarrow \quad U_{vdW} = -\frac{\pi\beta D}{6d^3} \tag{10}$$

The London-vdW model is presented as the potential energy of a single atom of a flexible electrode at a distance "d" from a fixed electrode. This energy proceeds from the interaction of an atom from a moving electrode with the entire fixed electrode. Hence, the adhesion forces between moving electrode atoms and the whole atoms of bellow fixed electrode are estimated using (Maugis 2000, Hamaker 1937):

$$F = \frac{\mathrm{d}U_{vdW}}{\mathrm{d}d} = \frac{\pi D\beta}{2d^4} \tag{11}$$

As the moveable electrode deflected, the gap distance will change as (d-w). Here, the "w" is the deflection of the moveable electrode. Then, the vdW force has the form:

$$f_{vdW} = \frac{\pi D\beta}{2(d-w)^4} \tag{12}$$

The Lennard-Jones interactions between two atoms lying on the same electrode (flexible electrode) are specified on the AIREBO potential terms. But, Eq. (12) defines the vdW interaction due to the attractive terms of Lennard-Jones, for simulating the effect of the fixed electrode on the flexible electrode.

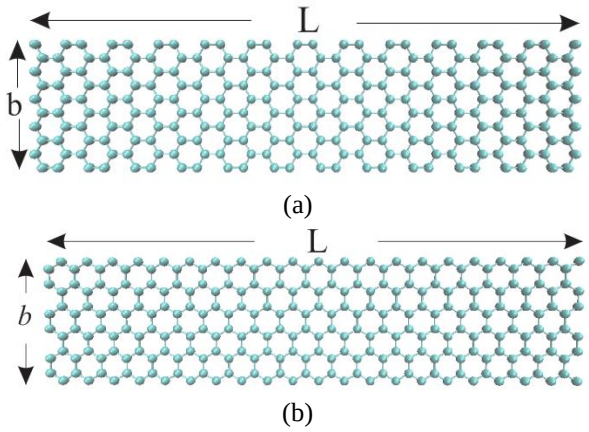


Fig. 3 (a) Armchair graphene sheet and (b) Zigzag graphene sheet

Table 1 Geometry of graphene sheet

Width, b, (nm)	1.8
Length, L, (nm)	20
Thickness, (nm)	0.345
Initial gap, G, (nm)	1.8

In MD analysis, the fixed electrode did not simulate. But the equivalent force of the fixed electrode was estimated and applied. We calculate the load due to vdW interaction between a single atom of moving electrode and the fixed plate. Each carbon atom in the graphene sheet will be affected by vdW force. The vdW force relation contains the position and displacement of each carbon atom. Therefore, the atom specifications have a direct role in the applied force, and at each time step of MD simulation, the atom positions must be updated.

5. Results and discussion

This part investigates the effective parameters in pull-in instability. Those parameters are as follows: the size effect by assuming the fringing effect of electrostatic force, vdW force effect, and the effect of gap distance. For molecular dynamics simulation, graphene sheets with two structures of armchair and zigzag are determined. Fig. 3 shows the graphene structure used in MD simulation. The geometry specifications of the graphene sheets depict in Table 1.

The following are the results of instability analysis in graphene. In small dimensions, considering the interaction between atoms can affect the electromechanical behavior of nanostructures. The interaction between the two moving and fixed electrodes, including electrostatic charges, causes graphene to deflect toward the fixed electrode. In the pull-in phenomenon, absorbing the graphene towards the lower electrode, the interatomic force opposed to the electrostatic force. As the electrostatic force increases, the force balance is lost, and the graphene deflects toward the below electrode. In this case, the pull-in instability will occur.

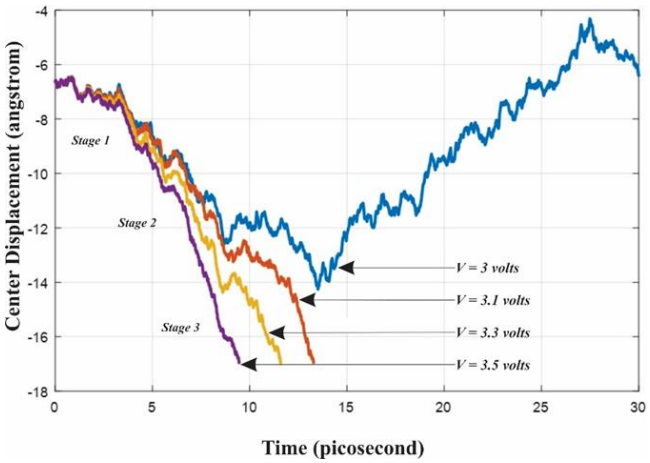


Fig. 4 Deflection of armchair graphene versus time for different voltages (volts) without fringing effect; gap distance = 18 angstrom

