Microsyst Technol (2016) 22:1115–1120
DOI 10.1007/s00542-015-2470-2

TECHNICAL PAPER

Vibration analysis of initially curved single walled carbon nanotube with vacancy defect for ultrahigh frequency nanoresonators

Mojtaba Amjadipour · Dzung Viet Dao · Nunzio Motta

Received: 1 February 2015 / Accepted: 10 February 2015 / Published online: 20 February 2015

Abstract Single walled carbon nanotubes (SWCNTs) are ideal choices for resonators due to its ultrahigh natural frequency. Fundamental frequency of resonators significantly affects their functionality and performance; therefore, an accurate prediction of SWCNTs' natural frequency is vital for designing and developing such devices. In reality, CNTs are not straight and perfect; indeed, they have some degree of vacancy defect and waviness, which occurs during growth and manipulation processes. This research investigates for the first time the combination effects of both initial curvature and vacancy defects on vibrational behaviour of SWCNTs in order to make the simulation closer to the "real world". In this study, an efficient method based on the molecular dynamics model and the finite element method is used to simulate wavy SWCNTs with vacancy defects. Zigzag carbon nanotube with chirality indices (5, 0) is considered. Accuracy of our modelling method is verified by comparing our results with the results obtained from previous studies in simulating ideal SWCNT natural frequency. The effects of vacancy, vacancy location, curvature and aspect ratio on natural vibration of the defected wavy SWCNTs have been investigated, and a parameter of critical waviness ratio has been defined for the first time to emphasize the combination effect of vacancies and waviness on the natural frequency of SWCNTs. Our results show that critical waviness is sensitive to the aspect ratio and indicate that by increasing the length of SWCNTs, the critical waviness ratio increases.

M. Amjadipour · N. Motta
Institute for Future Environments and School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Queensland, Australia

D. V. Dao (✉)
Queensland Micro and Nanotechnology Centre, Griffith University, Queensland, Australia
e-mail: d.dao@griffith.edu.au

1 Introduction

A significant body of literature has been devoted to Nano-electromechanical systems (NEMS) in the past few years because of the potential of such technologies to deliver device dimensions in the nanometre range, leading to low mass, high mechanical resonance frequency. To be successfully deployed in NEMS devices, components must be prepared from materials that meet specific chemical and physical properties. Since the discovery of carbon nanotubes (CNTs) (Iijima 1991), these materials have been under extensive investigation for their implementation as NEMS (Dao et al. 2010) and MEMS (Micro electromechanical systems) devices (Dau et al. 2010a, b).

CNTs have many of the desirable properties for NEMS, such as extremely high in-plane elastic modulus, high natural frequency and thermal conductivity. These properties, combined with their nanometer-size, ideal atomic structure, suggest that CNTs have potential applications as nanoresonators (Jensen et al. 2007, 2008; Poncharal et al. 1999; Bell et al. 2008). Nanoresonators are a subclass of resonance-based sensors being developed to meet the high-performance requirements of many sensing applications, including metal deposition monitors, chemical reaction monitors, biomedical sensors, mass detectors, etc., (Li and Chou 2003; Motta 2012; Goh et al. 2009). Reduction in the size of a resonator to the nano-scale increases its resonant frequency and reduces its energy consumption (De Los Santos 1999). For resonator-based sensors, higher resonant frequency leads to higher sensitivity (Jensen et al. 2008; Zhu et al. 2014; Shiraishi et al. 2013). Several examples of carbon nanotube oscillators highlighting these advantages have already been reported (Li and Chou 2003; Sazonova 2006; Ouakad and Younis 2011).

