Mechanical properties of multi-walled beryllium-oxide nanotubes: a molecular dynamics simulation study

Yaser Rostamiyan1 · Navid Shahab1 · Christos Spitas2 · Amin Hamed Mashhadzadeh2

Received: 3 March 2022 / Accepted: 29 August 2022 / Published online: 6 September 2022
© The Author(s), under exclusive licence to Springer-Verlag GmbH Germany, part of Springer Nature 2022

Abstract

Molecular dynamic (MD) simulation was employed to take the molecular fingerprint of mechanical properties of beryllium-oxide nanotubes (BeONTs). In this regard, the effect of the radius, the number of walls (single-, double-, and triple-walled), and the interlayer distance, as well as the temperature on the Young’s modulus, failure stress, and failure strain, are visualized and discussed. It was unveiled that larger single-walled BeON Ts have lower Young’s modulus in zigzag and armchair direction, and the highest Young’s modulus was obtained for the (8,0) zigzag and (4,4) armchair SWBeONTs as of 645.71 GPa and 624.81 GPa, respectively. Unlike Young’s modulus, however, the failure properties of the armchair structures were higher than those of zigzag ones. Furthermore, similar to SWBeONTs, an increase in the interlayer distance of double-walled BeON Ts (DWBeONTs) led to a slight reduction in Young’s modulus value, while no meaningful trend was found among failure behavior. For double-walled BeONTs (TWBeONTs), the elastic modulus was obviously higher in both armchair and zigzag directions compared to DWBeONTs.

Keywords Molecular dynamics · Beryllium-oxide nanotube · Young’s modulus · Multi-walled nanotube

Introduction

Non-carbon nanotubes, also called inorganic nanotubes, are a class of nanomaterials that have recently been widely considered by the researchers, similar to carbon nanotubes, due to their outstanding mechanical, optical, thermal, and electronic properties. These nanostructures mainly include metal-oxide nanotubes such as zinc-oxide (ZnO), beryllium-oxide (BeO), and titanium-oxide (TiO2); nitride-based nanotubes such as boron-nitride (BN), aluminum-nitride (AlN), and gallium-nitride (GaN); and also nanotubes composed of the elements of group VI periodic table such as silicon-carbide (SiC) and silicon-germanium (SiGe), widely considered in both theoretical and experimental research studies [1–7]. However, since the experimental approaches usually compel a high amount of expenditure on the research projects, theoretical studies have become more popular over the past few decades.

Ab initio–based density functional theory (DFT) and molecular dynamic (MD) simulation are the most used theoretical techniques for investigating the properties of nanotube structures, and the results of these methods have been reported to be close to those of experimental data [8, 9]. In this regard, Jun-Hua et al. investigated the mechanical properties of AlN nanotubes with both zigzag and armchair chirality using DFT and found that an increase in the diameter of both types of AlNNTs resulted in higher Young’s modulus as well as band gap energy [10]. Cong et al. studied the mechanical properties of different boron-nitride/aluminum nanocomposite by the employment of MD simulations. They reported that higher Young’s modulus, yield strain, and yield stress were obtained in nanotubes with higher diameters [11]. Liu et al. combined MD and DFT to probe the properties of single-walled SiGeNTs with zigzag and armchair chirality and reported that nanotubes with larger dimensions were more stable structures than those with smaller dimensions [12]. In a DFT study, ZnO nanotube was compared with the ZnO sheet with their adsorption properties by Hamed Mashahdzadeh and his coworkers.
They found that ZnO showed better adsorption capacity in nanotube form compared to sheet form [13].

Beryllium oxide (BeO) is a semiconducting oxide where its graphene form was firstly introduced by Contineza in the 1990s [14]. This nanostructure exhibits considerable properties such as high electrical resistivity, outstanding thermal conductivity, acceptable energy storage capability, and good hardness so that it has recently become a subject of many research studies [15–18]. Sorokin et al. made a comparison between the properties of BeO nanotubes and BeO graphene–like structures using a DFT research work. They found higher stability of these structures compared to single BeO molecules [19]. In another DFT-based study, Fathalian et al. considered the H$_2$ adsorption properties of zigzag BeONTs and showed these nanotubes would be suitable candidates for this purpose [20]. In addition to single nanotubes, the properties of some other nanostructures developed from these nanotubes including multi-walled, functionalized, doped, and defective structures have also been attractive for researchers. Anota et al. employed the DFT method to find out the effect of functionalization on the electronic behavior of BeONTs which were functionalized by the hydroxyl (–OH) group and found that the semiconducting properties of nanotubes remained almost unchanged after functionalization [21].