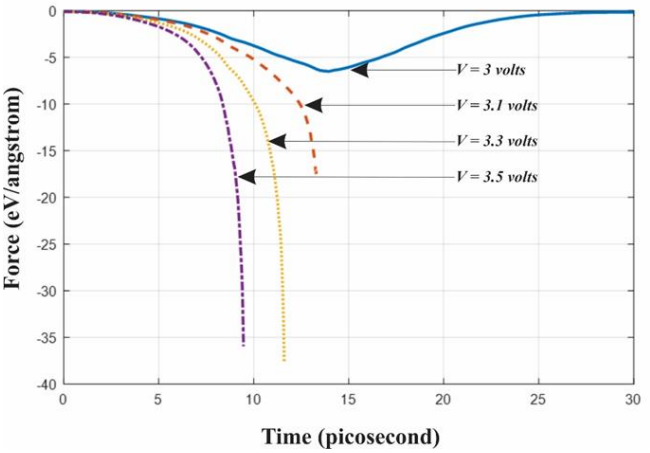


Fig. 5 Force variation during pull-in instability in armchair graphene without fringing field effect; gap distance = 18 angstrom

Fig. 4 illustrated the deflection of graphene atoms versus time. By neglecting the fringing effect on the electrostatic force, pull-in collapse occurred at a voltage equal to 3.1 volts. Then, by increasing the applied voltage, the amplitude of deflection will be increased and the time for reaching pull-in instability reduced.

In several stages, the movement of the graphene sheet is considered (Fig. 4). Graphene moves continuously and uniformly towards the fixed electrode at the beginning of the deflection (stage 1). In the next step, the graphene plate resists the electrostatic forces. In this stage, applying deformation to the graphene takes more time (stage 2). It's due to the equilibrium between intermolecular and electrostatic force. The third stage of motion occurs when electrostatic forces overcome the intermolecular force. The graphene eventually adheres to the fixed electrode (stage 3).

Fig. 5 shows the variation of force versus time without fringing field effect. With a voltage equal to 3 volts, pull-in does not happen. At voltage 3.1 volts, force increases and causes pull-in instability. Then, by increasing the voltage, the applied force will grow. At a Lower voltage, V = 3.1 volts, the applied force is equal to -17.5021 (eV/Angstrom).

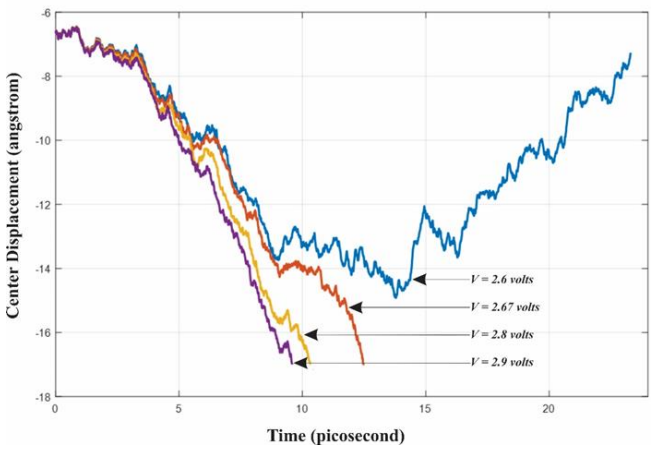


Fig. 6 Deflection of graphene versus time for different voltages with fringing effect; gap distance = 18 angstrom

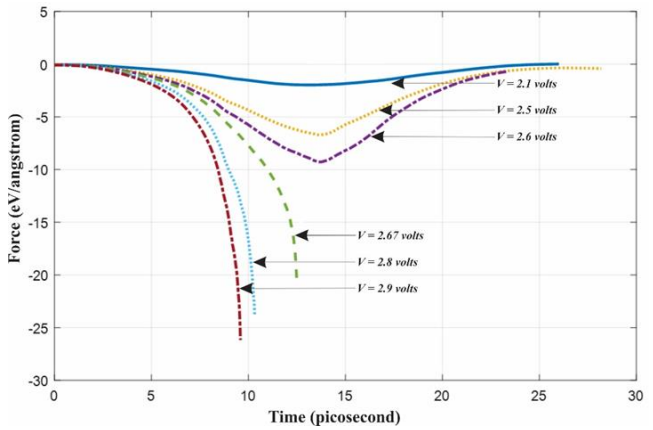


Fig. 7 Force variation during pull-in instability with fringing field effect; gap distance = 18 angstrom

More voltage reduced the time for the collapse of the graphene sheet.