In order to better understand and optimise CNTs nanoresonator design, detailed modelling of their behaviour is required. Due to the complexities of the fabrication process, producing perfectly straight CNTs with controlled geometry and orientation is difficult. Indeed, it has been indicated that CNTs are fabricated with some level of curvature or slack (Sazonova 2006). The curvature among nanotubes' structure can be seen in Fig. 1 (Qian et al. 2000). Gibson et al. (2007) stressed the importance of including the slack of CNTs in models and indicated that no consistent model has been presented to address this deficiency. Up to this point, most computational vibrational studies model CNTs to be perfectly straight; however, there are a few studies about the effect of waviness on vibrational behaviour of CNTs (Ouakad and Younis 2011; Farsadi et al. 2012; Imani Yengejeh et al. 2014).

Meanwhile, defects in nanotubes, including substitutional impurities, vacancies, and topologic defects, create heterogeneous structures, which can change the electronic, chemical, and mechanical properties of the carbon nanotubes (Suenaga et al. 2007). In turn, these different properties can influence the applications of such CNTs in NEMS and nanocomposites. Furthermore, the significant effect of vacancies on the natural frequencies of SWCNTs has been indicated in previous studies (Karami and Amjadipoor 2011; Ghavamian and Öchsner 2013). Karami and Amjadipour investigated the effect of vacancy defects on the natural frequency of SWCNTs using a model based on structural molecular mechanics. They scattered vacancies on the SWCNTs' structure for more realistic simulation, and their results indicated the significant effect of vacancies on vibrational behaviour of SWCNTs (Karami and Amjadipoor 2011).

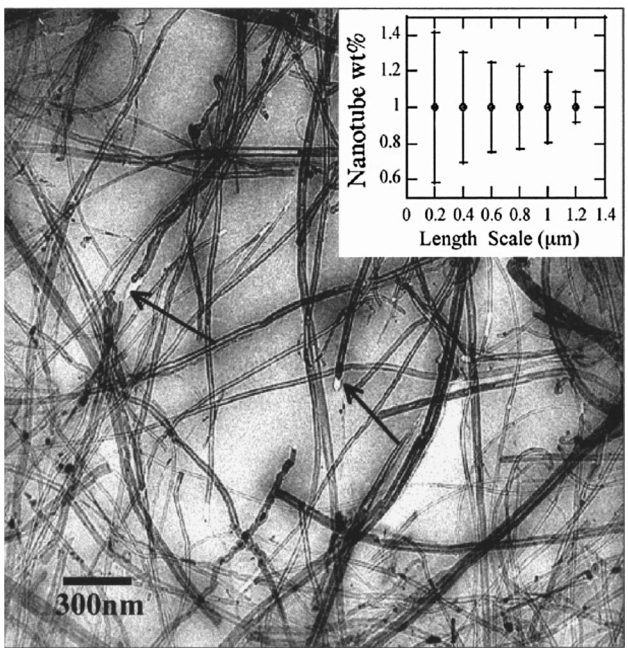

Fig. 1 Transmission electron microscope image showing waviness of nanotubes (Qian et al. 2000)

While previous research has considered the effect of curvature or the influence of defects in CNTs, to-date modelling the combination of these two effects on the vibrational characteristics of CNTs has not been reported. Therefore, in this paper, vibrational behaviours of SWCNTs under both the effects of waviness and vacancy defects have been investigated in order to approach the simulation of a "real-world" SWCNT. In this research, a model based on molecular dynamics and finite element method is developed. The foundation of this model is based on modeling methodology proposed by Li and Chou (2003) and an efficient model for vibration analysis of carbon nanotubes proposed by Georgantzinos et al. (2009). The simulation in this paper has been done using ANSYS.

2 Modelling and analysis method

In this paper for modelling SWCNTs a technique based on finite element method and molecular dynamics is used. This technique is based on the concept that CNT can be considered as a continuum having continuous distributions of mass and stiffness. Odegard et al. (2002) implemented an equivalent continuum model for prediction of property of nanostructure materials. Molecular mechanics model has been used for calculating extensional, torsional and bending rigidity of SWNTs using the potential energies (Bodily and Sun 2003). Li and Chou (2003) developed a similar method using continuum mechanics and molecular dynamics for determining the properties of CNTs. Thus we can simulate a SWCNT as a space frame model consists of mass and stiffness.