Fereidoon et al. considered Young’s modulus of zigzag and armchair one-, two-, and three-wall boron-nitride nanotubes (BNNTs) versus the number of walls using molecular dynamic (MD) simulations and found higher moduli versus adding more walls to the nanotube [22]. In a defect investigation work, Andressa et al. used the DFT technique for considering the effect of vacancy defects on the electronic levels of boron-nitride nanotubes and showed that vacancies could improve the electronic levels of this nanotube and make it an appropriate choice for adsorbing H$_2$ molecules [23]. MD was employed in another study by Yang et al. to consider the fracture mechanism of single-walled CNT under vacancy and Stone–Wales defects. Their results demonstrated that Stone–Wales defects decrease the nanotube concentration compared to vacancy defects [24].

In a previous work, we studied mechanical properties of multi-walled beryllium oxide (BeO) nanotubes and nanopapod using DFT computations [18]. However, DFT outcomes are just mathematical outcomes based on modulus performed at absolute temperature. To capture other mechanical properties as a function of time as well as to pattern fracture behavior in a scale which is close to the real case in a computationally cost-effective manner, one needs to use MD simulation [25, 26]. Moreover, mechanical properties of nanotubes are severely dependent on their length, which can be imaged in MD computational analysis [27]. Herein, we used MD simulation to study the effect of diameter, temperature, and the number of walls and on mechanical behavior of multi-walled BeO nanotubes in armchair and zigzag chirality. The Young’s modulus, failure stress, and failure strain of one-, two-, and three-walled BeO nanotubes were modeled and discussed at constant and variable temperature.

### Computational section

Molecular dynamic (MD) technique which is based on Newton’s second law using classical mechanics [28] was applied in this article to consider the mechanical properties of the armchair and zigzag one-, two-, and three-wall BeONTs. Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) was employed to model the under evaluation nanostructures as well as considering the long-range Coulomb atomic interactions. MD is able to provide scalable codes; it makes LAMMPS act on parallel platforms efficiently [29]. Visual molecular dynamics (VMD) indicator was selected to analyze the results obtained from simulation due to being an appropriate tool for supporting various formats and outputs particularly those obtained from LAMMPS. Selecting a suitable potential function is a critical factor for simulating through MD because this function directly affects the precision of the results. In this work, classical multi-body Tersoff potential was used to define the interactions among the elements of the simulated systems [30]. Since the interactions defined by Tersoff are based on the bond orders, this potential function is suitable for determining different bond states of atoms using the same parameters [30]. Furthermore, periodic boundary conditions should be applied along the axial direction by the employment of isoenthalpic-isobaric ensemble (NPT). The temperature varied between 300 and 1000 K for all single-walled structures and was set to 300 K for multi-walled and defective ones. Besides, the pressure was set to 1 bar, and we also applied non-equilibrium simulation mode to allow the ends of the BeONTs to move along the loading direction at a predefined and a consistent strain rate. In some of the previous studies, the most acceptable results were achieved when the time step was between 0.5 and 0.8 fs, and in other studies, this variable was adjusted between 0.1 and 1 fs for uniaxial tensile tests [28, 31]. To perform tensile tests by MD simulations, strain should be applied to the nanotubes at a constant rate, and, as far as we know, the failure of the under loading structure is related to the strain rate, so lower strain rates provide the system enough time to be relaxed [32]. Since the strain rates in the range of 0.0005 Ps$^{-1}$ and 0.01 Ps$^{-1}$ have extensively been employed in MD research studies [22, 27], we selected strain rate and time step equal to 0.01 Ps$^{-1}$ and 1 fs respectively. To consider the mechanical behavior, different single-walled, multi-walled, and defective BeONTs were put under uniaxial tensile loading to obtain
stress–strain evaluation plots, and the stress–strain relation was used to calculate the failure stress, failure strain, and Young’s modulus of all simulated BeO nanotubes.

**Results and discussion**

**Geometrical design**

To investigate the mechanical behavior of one-, two-, and three-wall BeONTs, all zigzag and armchair samples were designed under the MD framework. Figure 1 presents a schematic of the simulated nanotubes studied in the current article, and Table 1 includes all of the structures that were simulated along with their number of atoms. The average Be–O bond length was obtained equal to 1.57 Å and 1.58 Å for the zigzag and armchair structures respectively which are in good accordance with the results of the earlier studies [33–36].