Effect of the fringing field on pull-in instability of graphene sheet discussed in Figs. 6 and 7. The deflection in Fig. 6 is similar to Fig. 4. The difference is that by considering the fringing field effect, pull-in occurred in lower voltages. For the graphene sheet with specifications brought in Table 1, the pull-in voltage is 2.67 volts, recognizing the fringing field consequence.

Molecular dynamics studied the behavior of atoms under the electrostatic charges by allowing them to reach equilibrium. Carbon atoms in the structure of graphene have a natural vibration due to thermal energy. Fluctuations due to thermal energy in the presence of external forces cause a jump in displacement. Fig. 6 shows these jumps on the deflection.

As depicts in Fig. 7, pull-in happened with lower forces and lower voltages, considering the fringing effect. As shown, the lowest voltage of 2.67 (volts) causes a load of -20.3056 (eV/Angstrom) at a pull-in state. Based on Fig. 5, by considering the fringing effect correction in electrostatic force, a considerable increase in pull-in force is observed.

In practical cases for small actuators, the dimensions of mechanical electrodes are compared with the distance between two electrodes. The capacity created by the side

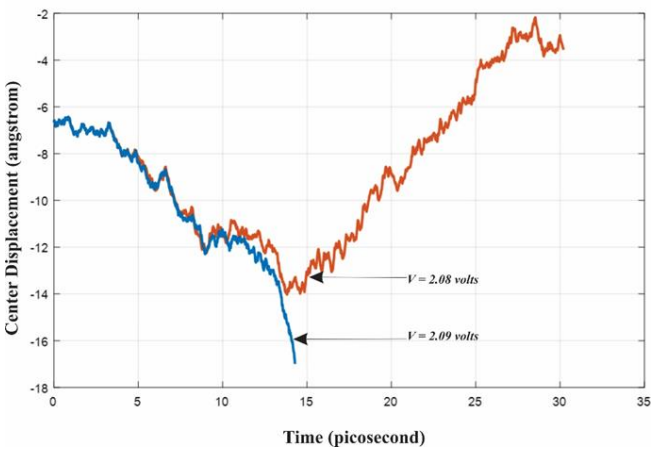


Fig. 8 Displacement of Armchair graphene sheet before & after pull-in with fringing effect and vdW force; gap distance = 18 A°

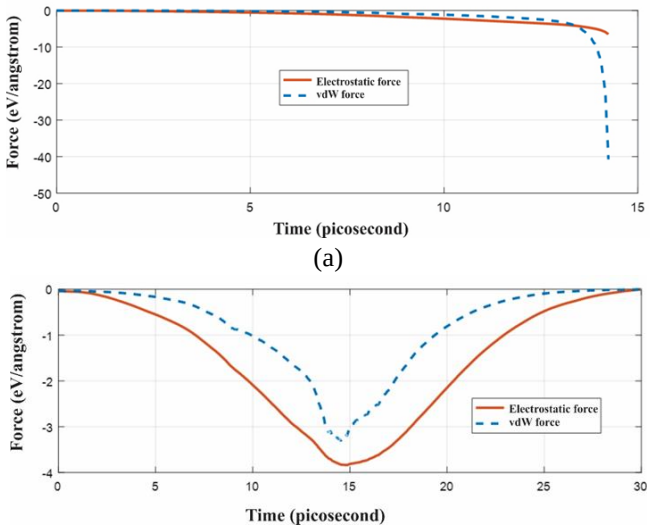


Fig. 9 (a) Armchair graphene force variation versus time "after" pull-in; V = 2.09 volts and gap distance = 18 A° and (b) Armchair graphene force variation versus time "before" pull-in; V = 2.08 volts and gap distance = 18 A°

Table 2 Pull-in voltages in graphene sheet (L = 20 nm, w = 1.8 nm, g = 1.8 nm)

Molecular simulation, Armchair graphene sheet	$V_{Pull\text{-}in}$ = 2.09 volts
Lin *et al*. 2019	$V_{Pull\text{-}in}$ = 2.05 volts

edges and even the back sides can play a significant role in the performance of actuators. The fringing effect has defined as the side edge effect. By adding the fringe effect to the electrostatic force, the force exerted on the graphene plate increases, which causes the pull-in phenomenon to occur at lower voltages.

Investigating the applied force to the graphene plate at different voltages (Fig. 7) shows that at lower voltage, the intermolecular forces will return the graphene plate to equilibrium. As shown in Fig. 7, as the voltage increases, the intermolecular forces continue to resist the electrostatic force. In this way, the graphene plate returns to its original state after some deformation. If the voltage exceeds a certain amount, the electrostatic force overcomes the interatomic forces, and the graphene plate sticks to the bottom plate, and finally, the pull-in instability occurs.