As the most part of atom mass is concentrated in nucleus, nucleus mass ($m_c = 1.9943 \times 10^{-26} kg$) is considered as atom mass and electron masses are neglected. In order to simulate atom mass, mass elements are located on carbon atoms positions in SWCNT structure. Bonding of carbon atoms is modelled by stiffness element.

Total steric potential energy, which is a summation of energies due to bonded interactions and nonbonded interactions, can be expressed as Eq. (1) (Rappé et al. 1992):

$$U = \sum U_r + \sum U_\theta + \sum (U_\varphi + U_\omega) + \sum U_{VDW} \qquad (1)$$

where U_r, U_θ, U_φ, U_ω and U_{VDW} are the energy terms due to bond stretching, bond angle bending, dihedral angle torsion, out-of-plane torsion and van der Waals interaction, respectively (Li and Chou 2003). In this research the van der Waals interaction is ignored, so the term related to it is omitted.

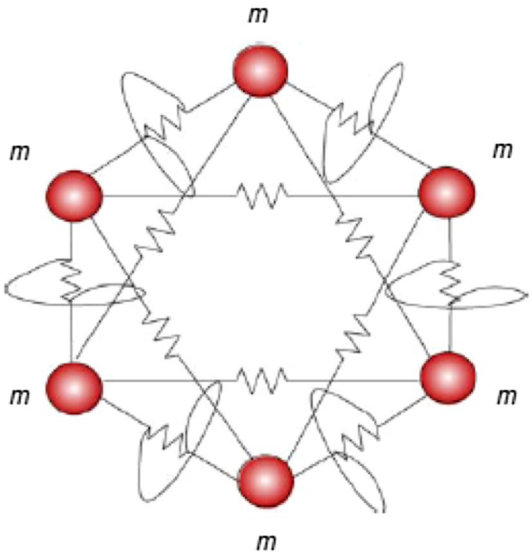

Fig. 2 Graphical demonstration of the hexagonal lattice (Georgantzinos et al. 2009)

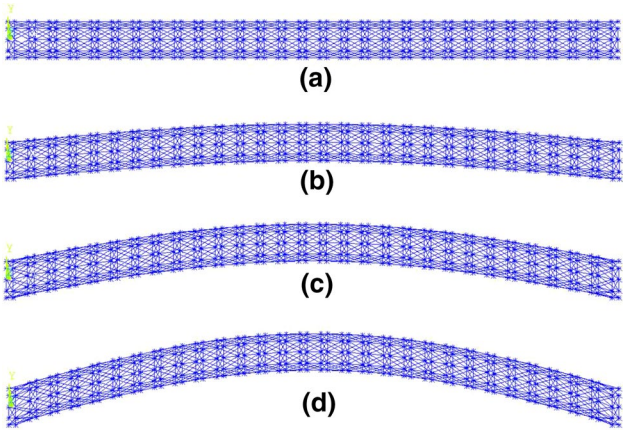

Fig. 3 Graphical demonstration of wavy SWCNT (5, 0) with aspect ratio of 15.9: **a** waviness ratio equal to 0, **b** waviness ratio equal to 0.03, **c** waviness ratio equal to 0.06, and **d** waviness ratio equal to 0.09

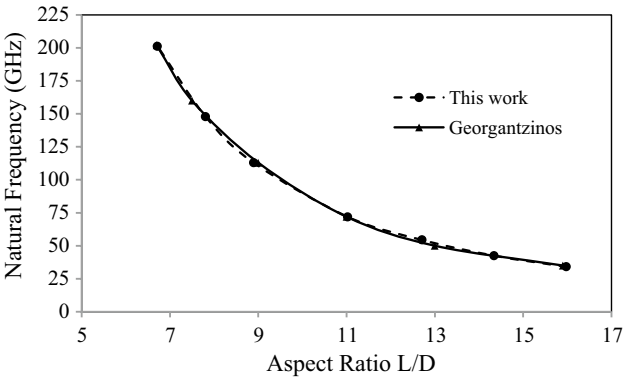

Fig. 4 Comparison of our result with the previous study (Georgantzinos et al. 2009) for a perfect SWCNT (5, 0) with clamped-free boundary condition