**Mechanical properties of single-walled BeONTs**

Concerning the mechanical properties of single-walled BeO nanotubes, seven zigzag nanotube structures including (8,0), (10,0), (12,0), (14,0), (16,0), (18,0), and (20,0) and five armchair structures including (4,4), (6,6), (8,8), (10,10), and (12,12) were simulated using MD. To calculate Young’s modulus, we put all samples under uniaxial tensile loading, and stress–strain curves were plotted accordingly. A schematic of a double-walled nanotube under tensile...
loading is presented in Figs. 2, and 3a shows a stress–strain curve which is plotted for zigzag structure (8,0). As seen, the stress–strain relation is not linear, so to calculate Young’s modulus, we fitted a second-order polynomial to the linear part of the stress–strain plot regarding Fig. 3b. The elastic modulus was calculated through the following equation:

$$\sigma = \frac{\partial U}{\partial \epsilon} = D\epsilon^2 + E\epsilon + C$$  \hspace{1cm} (1)$$
in which $D$ is the third-order elastic modulus, $E$ is entitled to Young’s modulus, and $C$ is the residual stress of BeO nanotubes. This process is repeated throughout the manuscript to find out the moduli of double-walled and triple-walled BeONTs as well. Furthermore, since failure starts when the stress reaches the highest value, the highest stress value on the stress–strain plot (peak point) introduces the failure stress, and the corresponding strain value would be the failure strain of the nanostructure. Young’s modulus, failure stress, and failure strain of all single-walled structures are collected in Fig. 4. We can see that an increase in the tubes’ diameter resulted in a small decrease in Young’s modulus of both chirality while failure properties remained almost unchanged. Young’s modulus of the zigzag structures was higher than those of the armchair ones with the close radius. The highest obtained moduli belonged to the zigzag structure (8,0) and armchair structure (4,4) with the magnitudes of 645.71 GPa and 624.81 GPa respectively. This property decreased by nearly 7% for both considered chirality. Unlike Young’s modulus, failure stress and failure strain of the armchair BeONTs were higher than those of zigzag BeONTs in every considered structure. According to Fig. 4, we see that these properties showed some negligible fluctuations versus an increase in the nanotubes’ diameter, and we could observe no
meaningful trend. The similar trend for all mechanical properties was reported for Silicon–Germanium nanotubes (SiGeNT) by Dadrasi et al. [37]. Moreover, in another work, Memarian et al. [27] reported that all of the mechanical properties of the SiC nanotubes in the armchair direction are higher than those of the zigzag. In another study, Salmankhani et al. [38] reported that failure stress and failure strain for C3N nanotube in armchair direction are significantly higher than those for zigzag. To provide a better comprehension of the failure process, a snapshot of the failure process that is presented for a zigzag (8,0) structure is displayed in Fig. 5. The figure demonstrates that failure started at the tube length of 56.016 Å and continued until the complete rupture of the structure at the tube length of 63.114 Å, so a total of 19% length increment occurred between the starting and the finishing points of the failure process. To make a comparison with earlier studies about the effect of radius on Young’s modulus, Hao et al. considered the Young’s modulus of the zigzag and armchair AINNTs under MD and reported that radius increment resulted in elastic modulus increment of the zigzag structures while it did not change the moduli of the armchair configuration considerably [10]. Similarly, in another MD research, Memarian et al. showed an increase in Young’s modulus of both zigzag and armchair SWCNTs versus growth in the tubes’ diameter [27]. Setoodeh et al., in their MD study, showed that the changes in Young’s modulus of SWSiGeNTs versus radius were insignificant [39]. Furthermore, to investigate the effect of temperature on the mechanical properties of BeONTs, (10,10) armchair and (18,0) zigzag structures were put under uniaxial loading while the temperature varied from 300 to 1000 K constantly, and the results are shown in Fig. 6. As we expected, Young’s modulus of both chirality reduced via temperature rising gradually so the lowest magnitudes of this property were seen at 1000 K with the magnitudes of 507.89 GPa and 528.64 GPa for (18,0) and (10,10), respectively. This could be associated with the higher vibration of the nanotube’s elements as a result of the temperature increment which increases the instability of the system. Also, unlike the radius variation which