In the following, the vdW forces added to the electrostatic force with the fringing field. When the distance between two electrodes is below 20 nm, the vdW force must consider. The gap distance in this research is g = 18 Ao. Fig. 8 shows the deflections of the Armchair graphene sheet for several amounts of applied voltages. In voltage of 2.08 volts, graphene sheet after some steps reached the minimum deflection. Then the graphene sheet arose to the last stable level. This behavior is directly related to the force is applied to the graphene sheet. As depicted in Fig. 9, up to time about 14.7 (picosecond), the actuation force grows until the sheets reach maximum deflection (according to Eq. (12)).

Afterward, because the force is not enough for making collapse in the graphene sheet, the actuation force begins to decrease, and the sheet refers to its stable state. According to Fig. 9, until pull-in has not occurred, the vdW force is lower than the electrostatic force. But in pull-in voltage, V = 2.09 volts, when the upper electrode is near to fixed one, the effect of vdW force increased. And after a specified time step, the amount of vdW force became more than the electrostatic force.

Comparison of Fig. 9(b) shows that, at a voltage lower than the pull-in voltage, the van der Waals force is less than the electrostatic force at all stages of graphene deformation. At pull-in voltage, as graphene sheet deflected, the gap distance between two electrodes decreased, and the van der Waals force increased. In this stage, the van der Waals force will exceed the electrostatic force. The results reveal that, by considering vdW interaction and fringing effect in the MD model, the pull-in parameters will be close to the presented results in reference (Lin *et al*. 2019). Therefore, proposed model predicts pull-in instability accurately and illustrates the significance of the chirality and gap distance on the behavior of nanostructures.

Table 2 shows the comparison between pull-in voltages in which obtained from molecular dynamics simulation presented in our study and analytical results brought in reference (Lin *et al*. 2019)

Considering the van der Waals force reduces the instability voltage of the graphene sheet. We found that the influence of the van der Waals force on the pull-in instability of the graphene sheet depends on the geometrical specifications of graphene, such as the chirality and gap distance, etc.

Another issue is the structural effect of the graphene sheet on the pull-in voltages. In this section, we want to study the effect of the atoms' arrangement on the pull-in behavior of the zigzag structure of graphene and compare it with the behavior of the armchair graphene. Fig. 10 shows the deflection of the graphene sheet at a zigzag structure with two different voltages. At voltage of 2.38 volts, the graphene plate reaches a minimum deflection. It then returns to a stable energy level. By increasing the voltage, in V = 2.42 volts, the movable electrode sticks to the fixed

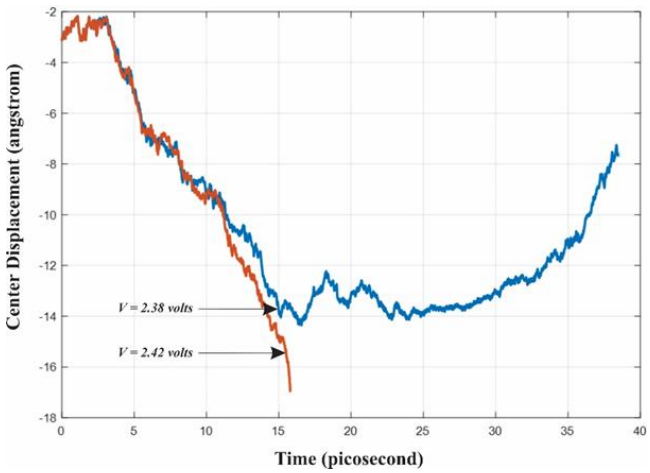
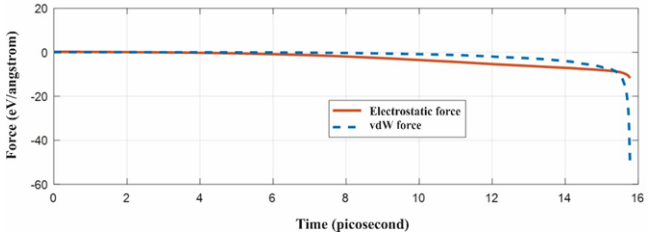
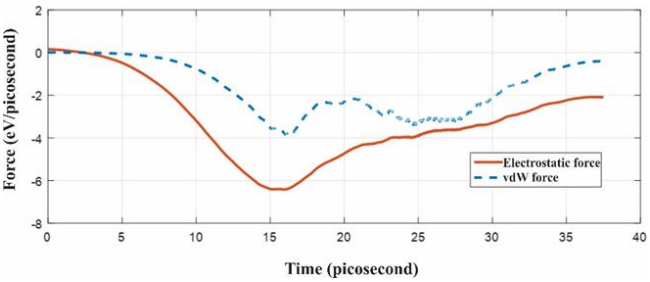


Fig. 10 Deflection in zigzag graphene before and after pull-in instability



(a)



(b)

