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Analyzing the effect of adsorption of Flavin Mononucleotide biomolecule on the natural frequency of biocompatible boron-nitride nanotubes

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ABSTRACT: In this study, natural frequency of single- and double-walled boron-nitride nanotubes under physical adsorption of Flavin Mononucleotide molecules are investigated employing the molecular dynamics simulations in vacuum and aqueous environments. The effects of different boundary conditions and geometrical parameters on the natural frequency have been explored. According to the results, the physical adsorption of polymers reduces the natural frequency of boron-nitride nanotubes which is considerable in the case of boron-nitride nanotubes with fully clamped boundary conditions. Moreover, it has been observed that the frequency shift for clamped-free boundary condition in an aqueous environment due to change in mode-shape which is the result of van der Waals interaction with environment, is positive. Also, it is observed that frequency shift of single-walled boron-nitride nanotubes with smaller aspect ratios is higher than that of single-walled boron-nitride nanotubes with higher aspect ratios and double-walled boron-nitride nanotubes. Considering the aqueous environments, frequency shift considerably increases, whereas the slope of variation with the weight percentage decreases. The result of this study can be used as the benchmark for further studies in nanoelectromechanical systems to design more efficient molecular recognition nanobiosensors in aqueous environments.

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1- Introduction

Proposing the inorganic analogous of Carbon NanoTubes (CNTs) [1], i.e. Boron Nitride NanoTubes (BNNTs) with unique properties such as a wide band gap, high thermomechanical properties together with chemical stability [2] demonstrates that BNNTs can be used as an alternative to CNTs in NanoElectroMechanical systems (NEMS) [3] due to their some comparable properties [4]. Although these unique properties together with non-cytotoxicity make them more efficient for nanobiotechnology [5], chemical inertness and their insolubility in various solvents restrict their potential applications considerably. Different investigations have declared that these restrictions can be eliminated by functionalizations. Accordingly, the intrinsic properties and behavior of the host nanostructure are altered noticeably [6]. Considering BNNTs, magnetic and electrical properties of functionalized BNNTs are altered as their solubility is improved remarkably [7]. The phosphorylated derivative of vitamin B2 called Flavin MonoNucleotide (FMN) is a fairly small molecule that can interact with BNNTs. According to the experimental proofs, BNNTs under physical adsorption of FMN molecules can emit stable green fluorescent in a wide range of local conditions which make them so promising in biological nanomarkers and nanosensors [8]. In this investigation, the mechanical vibrational behavior of single- and double-walled BNNTs under physical adsorption of FMN is studied. The Molecular Dynamics (MD) simulations are carried out and the natural frequency of functionalized BNNTs is determined. The influences of different boundary conditions, radius, weight percentage of FMN and number of walls on the natural frequency are explored. Also, the effects of different environments, i.e. vacuum and aqueous environments, are studied.

2- Methodology and Model

2.1. Simulation details

Employing Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package [9], all MD simulations are performed. To this end, AMBER force field [10] was selected to perform simulations in canonical ensemble. Velocity-Verlet integrator algorithm together with Nose-hoover thermostat algorithm is selected to solve the Newtonian equations of motion in constant temperature (300K) with the time step of 1 fs [11]. After initial minimization, the system is relaxed for up to 300 ps to reach its equilibrium state at 300 K. Then, the nanotubes are allowed to vibrate freely. During the simulation, the coordinates of the center of mass of nanotubes are stored and the natural frequency is obtained by implementation of Fast Fourier Transform (FFT) [12].

2.2. Simulation models

Molecular structure of FMN molecule can be found in [13]. In order to perform the simulations, two SWBNNTs,

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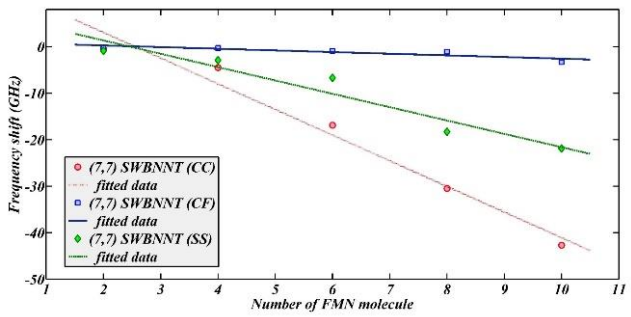