In this study, for bond simulation, a configuration of nano springs has been employed. This technique has been introduced by Georgantzinos et al. (2009). These springs are connected to two nodes, which have six degrees of freedom per node. The required spring stiffness coefficients can be produced according to Castigliano's theorem from the potential energies. The types of springs used are demonstrated in Fig. 2. One axial spring and one torsional spring have been used for simulation of the stretching (k_r) and torsion k_τ bond interaction. The angle bending interaction has been simulated using a set of axial springs k_b, and their stiffness can be calculated from bond-angle bending force constant (k_θ) (Georgantzinos et al. 2009).

The capability and efficiency of this molecular structural mechanics method have been verified in the vibrational analysis of single walled carbon nanotubes (Li and Chou 2003; Georgantzinos et al. 2009).

It has been reported in the literature that sinusoidal function shows more compatibility with the real curvature of SWCNT (Gibson et al. 2007), so in this study the waviness has been simulated using Eq. (2):

$$Z = e \times sin\left(\frac{\pi x}{L}\right) \tag{2}$$

where x is the spatial coordinate, L is the length of the carbon nanotube and e is the amplitude of its waviness. For the investigation of the effect of waviness, a parameter waviness ratio (e/L) has been introduced. The SWCNT simulation models with different waviness ratios have been developed as shown in Fig. 3.

Vacancy ratio $V_r = \frac{n_1}{n} \times 100$ has been introduced to present the vacancies, where n_1 denotes the number of nodes that have been vanished due to vacancy modelling, and n is the number of total nodes in the CNT's structure. Creation of vacancies has a limitation; two neighbour nodes cannot be eliminated together. For vacancy simulation, related elements were omitted in the frame like model.

Furthermore, in order to investigate the changes in the vibrational behaviour of SWCNTs, a parameter called natural frequency shift $\Delta f = f_d - f_p$ is defined, where f_d represents the natural frequency of the defected one, and f_p denotes the natural frequency of the perfect and straight SWCNT.

The equation of motion for the free vibration of undamped structure is:

$$[M]\{\ddot{y}\} + [K]\{y\} = 0 \tag{3}$$

where [M] and [K] are, respectively, the global mass and stiffness matrices; {y} and $\{\ddot{y}\}$ represent the nodal

displacement vector and acceleration vector, respectively. The global matrices of the structure can be assembled from the elemental matrices. For assembling nodes, finite element method is used. The natural frequencies f and mode shapes are determined from the solution of the eigenproblem (Li and Chou 2003; Georgantzinos et al. 2009).

For the verification of the modelling technique, our results are compared with the result obtained by Georgantzinos et al. (2009) as shown in Fig. 2. Perfect SWCNT with chirality index (5, 0) and clamped-free boundary condition is considered. As shown in Fig. 4, our results are close to those reported by Georgantzinos et al. (2009).

3 Results

Figure 5 shows natural vibration frequency shift of SWCNT with chirality index (5, 0). Clamped-free boundary condition with aspect ratio (L/D) equal to 15.9 and different waviness ratios and vacancy ratios have been considered.

As shown in Fig. 5, a SWCNT (5, 0) with waviness ratio equals to 0.09 and vacancy ratio equals to 0.01 has a natural frequency of 2.67 GHz lower than that of the perfect one. This shows the important effect of such defects on the vibrational behaviour of SWCNTs. It is clear from Fig. 5 that as the waviness ratio increases, natural frequency decreases. By comparing natural frequency shift of wavy one with wavy-vacancy defected one, it can be seen that vacancies have the dominant effect on the natural frequency until the waviness ratio equals to 0.082, and from this point onward, the effect of waviness surpasses the effect of vacancies. Therefore, for a specific vacancy ratio, the waviness ratio at which the effect of waviness equals to the effect of vacancies is defined as the critical waviness ratio $(e/L)_{cr}$.