Fig. 11 (a) Forces variation in zigzag graphene, after pull-in happening; V = 2.42 volts and gap distance = 18 angstrom and (b) Forces variation in zigzag graphene, before pull-in happening; V = 2.38 volts and gap distance = 18 angstrom

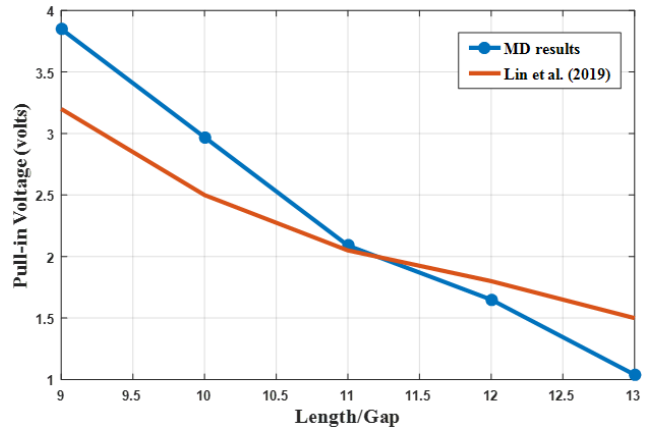
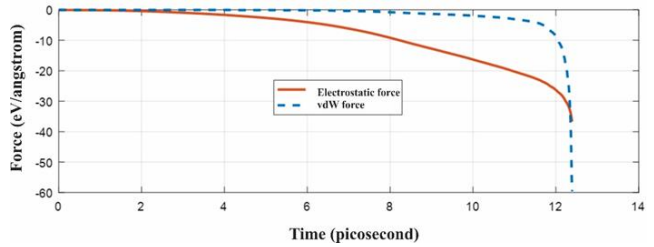
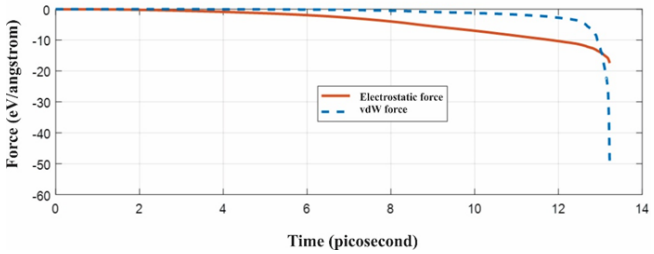


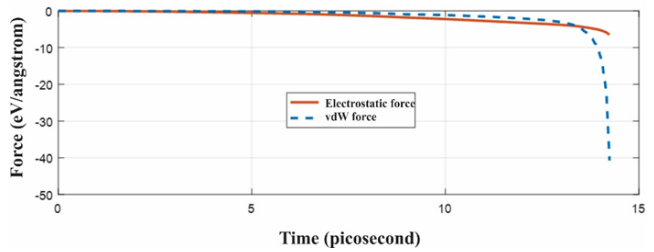
Fig. 12 Pull-in voltage variation versus length to gap ratio (L/g)



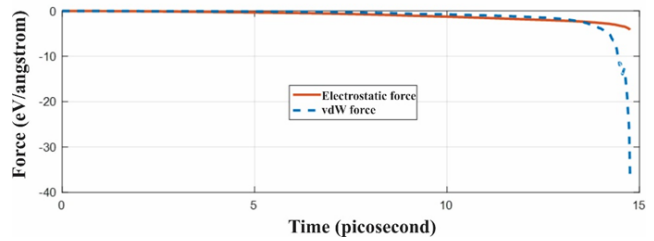
(a)



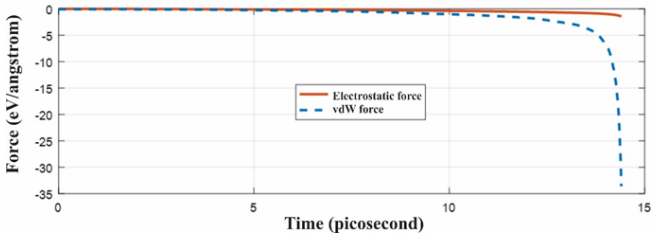
(b)



(c)



(d)



(e)

Fig. 13 Force variation in pull-in instability; (a) $V_{pull\text{-}in}$ = 3.85 volts and gap distance = 22.22 angstrom; (b) $V_{pull\text{-}in}$ = 2.97 volts and gap distance = 20 angstrom; (c) $V_{pull\text{-}in}$ = 2.09 volts and gap distance = 18 angstrom; (d) $V_{pull\text{-}in}$ = 1.65 volts and gap distance = 16.16 angstrom and (e) $V_{pull\text{-}in}$ = 1.04 volts and gap distance = 15.38 angstrom

electrode, and the pull-in instability happened. The electrostatic and vdW force depicts in Figs. 11(a) and 11(b). In this investigation, the zigzag graphene sheet is stiffer than the armchair structure. Therefore, the pull-in instability happened with higher voltages.