Fig. 1. Frequency shift of (7,7) functionalized SWBNNTs with different boundary conditions in vacuum

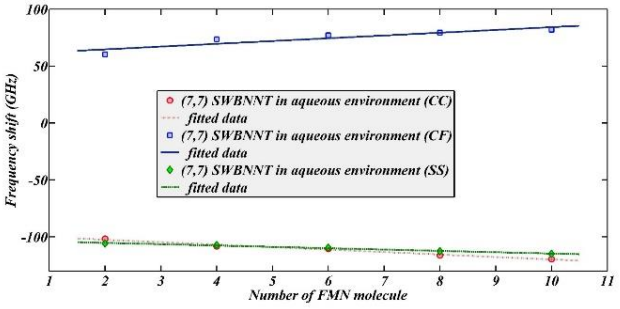

Fig. 2. Frequency shift of (7,7) functionalized SWBNNTs with different boundary conditions in aqueous environment

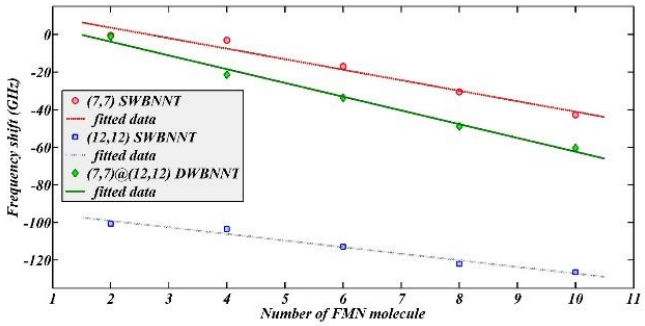

Fig. 3. Frequency shift of functionalized SWBNNTs and DWBNNTs with CC boundary conditions in vacuum

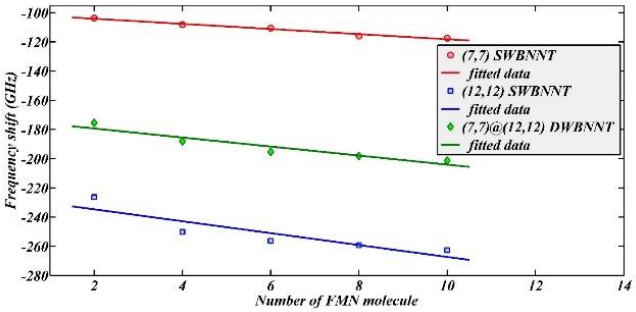

Fig. 4. Frequency shift of functionalized SWBNNTs and DWBNNTs with CC boundary conditions in aqueous

i.e. (7,7) and (12,12), and a (7,7)@(12,12) DWBNNTs with the length of ~100 Å are selected and the FMN molecules are placed near the walls of BNNTs as in [13]. It should be noted that different boundary conditions are taken into consideration, i.e. fully clamped (CC), fully Simply-Support (SS) and Clamped-Free (CF). Also, the density of aqueous environment is selected to be 1 gr/(cm^3).

3- Results and Discussion

3.1. Effect of boundary conditions

In the case of functionalized BNNTs, it is observed that the natural frequency of BNNTs decreases as FMN molecule is physically adsorbed to the walls of CNTs. Fig. 1 reveals the frequency shift of functionalized (7,7) BNNT with different boundary conditions.

The calculations of natural frequency of functionalized BNNTs in aqueous environments with different boundary conditions demonstrate that the magnitude of frequency shift is higher than that of functionalized BNNT in vacuum as depicted in Fig. 2. Note that all frequency shifts are calculated according to the natural frequency of pure BNNT in vacuum. It should be noted that the positive frequency shift occurs in the case of nanotubes with CF boundary conditions in aqueous environment due to not vibrating in its first mode [9].

3.2. Effect of geometrical parameters

To study the effects of radius, and number of walls on the natural frequency of functionalized BNNTs, SWBNNTs and DWBNNTs are selected with CC boundary conditions. By physical adsorption of FMN molecules on BNNTs, natural frequency of BNNTs decreases as illustrated in Fig. 3. Accordingly, it is observed that frequency shift of DWBNNT is between that of constituent inner and outer tube of DWBNNT.