---

**Fig. 4**  
(a) Young’s modulus, (b) failure stress, and (c) failure strain of SWBeONTs under uniaxial tensile test at 300 K

---

**Fig. 5** Snapshots of a continuous zigzag SWBeONT (8,0) failing under tensile loading condition at 300 K (unit in Angstrom for length)
had not affected the failure properties significantly, failure stress and failure strain of both mentioned BeONTs decreased by temperature increase. Similar results were reported by Setoodeh et al. about the buckling load of SiGeNTs via temperature growing [39]. In the above mentioned MD research, Memarian et al. showed a reduction in Young’s modulus and failure properties of SWCNT via temperature rising [27]. In another work by Dadras et al. [37], reduction trend in all mechanical properties by increasing the temperature was observed for SiGeNT. Moreover, they reported that the mechanical properties of SiGeNT (10,10) are higher than (18,0) in all the studied temperatures. In another MD study, similar reduction for all mechanical properties was observed for CNT and C₃N nanotube [38].

Mechanical properties of double-walled BeONTs

At this stage, we modeled four zigzag double-walled structures including (8,0)@(14,0), (8,0)@(15,0,), (8,0)@(16,0), and (8,0)@(17,0) and three armchair structures including (4,4)@(8,8), (4,4)@(9,9), and (4,4)@(10,10) as shown in Fig. 7. Interlayer distance has undoubtedly increased with an increase in the based nanotubes’ radius. As well as the previous section, all double-walled structures were put under uniaxial tensile loading, and the obtained results are illustrated in Fig. 8. Regarding Fig. 8, we can see that armchair and zigzag structures revealed contradictory behavior via interlayer distance. Similar to single-walled structures, Young’s modulus of zigzag DWBeONTs generally reduced (except one point) via an increase in the interlayer distance while this property rose constantly via the increase in interlayer distance of the armchair structures. The highest calculated values of Young’s modulus belonged to (8,0)@(15,0,) zigzag and (4,4)@(10,10) armchair DWBeONTs with the magnitudes of 659.75GPa and 640.67GPa, respectively. In an MD theoretical approach, Fereidoon et al. found a reduction in Young’s modulus of both armchair and zigzag DWBNNTs via interlayer distance rising [15]. Furthermore, the failure properties of the zigzag double-walled structures did not show a significant trend as well as single-walled ones while the failure stress and failure strain of the armchair DWBeONTs increased slightly similar to what we had already observed for Young’s modulus of this chirality. Besides, a snapshot of the failure process of zigzag (8,0)@(14,0) structure is presented in Fig. 9. This figure demonstrates that the failure of the double-walled structure which started from the inner layer occurred at the same length increment compared to the single-walled one (19% against 19%), and the inner layer failed sooner than the outer one.

Mechanical properties of triple-walled BeONTs

To study more about the effect of adding walls on the properties of nanotubes, a triple-walled (8,0)@(14,0)@(20,0) zigzag BeONT and a triple-walled (4,4)@(8,8)@(12,12) armchair BeONT were simulated using MD as seen in Fig. 10. By putting both samples under uniaxial tensile loading, we obtained the values of Young’s modulus equal to 668.04 GPa and 647.57 GPa for zigzag and armchair TWBeONTs, respectively. These results are in agreement with those of single-walled and double-walled results which had demonstrated higher modulus for the zigzag BeONTs compared to armchair ones. Similarly, failure properties of the armchair TWBeONTs were higher than those of zigzag ones similar to what we had already found in SWBeONTs (see Fig. 4). The variation of Young’s modulus with adding walls is displayed in Fig. 11. This figure confirms that with raising the number of walls from one to two and then three, Young’s modulus of both chirality increased slightly so adding
walls could result in nanotubes with better mechanical properties. In the MD research, Dadrasi and his co-workers observed that by increasing the number of layers in SiGENTs, Young’s modulus increased for both armchair and zigzag directions, which is in agreement with the present results [37]. Moreover, they demonstrated that Young’s zigzag configuration modulus is higher than the zigzag ones.