Figure 6 indicates that for SWCNT (5, 0) with the aspect ratio equals to 10.3, when waviness ratio is 0.09 and vacancy ratio is 0.01, the natural frequency shift is −10.2 GHz. By comparing Figs. 5 and 6, the significant effect of aspect ratio on the impact of the vacancy defect and waviness on the principle frequency of SWCNTs can be observed. It can be noted that by decreasing the length of SWCNT, the critical waviness ratio $(e/L)_{cr}$ decreases, as at vacancy ratio of 0.01, this is equal to 0.028 for the aspect ratio of 10.3, whereas it is equal to 0.082 for the aspect ratio of 15.9. By considering this, it can be concluded that in short SWCNTs the waviness represents the dominant effect on the natural frequency.

For analysing the effect of vacancy location on the vibrational behaviour of SWCNTs, vacancies are simulated in two different positions within the structure of SWCNT (5, 0) with the aspect ratio of 13.2. For this purpose, a parameter of vacancy location x/L has been defined, where x denotes the distance of the vacancies from the closest end of SWCNT and L is the length of SWCNT. According to Fig. 7, the natural frequency of SWCNT with aspect ratio equal to 13.2 and waviness ratio equal to 0.09 is 2.2 GHz lower than that of the straight one with no defects, and

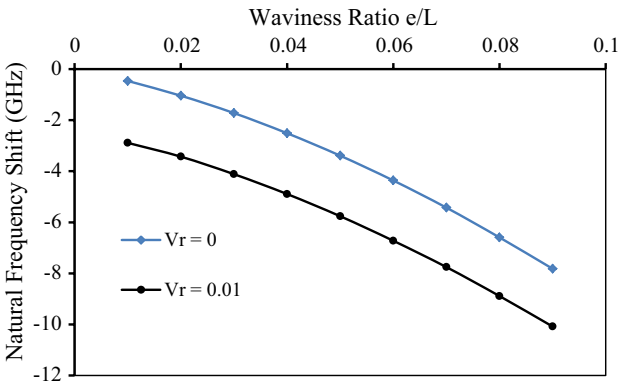

Fig. 6 Natural frequency shift of SWCNT (5, 0) with the aspect ratio of 10.3 and clamped free boundary condition

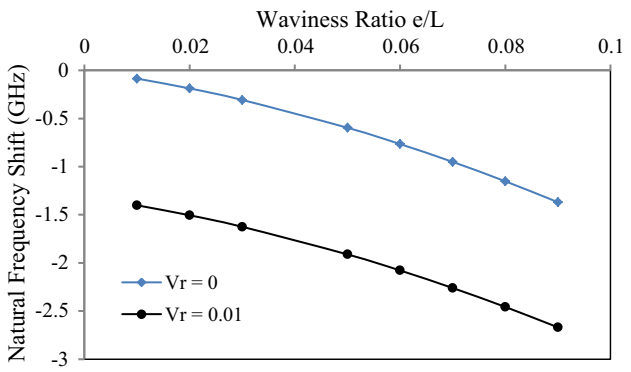

Fig. 5 Natural frequency shift of SWCNT (5, 0) with the aspect ratio of 15.9 and clamped-free boundary condition

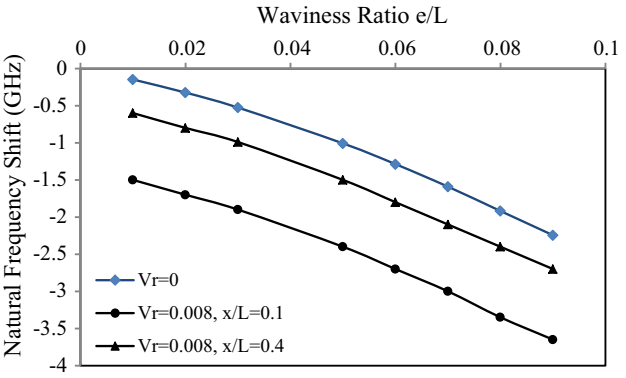

Fig. 7 Natural frequency shift of SWCNT (5, 0) with the aspect ratio of 13.2 and clamped-free boundary condition