Performing the simulations in aqueous environments reveals that the frequency shift considerably increases, whereas the sensitivity of frequency shift to the number of FMN molecules (weight percentage) decreases as presented in Fig. 4. Based on this Figure, it is shown that the frequency shift of DWBNNT is higher than that of DWBNNTs in vacuum and becomes closer to that of its outer constituent SWBNNT. Comparing the frequency shifts for BNNTs in vacuum and aqueous environments indicates that the frequency shift of DWBNNTs and SWBNNTs with higher aspect ratios is altered more considerably than that of SWBNNTs with smaller aspect ratios.

4- Conclusions

Based on the MD simulations, vibrational characteristics of functionalized SWBNNTs and DWBNNTs with FMN molecule was investigated and the effects of different boundary conditions, radius and number of walls were explored considering vacuum and aqueous simulation environments. According to the simulation results, non-covalent functionalization reduces the natural frequency of BNNTs. Also, it was observed that BNNT with CC

boundary conditions is more sensitive to functionalization than BNNTs with other boundary conditions. It was found that with a similar length, the frequency shift of SWBNNTs with smaller radius is higher than other SWBNNTs with smaller radius and DWBNNTs. Further, it was demonstrated that the presence of water molecules results in a higher reduction in natural frequency, whereas it reduces the slope of variation of frequency shift with the weight percentage of FMN molecules.

References

[1] A. Rubio, J. L. Corkill, M. L. Cohen, Theory of graphitic boron nitride nanotubes, Physical Review B 49 (1994) 5081-5088.

[2] R. Ansari, S. Ajori, A molecular dynamics study on the vibration of carbon and boron nitride double-walled hybrid nanotubes, Applied Physics A 120 (2015) 1399-1406.

[3] M.F.L. De Volder, S.H. Tawfick, R.H. Baughman, A.J. Hart, Carbon Nanotubes: Present and Future Commercial Applications, Science 339 (2013) 535-539.

[4] H.M. Sedighi, and M. Malikan, Stress-driven nonlocal elasticity for nonlinear vibration characteristics of carbon/boron-nitride hetero-nanotube subject to magneto-thermal environment. Physica Scripta, 95(5) (2020) 055218.

[5] C.Y. Zhi, Y. Bando, C.C. Tang, Q. Huang, D. Golberg, Boron nitride nanotubes: functionalization and composites, Journal of Materials Chemistry 18 (2008) 3900–3908.

[6] R. Ansari, S. Ajori, S. Rouhi, Structural and elastic properties and stability characteristics of oxygenated carbon nanotubes under physical adsorption of polymers' Applied Surface Science, 332 (2015): 640-647.

[7] S.H. Kang, S.W. Jeon, S.Y. Moon, Y.J. Yoon, and T.H. Kim, Fabrication of Non-Covalently Functionalized Boron Nitride Nanotubes with High Stability and Water-Redispersibility. The Journal of Physical Chemistry Letters, 11 (2020) 4511–4516

[8] Z. Gao, C. Zhi, Y. Bando, D. Golberg, T. Serizawa, Noncovalent functionalization of disentangled boron nitride nanotubes with flavin mononucleotides for strong and stable visible-light emission in aqueous solution". ACS applied materials & Interfaces, 3 (2011) 627.

[9] S.J. Plimpton, Fast parallel algorithms for short-range molecular dynamics, Journal of computational physics, 117 (1995) 1-19.

[10] C. Grindon, S. Harris, T. Evans, K. Novik, P. Coveney, C. Laughton, Large-scale molecular dynamics simulation of DNA: implementation and validation of the AMBER98 force field in LAMMPS, Philosophical Transactions of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences, 362 (2004) 1373-1386.

[11] W.G. Hoover, Canonical dynamics: Equilibrium phase-space distributions, Physical review A 31 (1985) 1695-1697.

[12] R. Ansari, S. Ajori, and A. Ameri, On the vibrational characteristics of single-and double-walled carbon nanotubes containing ice nanotube in aqueous environment. Applied Physics A, 121(1) (2015) 223-232.

[13] R. Ansari, S. Ajori, and A. Ameri, Stability characteristics and structural properties of single-and double-walled boron-nitride nanotubes under physical adsorption of Flavin mononucleotide (FMN) in aqueous environment using molecular dynamics simulations. Applied Surface Science, 366 (2016) 233-244.

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