**Conclusion**

In the present work, we employed molecular dynamic (MD) simulation to evaluate the mechanical properties of single-, double-, and triple-walled beryllium-oxide nanotubes (BeONTs) in armchairs and zigzag directions. We found that Young’s modulus of single-walled BeONTs decreased via the increase in radius as well as temperature so that the highest obtained values of this property occurred in the zigzag structure (8,0) and armchair structure (4,4) with the magnitudes of 645.71 GPa and 624.81 GPa respectively. Failure strain of the SWBeONTs while temperature growth dwindled these properties for both chirality slightly. Unlike Young’s modulus, the failure properties of the armchair structure were better than those of the zigzag structures. Furthermore, concerning the modulus of DWBeONTs, an interlayer distance increment resulted in Young’s modulus reduction as same as SWBeONTs. Moreover, adding another wall to double-walled BeONTs
Fig. 9 Snapshots of a continuous zigzag DWBeONT (8,0)@(14,0) failing under tensile loading condition at 300 K (unit in Angstrom for length)

Fig. 10 The schematics of TWBeONTs a zigzag (8,0)@(14,0)@(20,0) and b armchair (4,4)@(8,8)@(10,10) with different interlayer distance (unit in Angstrom for length)
improved the young's modulus of both chiralities so that the modulus of the triple-walled structures (8,0)@(14,0)@(20,0) and (4,4)@(8,8)@(12,12) with the corresponding magnitudes of 668.04 GPa and 647.57 GPa were higher than those of DWBeONTs (8,0)@(14,0) and (4,4)@(8,8) with the values of 649.69 GPa and 636.12 GPa as well as SWBeONTs (8,0) and (4,4) with the magnitudes of 645.71 GPa and 624.81 GPa respectively.

**Author contribution** Navid Shahab analyzed the data, discussed the results, and designed the figures and table. Yasser Rostamiyan analyzed and rechecked the results for correctness and supervising. Christos Stephanos supervising and wrote the initial draft. Amin Hamed Mashhadzadeh designed the case study, wrote the LAMMPS code of the present article, and carried out the computational measurements. All the authors have read and agreed to the published version of the manuscript.

**Data availability** Available by the corresponding author per request through the email (amin.hamed.m@gmail.com).

**Code availability** Available by the corresponding author per request through the email (amin.hamed.m@gmail.com).

**Declarations**

**Competing interests** The authors declare no competing interests.

**References**

1. Samadipakchin P, Mortaheb HR, Zolfaghari A (2017) ZnO nanotubes: preparation and photocatalytic performance evaluation. J Photochem Photobiol, A 337:91–99. [https://doi.org/10.1016/j.jphotochem.2017.01.018](https://doi.org/10.1016/j.jphotochem.2017.01.018)

2. Marana NL, Casassa S, Longo E, Sambrano JR (2018) Computational simulations of ZnO@GaN and GaN@ZnO core@shell nanotubes. J Solid State Chem 266:217–225. [https://doi.org/10.1016/j.jssc.2018.07.023](https://doi.org/10.1016/j.jssc.2018.07.023)

3. Nia BA, Shahrokhi M (2018) Dilute magnetic semiconductor and half-metal behaviors in C-codoped BeO nanotubes: a first principles simulations. Chin J Phys 56:3039–3045. [https://doi.org/10.1016/j.jchemphys.2018.10.013](https://doi.org/10.1016/j.jchemphys.2018.10.013)

4. DE Kim D Pak (2019) Ti plate with TiO2 nanotube arrays as a novel cathode for nitrate reduction. Chemosphere. [https://doi.org/10.1016/j.chemosphere.2019.04.071](https://doi.org/10.1016/j.chemosphere.2019.04.071)

5. Taguchi T, Igawa N, Yamamoto H, Jitsukawa S (2005) Synthesis of silicon carbide nanotubes. J Am Ceram Soc 88:459–461. [https://doi.org/10.1111/j.1551-2916.2005.00066.x](https://doi.org/10.1111/j.1551-2916.2005.00066.x)

6. Krause M, Müßlich A, Zak A, Seifert G, Gemming S (2011) High resolution TEM study of WS2 nanotubes. Phys Status Solidi (b) 248:2716–2719. [https://doi.org/10.1002/pssb.201000076](https://doi.org/10.1002/pssb.201000076)

7. Jiang Z, Xie T, Wang GZ, Yuan XY, Ye CH, Cai WP et al (2005) GeO2 nanotubes and nanorods synthesized by vapor phase reactions. Mater Lett 59:416–419. [https://doi.org/10.1016/j.matlet.2004.09.036](https://doi.org/10.1016/j.matlet.2004.09.036)

8. Ganji M, Sharifi N, Ahangari MG (2014) Adsorption of H2S molecules on non-carbonic and decorated carbonic graphene: a van der Waals density functional study. Comput Mater Sci 92:127–134