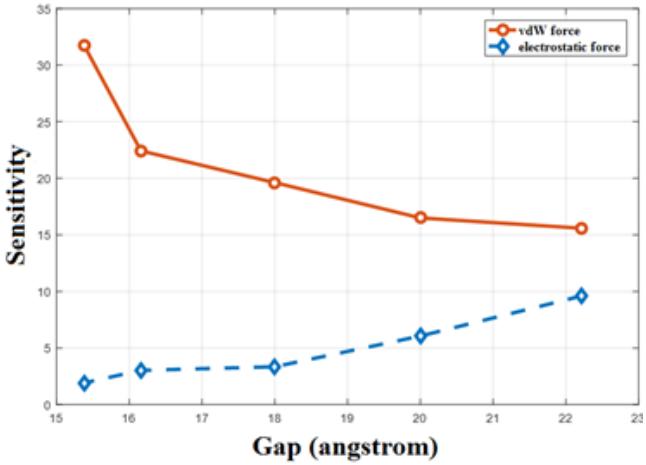


Fig. 14 The sensitivity of actuating forces to the gap distance

Fig. 11(b) shows that in zigzag graphene without the pull-in instability, the van der Waals force is less than the electrostatic force. The effect of length to gap distance ratio (L/G) on the pull-in parameters of the graphene sheet had estimated. Fig. 12 shows that by increasing the amount of L/G, the pull-in voltage decreased. The results are in good agreement with the reference (Lin *et al*. 2019). As the length-to-distance ratio between the two plates increases, the pull-in voltage decreases. Graphene with larger dimensions, at a fixed gap, bends faster and sticks to the lower electrode.

According to Fig. 12, at a constant gap, the pull-in voltage decreases with increasing the length of graphene. If the length of the graphene sheet increased, the flexibility is enhanced, and the sheet bends more easily. As mentioned before, the discrete structure of graphene has been considered. It is the reason for the difference between the results of this study and the reference results. But, in the reference, authors used the size-dependent-based continuum theories. They modeled the graphene sheet as a thin layer and used Bernoulli-Euler beam theory to study pull-in instability.

Fig. 13 clearly shows that the obtained pull-in voltage is directly affected by the van der Waals force. The portion and effect of van der Waals force increase as the gap distance decreases. Therefore, more analysis requires for predicting the relation between applied force and the gap distance. The sensitivity of the nano switch for electrostatic and van der Waals forces is calculated based on the following formula, deviation as the output divided by excitation voltage as input (Fig. 14). We need less gap to increase the sensitivity of the van der Waals force and reduce the pull-in voltage. For the electrostatic force, gap distance increased the sensitivity, but in this condition, the pull-in voltage increases, which is not desirable. As shown in Figs. 13 and 14, the gap distance should be shorter to require less voltage in pull-in instability and to be able to take advantage of the nano switch sensitivity to van der Waals force.

This case study shows that the actuators are very sensitive to the vdW forces in small gap distances. Therefore, ignoring the effect of molecular attraction (vdW) for a wide range of real applications can cause a significant error in calculating the pull-in voltage of nanomaterials at a gap distance below 18 nm.

6. Conclusions

In this study, the molecular dynamics simulation of pull-in instability in a single-layer graphene sheet has been performed. The results presented the influences of the applied voltage and intermolecular forces on the pull-in behavior of nano-actuator. The AIREBO potential defined the atom interactions. The applied loads are composed of electrostatic and vdW forces. It depicts that the pull-in behavior depends on the fringing field effect, relating to the size effect. Additionally, results show that by reducing the gap distance, the portion of the vdW force increased. Furthermore, the presented analysis illustrated the variation of pull-in voltage, deflection of atoms in the graphene sheet, electrostatic and vdW forces versus the system parameters.

The vdW force causes the reduction of the time and the voltage required to reach pull-in instability. The effect of geometry parameters, such as armchair and zigzag and length to gap distance ratio onto pull-in voltage, was investigated. Results indicated that the required pull-in voltage reduced when the length-to-gap ratios increased. Results showed that the zigzag structure is stiffer than the armchair structure. Therefore, the zigzag graphene sheet had increasing effects on the pull-in parameters. The evaluation of the sensitivity of the forces to the gap distance shows that to take advantage of the van der Waals force effect, we must reduce the gap distance. Then, the pull-in voltage will also decrease.

Furthermore, for the graphene sheet, pull-in voltage and minimum gap distance, as fundamental design parameters of actuators, have been determined. The results of MD analysis were compared and validated with those obtained by previous semi-analytical results and had good agreement with previous works.