the frequency shift is −3.7 GHz for the wavy vacancy defected one with vacancy ratio equals to 0.008 and the vacancy location is 0.1. By comparing the natural frequency shift of the one with vacancy location of 0.1 and the one with vacancy location of 0.4, it can be noted that as the vacancies approach the peak of the waviness, the natural frequency shift decreases and the critical waviness ratio decreases, too. Furthermore, by comparing Figs. 5 and 7, the significant effect of aspect ratio on the influence of the vacancy defect and waviness on the principle frequency of SWCNTs can also be seen. The critical waviness ratio $(e/L)_{cr}$ for this SWCNT with vacancy ratio equal to 0.008 is found to be 0.062 at vacancy location of 0.1 and 0.032 at vacancy location of 0.4.

4 Conclusions

By using an efficient modelling technique based on the molecular mechanics method, we investigated the combination effect of vacancy defect and waviness on the natural vibration of SWCNTs with chiral indices (5, 0). Results indicate that vacancies and waviness significantly affect the fundamental frequency of SWCNTs. By increasing the waviness ratio and vacancy ratio, the natural frequency decreases. The aspect ratio also affects the effect of waviness and vacancy defects on the vibrational behaviour of SWCNTs. Furthermore, the critical waviness ratio decreases by decreasing the length of SWCNT, which indicates that by increasing the length of SWCNTs, the effect of vacancies is getting more noteworthy compared to the effect of waviness on the natural frequency of SWCNTs. In other words, in shorter SWCNTs, waviness has more dominant effect on the natural frequency compared to vacancies. In addition, the effect of vacancy location on the vibrational behaviour of wavy-vacancy defected SWCNTs have been studied, and the results showed that when vacancies are further from the peak of the waviness, the critical waviness ratio decreases. These findings can help researchers to understand the combination effect of waviness and vacancy defects on the natural frequency of SWCNTs, and therefore, to develop more accurate CNT-based nanoresonators.

References

Bell JM, Goh RGS, Waclawik ER, Giulianini M, Motta N (2008) Polymer-carbon nanotube composites: basic science and applications. Mater Forum 32:144–152

Bodily BH, Sun CT (2003) Structural and equivalent continuum properties of single-walled carbon nanotubes. Int J Mater Prod Technol 18(4):381–397

Cornell WD, Cieplak P, Bayly CI, Gould IR, Merz KM, Ferguson DM, Kollman PA (1995) A second generation force field for the simulation of proteins, nucleic acids, and organic molecules. J Am Chem Soc 117(19):5179–5197

Dao DV, Bui TT, Nakamura K, Dau VT, Yamada T, Hata K, Sugiyama S (2010) Towards highly sensitive strain sensing based on nanostructured materials. Adv Nat Sci Nanosci Nanotechnol 1(4):045012

Dau VT, Yamada T, Dao DV, Tung BT, Hata K, Sugiyama S (2010a) Integrated CNTs thin film for MEMS mechanical sensors. Microelectron J 41(12):860–864

Dau VT, Dao DV, Yamada T, Tung BT, Hata K, Sugiyama S (2010b) Integration of SWNT film into MEMS for a micro-thermoelectric device. Smart Mater Struct 19(7):075003

De Los Santos HJ (1999) Introduction to micorelectromechanical (MEM) microwave systems(Book). Artech House, Norwood, p 1999

Farsadi M, Öchsner A, Rahmandoust M. (2012) Numerical investigation of composite materials reinforced with waved carbon nanotubes. J Compos Mater: 0021998312448495

Georgantzinos SK, Giannopoulos GI, Anifantis NK (2009) An efficient numerical model for vibration analysis of single-walled carbon nanotubes. Comput Mech 43(6):731–741