9. Ahangari MG, Fereidoon A, Jahanshahi M, Ganji M (2013) Electronic and mechanical properties of single-walled carbon nanotubes. J Phys Condens Matter 25:455301.
nanotubes interacting with epoxy: a DFT study. Physica E 48:148–156. https://doi.org/10.1016/j.physe.2012.01.013
10. Hao J-H, Wang Y-F, Yin Y-H, Jiang R, Wang Y-F, Jin Q-H (2015) An ab initio study of the size-dependent mechanical behaviour of single-walled AlN nanotubes. Solid State Sci 45:30–34. https://doi.org/10.1016/j.solidstatesciences.2015.05.001

11. Cong Z, Lee S (2018) Study of mechanical behavior of BNNT-reinforced aluminum composites using molecular dynamics simulations. Compos Struct 194:80–86. https://doi.org/10.1016/j.compstruct.2018.03.103

12. Liu X, Cheng D, Cao D (2009) The structure, energetics and thermal evolution of SiGe nanotubes. Nanotechnology 20:315705. https://doi.org/10.1088/0957-4484/20/31/315705

13. Hamed Mashhadzadeh A, Fathalian M, Ghorbanzadeh Ahangari M, Shahavi MH (2018) DFT study of Ni, Cu, Cd and Ag heavy metal atom adsorption onto the surface of the zinc-oxide nanotube and zinc-oxide graphene-like structure. Mater Chem Phys 220:366–373. https://doi.org/10.1016/j.matchemphys.2018.09.016

14. Continenza A, Wentzcovitch R, Freeman AJ (1990) Theoretical investigation of graphitic BeO. Phys Rev B 41:3540–3544. https://doi.org/10.1103/PhysRevB.41.3540

15. Hamed Mashhadzadeh A, Ghorbanzadeh Ahangari M, Dadrasi A, Fathalian M (2019) Theoretical studies on the mechanical and electronic properties of 2D and 3D structures of Beryllium-Oxide graphene and graphene nanobud. Appl Surf Sci 476:36–48. https://doi.org/10.1016/j.apsusc.2019.01.083

16. Zarghami Dehaghani M, Hamed Mashhadzadeh A, Salmankhani A, Karami Z, Dadrasi A, Habibzadeh S, Ganjali MR et al (2020) Fracture toughness and crack propagation behavior of nanoscale beryllium oxide graphene-like structures: a molecular dynamics simulation analysis. Eng Fract Mech 235:107194. https://doi.org/10.1016/j.engfracmech.2020.107194

17. Zarghami Dehaghani M, Salmankhani A, Hamed Mashhadzadeh A, Habibzadeh S, Abida O, Reza Saeb M (2021) Fracture mechanics of polycrystalline beryllium oxide nanosheets: a theoretical basis. Eng Fract Mech 244:107552. https://doi.org/10.1016/j.engfracmech.2021.107552

18. Rostamiyan Y, Mohammadi V, Hamed Mashhadzadeh A (2020) Mechanical, electronic and stability properties of multi-walled beryllium oxide nanotubes and nanopeapods: a density functional theory study. J Mol Model 26:76. https://doi.org/10.1007/s00894-020-4288-5

19. Sorokin P, Fedorov A, Chernozatonskii L (2006) Struct prop BeO nanotubes 48:398–401. https://doi.org/10.1134/S10783406062034X

20. Fathalian A, Kanjouri F, Jalilian J (2013) BeO nanotube bundle as a gas sensor. Superlattice Microst 60:291–299. https://doi.org/10.1016/j.spmi.2013.04.028

21. Chigo Anota E, Coccoletzi GH (2013) Electronic properties of functionalized (5,5) beryllium oxide nanotubes. J Mol Graph Model 42:115–119. https://doi.org/10.1016/j.jmgm.2013.03.007

22. Fereidoon A, Mostafaei M, Ganjidi MD, Memarian F (2015) Atomistic simulations on the influence of diameter, number of walls, interlayer distance and temperature on the mechanical properties of BNNTs. Superlattice Microst 86:126–133. https://doi.org/10.1016/j.spmi.2015.07.036

23. Bevilacqua AC, Rupp CJ, Baiere RJ (2016) First principles study on defective BN nanotubes for water splitting and hydrogen storage. Chem Phys Lett 653:161–166. https://doi.org/10.1016/j.cplett.2016.04.093