References

Abdi, J., Koochi, A., Kazemi, A. and Abadyan, M. (2011), "Modeling the effects of sizedependence and dispersionforces on the pull-in instability of electrostatic cantilever NEMS using modified couple stress theory", *Smart Mater. Struct.*, **20**(5), 055011.

Ansari, R., Ajori, S. and Hassani, R. (2016), "A molecular dynamics investigation into the size-dependent buckling behavior of a novel three-dimensional metallic carbon nanostructure", *Superlattice Microst.*, **97**, 125-131. https://doi.org/10.1016/j.spmi.2016.06.012.

Ansari, R., Gholami, R., Shojaei, M.F., Mohammadi, V. and Darabi, MA. (2012), "Surface stress effect on the pull-in instability of hydrostatically and electrostatically actuated rectangular nanoplates with various edge supports", *J. Eng. Mater. Technol.*, **134**(4), 041013. https://doi.org/10.1115/1.4007260.

Attia, M.A. and Mohamed, S.A. (2019), "Coupling effect of surface energy and dispersion forces on nonlinear size-

dependent pull-in instability of functionally graded micro-nanoswitches", *Acta Mech*., **230,** 1181-1216. https://doi.org/10.1007/s00707-018-2345-6.

Batra, R.C., Porfiri, M. and Spinello, D. (2008), *Pull-In Instability in Elecrostatically Actuated MEMS*, Imperial College Press, London, U.K.

Batra, R.C., Porfiri, M. and Spinello, D. (2006), "Capacitance estimate for electrostatically actuated narrow microbeams", *Micro Nano Lett*., **1**(2), 71-73. https://doi.org/10.1049/mnl:20065046.

Cheng, J., Zhe, J. and Wu, X. (2003), "Analytical and finite element model pull-in study of rigid and deformable electrostatic microactuators", *J. Micromech. Microeng*., **14**(1), 57-68. https://doi.org/10.1088/0960-1317/14/1/308.

Dequesnes, M., Rotkin, S. and Aluru, N. (2002), "Calculation of pull-in voltages for carbonnanotube- based nanoelectromechanical switches", *Nanotechnology*., **13**(1), 120-131. https://doi.org/10.1088/0957-4484/13/1/325.

Farazinand, A. and Mohammadimehr, M. (2020), "Nano research for investigating the effect of SWCNTs dimensions on the properties of the simulated nanocomposites: A molecular dynamics simulation", *Adv. Nano Res*., **9**(2), 83-90. http://doi.org/10.12989/anr.2020.9.2.083.

Fakhrabadi, M.M.S., Khorasani, P.K., Rastgoo, A. and Ahmadian, M.T. (2013), "Molecular dynamics simulation of pull-In phenomena in carbon nanotubes with stone-wales defects", *Solid State Commun*., **157,** 38-44. https://doi.org/10.1016/j.ssc.2012.12.016.

Genoese, A., Genoese, A. and Salerno, G. (2020), "In-plane and out-of-plane tensile behavior of single-layer graphene sheets: A new interatomic potential", *Acta Mech*., **231**(7), 2915-2930. https://doi.org/10.1007/s00707-020-02680-0.

Gupta, R.K. (1997), "Electrostatic pull-in test structure design for in-situ mechanical property measurements of microelectromechanical systems", Ph.D. Dissertation, Massachusetts Institute of Technology (MIT), Cambridge, Massachusetts, U.S.A.

Guo, J.G. and Zhao, Y.P. (2004), "Influence of van der Waals and Casimir forces on electrostatic torsional actuators", *J. Microelectromech. S*., **13**(6), 1027-1035. http://doi.org/10.1109/JMEMS.2004.838390.

Hamaker, H.C. (1937), "The London-van der Waals attraction between spherical particles" *Physica*, **4**(10), 1058-1072. https://doi.org/10.1016/S0031-8914(37)80203-7

Yang, J., Jia, X.L. and Kitipornchai, S. (2008), "Pull-in instability of nano-switches using nonlocal elasticity theory", *J. Phys. D Appl. Phys*., **41**(3), 035103. https://doi.org/10.1088/0022-3727/41/3/035103.

Korobeynikov, S.N., Alyokhin, V.V. and Babichev, A.V. (2018), "Simulation of mechanical parameters of graphene using the DREIDING force field", *Acta Mechanica*., **229**(6), 2343-2378. https://doi.org/10.1007/s00707-018-2115-5.

Kuang, J.H. and Chen, C.J. (2005), "Adomian decomposition method used for solving nonlinear pull-in behavior in electrostatic micro-actuators", *Math. Comput. Model*., **41**, 1479-1491. https://doi.org/10.1016/j.mcm.2005.06.001.