Ghavamian A, Öchsner A (2013) Numerical modeling of eigenmodes and eigenfrequencies of single-and multi-walled carbon nanotubes under the influence of atomic defects. Comput Mater Sci 72:42–48

Gibson RF, Ayorinde EO, Wen YF (2007) Vibrations of carbon nanotubes and their composites: a review. Compos Sci Technol 67(1):1–28

Goh RG, Bell JM, Motta N, Ho PKH, Waclawik ER (2009) < i > p </i > -Channel, < i > n </i > -Channel and ambipolar field-effect transistors based on functionalized carbon nanotube networks. Superlattices Microstruct 1:347–356

Iijima S (1991) Helical microtubules of graphitic carbon. Nature 354(6348):56–58

Imani Yengejeh S, Delgado JM, de Lima AGB, Öchsner A. (2014). Numerical Simulation of the Vibration Behavior of Curved Carbon Nanotubes. Adv Mater Sci Eng. doi:10.1155/2014/815340

Jensen K, Weldon J, Garcia H, Zettl A (2007) Nanotube radio. Nano Lett 7(11):3508–3511

Jensen K, Kim K, Zettl A (2008) An atomic-resolution nanomechanical mass sensor. Nat Nanotechnol 3(9):533–537

Jorgensen WL, Severance DL (1990) Aromatic-aromatic interactions: free energy profiles for the benzene dimer in water, chloroform, and liquid benzene. J Am Chem Soc 112(12):4768–4774

Karami Mohammadi A, Amjadipoor M (2011) Effect of vacancy defect on natural vibration of single walled carbon nanotube as ultrahigh nanoresonators. J Vibroeng JVE 3:414–422

Li C, Chou TW (2003a) Single-walled carbon nanotubes as ultrahigh frequency nanomechanical resonators. Phys Rev B 68(7):073405

Li C, Chou TW (2003b) A structural mechanics approach for the analysis of carbon nanotubes. Int J Solids Struct 40(10):2487–2499

Motta N (2012) Nanostructures for sensors, electronics, energy and environment. Beilstein J Nanotechnol 3(1):351–352

Nasdala L, Ernst G (2005) Development of a 4-node finite element for the computation of nano-structured materials. Comput Mater Sci 33(4):443–458

Odegard GM, Gates TS, Nicholson LM, Wise KE (2002) Equivalent-continuum modeling of nano-structured materials. Compos Sci Technol 62(14):1869–1880

Ouakad HM, Younis MI (2011) Natural frequencies and mode shapes of initially curved carbon nanotube resonators under electric excitation. J Sound Vib 330(13):3182–3195

Poncharal P, Wang ZL, Ugarte D, De Heer WA (1999) Electrostatic deflections and electromechanical resonances of carbon nanotubes. Science 283(5407):1513–1516

Qian D, Dickey EC, Andrews R, Rantell T (2000) Load transfer and deformation mechanisms in carbon nanotube-polystyrene composites. Appl Phys Lett 76(20):2868–2870

Rappé AK, Casewit CJ, Colwell KS, Goddard Iii WA, Skiff WM (1992) UFF, a full periodic table force field for molecular mechanics and molecular dynamics simulations. J Am Chem Soc 114(25):10024–10035

Sazonova VA (2006) A tunable Carbon Nanotube Resonator. Ph.D. Thesis, Department of Physics, Cornell University

Shiraishi N, Ikehara T, Dao DV, Sugiyama S, Ando Y (2013) Fabrication and testing of polymer cantilevers for VOC sensors. Sens Actuat A 202:233–239

Suenaga K, Wakabayashi H, Koshino M, Sato Y, Urita K, Iijima S (2007) Imaging active topological defects in carbon nanotubes. Nat Nanotechnol 2(6):358–360

Zhu Y, Dao DV, Woodfield P (2014) A fluid density sensor based on a resonant tube. Adv Natural Sci Nanosci Nanotechnol 5(3):035010