24. Yang L, Greenfeld I, Wagner HD (2016) Toughness of carbon nanotubes conforms to classic fracture mechanics. Sci Adv 2:e1500969. https://doi.org/10.1126/sciadv.1500969

25. Zarghami Dehaghani M, Esmaeili Safa M, Yousefi F, Salmankhani A, Karami Z, Dadrasi A et al (2021) Fracture behavior of SiGe nanosheets: mechanics of monocrystalline vs. polycrystalline structure. Eng Fract Mech 251:107782. https://doi.org/10.1016/j.engfracmech.2021.107782

26. Salmankhani A, Karami Z, Hamed Mashhadzadeh A, Zarghami Dehaghani M, Reza Saeb M, Fierro V et al (2021) A theoretical scenario for the mechanical failure of boron carbide nanotubes. Comput Mater Sci 186:110022. https://doi.org/10.1016/j.commatsci.2020.110022

27. Memarian F, Fereidoon A, Khodaei S, Mashhadzadeh AH, Ganji MD (2017) Molecular dynamic study of mechanical properties of single/double wall SiCNTs: consideration temperature, diameter and interlayer distance. Vacuum 139:93–100. https://doi.org/10.1016/j.vacuum.2017.02.014

28. Zhang Y, Huang H (2008) Stability of single-wall silicon carbide nanotubes – molecular dynamics simulations. Comput Mater Sci 43:664–669. https://doi.org/10.1016/j.commatsci.2008.01.038

29. Grindon C, Harris S, Evans T, Novik K, Coveyney P, Laughton C (2004) Large-scale molecular dynamics simulation of DNA: implementation and validation of the AMBER98 force field in LAMMPS. Philos Trans R Soc Lond Ser Math Phys Eng Sci 362:1373–86. https://doi.org/10.1098/rsta.2004.1381

30. Tersoff J (1988) New empirical approach for the structure and energy of covalent systems. Phys Rev B 37:6991–7000. https://doi.org/10.1103/PhysRevB.37.6991

31. Cumings J, Zettl A (2000) Mass-production of boron nitride double-wall nanotubes and nanococonuts. Chem Phys Lett 316:211–216. https://doi.org/10.1016/S0009-2614(99)01277-4

32. Barick A, Tripathy D (2011) Effect of organically modified layered silicate nanoclay on the dynamic viscoelastic properties of thermoplastic polyurethane nanocomposites. Appl Clay Sci 52:312–321. https://doi.org/10.1016/j.clay.2011.03.010

33. Jalilian J, Safari M, Naderizadeh S (2016) Buckling effects on electronic and optical properties of BeO monolayer: first principles study. Comput Mater Sci 117:120–126. https://doi.org/10.1016/j.commatsci.2016.01.032

34. Sherafati M, Shokuh Rad A, Ardjmand M, Heydarinasab A, Peyravi M, Mirzaei M (2018) Beryllium oxide (BeO) nanotube provides excellent surface towards adenine adsorption: a dispersion-corrected DFT study in gas and water phases. Curr Appl Phys 18:1059–1065. https://doi.org/10.1016/j.cappend.2018.05.024

35. Rastegar SF, Ahmadi Peyghan A, Soleymanabadi H (2015) Ab initio studies of the interaction of formaldehyde with beryllium oxide nanotube. Physica E 68:22–27. https://doi.org/10.1016/j.physe.2014.12.005

36. Shahrokhi M, Leonard C (2016) Quasi-particle energies and optical excitations of wurtzite BeO and its nanosheet. J Alloy Comp 682:254–262. https://doi.org/10.1016/j.jallcom.2016.04.288

37. Dadrasi A, Albooyeh AR, Hamed Mashhadzadeh A (2019) Mechanical properties of silicon-germanium nanotubes: a molecular dynamics study. Appl Surf Sci 498:143867. https://doi.org/10.1016/j.apsusc.2019.143867

38. Salmankhani A, Karami Z, Hamed Mashhadzadeh A, Saeb MR, Fierro V, Celzard A (2020) Mechanical properties of C3N nanotubes from molecular dynamics simulation studies. Nanomaterials 10:894

39. Setoodeh A, Attarian H, Jahanshahi M (2011) Mechanical properties of silicon-germanium nanotubes under tensile and compressive loadings. J Nano Res 15:105–114. https://doi.org/10.4028/www.scientific.net/JNanoR.15.105

Publisher’s note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.