Kumar, B.R. (2018), "Investigation on mechanical vibration of double-walled carbon nanotubes with inter-tube Van der waals forces", *Adv. Nano Res*., **6**(2), 135-145. http://doi.org/10.12989/anr.2018.6.2.135.

Ke, C.H., Pugno, N., Peng, B. and Espinosa, H.D. (2005), "Experiments and modeling of carbon nanotube-based NEMS devices", *J. Mech. Phys. Solids*., **53**(6), 1314-1333. https://doi.org/10.1016/j.jmps.2005.01.007.

Leite, F.L., Bueno, C.C., Da-Róz, A.L., Ziemath, E.C. and Oliveira, O.N. (2012), "Theoretical models for surface forces and adhesion and their measurement using atomic force microscopy", *Int. J. Mol. Sci*., **13**(10), 12773-12856. https://doi.org/10.3390/ijms131012773.

Lv, J., Bai, M. and Cui, W. (2011), "The molecular dynamic simulation on impact and friction characters of nanofluids with many nanoparticles system", *Nanosc. Res. Lett*., **6**(1), 1-8. https://doi.org/10.1186/1556-276X-6-200.

Lin, M., Lee, S. and Chen, C. (2019), "Nonlocal effect on the pull-in instability analysis of graphene sheet nano-beam actuator", *J. Mech*., **35**(5), 767-778. https://doi.org/10.1017/jmech.2018.41.

Lu, P., Lee, H.P., Lu, C. and Zhang P.Q. (2007), "Application of nonlocal beam models for carbon nanotubes", *Int. J. Solids Struct*., **44**(16), 5289-5300. https://doi.org/10.1016/j.ijsolstr.2006.12.034.

Lin, W.H. and Zhao, Y.P. (2003), "Dynamic behavior of nanoscale electrostatic actuators", *Chinese. Phys. Lett*., **20**, 2070-2073. https://doi.org/10.1088/0256-307X/20/11/049.

Mousavi, T., Bornassi, S. and Haddadpour H. (2013), "The effect of small scale on the pull-in instability of nano-switches using DQM", *Int. J. Solids. Struct*., **50**(9), 1193-1202. https://doi.org/10.1016/j.ijsolstr.2012.11.024.

Maugis, D. (2000), *Contact, Adhesion, and Rupture of Elastic Solids*, Springer-Verlag, Berlin, Germany.

Nazemnezhad, R., Zare, M., Hosseini-Hashemi, S. and Shokrollahi, H. (2016), "Molecular dynamics simulation for interlayer interactions of graphene nanoribbons with multiple layers", *Superlattice Microst*., **98**, 228-234. https://doi.org/10.1016/j.spmi.2016.08.036.

Plimpton, S.J. (1995), "Fast parallel algorithms for short-range molecular dynamics", *J. Comput. Phys.* **117**(1), 1-19. https://doi.org/10.1006/jcph.1995.1039.

Ramezani, A., Alasty, A. and Akbari, J. (2007), "Closed-form solutions of the pull-in instability in nano-cantilevers under electrostatic and intermolecular surface forces", *Int. J. Solids Struct*., **44**(14), 4925-4941. https://doi.org/10.1016/j.ijsolstr.2006.12.015.

Rotkin, S.V. (2002), "Analytical calculations for nanoscale electromechanical systems", *Electrochem. Soc. Proc*., **6**, 90-97.

Rokni, H. and Lu, W. (2013), "A continuum model for the static pull-in behavior of graphene nanoribbon electrostatic actuators with interlayer shear and surface energy effects", *J. Appl. Phys*., **113**(15), 153512. https://doi.org/10.1063/1.4800543.

Sedighi, H.M., Daneshmand, F. and Zare, J. (2014), "The influence of dispersion forces on the dynamic pull-in behavior of vibrating nano-cantilever based NEMS including fringing field effect", *Arch. Civil Mech. Eng*., **14**(4), 766-775. https://doi.org/10.1016/j.acme.2014.01.004.

Sutrakar, V.K., Subramanya, N. and Mahapatra, D.R. (2015), "Crack growth prediction and cohesive zone modeling of single crystal aluminum: A molecular dynamics study", *Adv. Nano Res*., **3**(3), 143-168. http://doi.org/10.12989/anr.2015.3.3.143.

Stuart, S.J., Tutein, A.B. and Harrison, J.A. (2000), "A reactive potential for hydrocarbons with inter-molecular interactions", *J. Chem. Phys*., **112**(14), 6472. https://doi.org/10.1063/1.481208.

Taghavi, N. and Nahvi, H. (2013), "Pull-in instability of cantilever and fixed-fixed nano-switches", *Eur. J. Mech. A Soild*, **41**, 123-133. https://doi.org/10.1016/j.euromechsol.2013.03.003.

CC