ELK Asia Pacific Journals

ELK Asia Pacific Journals – 978-93-85537-06-6
ARIMPIE -2017

Parametric Variation Based Mechanical Charactrization of Nanocomposites

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Abstract—Since the revelation of carbon nanotubes (CNT) in 1991 and boron nitride nanotube (BNNT) in 1994. CNTs and BNNTs possess properties, which make them an excellent reinforcing material. In present work, single wall nanotubes (CNT & BNNT) are analyzed for their mechanical properties when used as the reinforcement in matrix material. To perform this analysis polyethylene and polycarbonatematrix materials are considered, which proves the possible bonding with nanotube material. The analysis has been performed for the estimation of Poisson's ratio and Young's modulus of the nano-composites using CNTs and BNNTs as reinforcing material. Also, the parametric variational analysis considering variation in diameter and length has been performed to analyze theeffect on Poisson's ratio and Young's modulus. The obtained results shows that as the length increases the Young's modulus decreases for considered nanotubes as reinforcing material as well as for the considered matrix materials. When diameter increases the value of Young's modulus increases. The effect on the Poison's ratio due to variation in diameter and length of the nanotubes is not of much significant. The present continuum modeling based simulation approach is found to be useful for the mechanical characterization of CNT and BNNT based nanocomposites.

Keywords—CNT, BNNT, Nanocomposite, Mechanical Characterization.

I. INTRODUCTION (*HEADING 1*)

Carbon nanotubes were discovered by Iijima [1], and Boron nitride nanotube was first synthesis by Nasreen[2]. Both nanotubes are capable of resisting high strain withoutbreaking. CNTs and BNNTsbased nano-composites are advanced composite materialswith promising high strength and wear resistance but predicting their propertiesround about exact value is an ongoing task.Many researchers are working to doso. Extreme work is being done to use nanotubes as the reinforcing agent andto boost the properties of the composite materials. Nanotubes are having three types of atomic structures armchair, zigzag and chiral with the configuration of a single-wall nanotube and multiwall nanotube.

Nanotube has excellent mechanical, thermal and electrical properties and can bean ideal candidate for composite reinforcement. Whereas when it comes to BNNT itis an electrical insulator with the band gap of 5.5eV in addition to usage over high temperatures above 700˚C CNT is not the better option. CNT oxidizes at 400-600˚C and burns completely at 700˚C. So, whenever the application of the composite is athigh temperature with oxidizing environment BNNT are more suitable [3].

CNT and BNNT possess exceptional mechanical properties with CNT 1TPa and forBNNT its 0.7 to 0.9 Tpa. Further, the thermal properties for CNT is found outto be 6000W/mK but for BNNT 2 papers predicted different values one higher andthe other lower. Still, the BNNT has a better thermal and oxidation stability thanCNT. The electrical properties for BNNT and CNT turn different, where BNNT is aninsulator whereas the CNT is a good conductor. BNNT can be used as the insulation fillers, and CNT can be utilized as a conductor [3].

II. MODELLING APPROACH

The computational approach can play a significant role in the development of nanotube based composite by providingsimulation results to help on the understanding, analysis and design of such Nano composites. At the nanoscale, analytical models are difficult to establish or too complicated to solve, and tests are extremely difficult andexpensive to conduct.

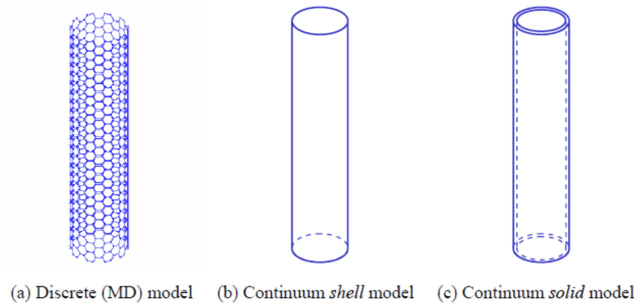

Fig 1: Computational models of an individual carbon nanotube [4]

Molecular dynamics simulation is accurate when studying the material properties at the nanoscale. In this approach the atoms are considered as individual particles and the force among them are calculated using potential theories. The equilibrium or dynamic equation for each particle is established for determining the displacement fields under given loads. These fundamentals approach have provided abundantsimulation result for understanding the behavior of individual or bundled nanotubes.The Molecular dynamics approach can provide abundant information about themechanical behavior of the Nano composite but currently, are limited to small size andshort time scale due to its computational expense for convergence requirement.
Continuum mechanics is the best among all; it is very feasible, cost effective and an efficient approach at present to characterize large-scale nanotube based compositefor mechanical properties using the finite element modeling and simulations. Thecontinuum mechanics approach has been applied successfully for simulating the mechanical response of individual nanotubes which are treated as a beam, thin shellsor solids in cylindrical shapes [5-8]. This approach has been employed by many researchers for to study of simulating individual nanotube, and it has was found thatthe only feasible approach at present to obtain preliminary results for characterizing nanotube-reinforced Nano composite.

III. METHODOLOGY

A composite with RVE's is proposed with BNNT and CNT Nanotube as the reinforcement. The model is prepared to keep in mind the interface bonding between polymer and nanotube which in turn gives rise to increasing the overall Mechanical, Thermal and Electrical property of the Composite. It has been demonstrated that just 1% (by weight) of Nanotube added in a matrix material, the stiffness of the resulting composite can be increased between 36% to 42% and the tensile strength by 25% [5].

The matrix material is polycarbonate and polyethylene, this material is bonded with the nanotube CNT and BNNT, and this bonding is justified by this reference [9-12]. Each matrix material is taken and bonded with the nanotube, and the result is taken out. This result is plotted and compared with the different matrix material to get a better idea which is better among CNT and BNNT.

In this work, the analysis of Nano composite with a single wall is done. Which includes matrix polymer and nanotube which are bonded without the interface modeling, and the result is compared with the result of the published paper [13].

1. *Modeling CNT/BNNT with Matrix Material*

CNT and BNNT are modeled as per the paper [13]. As the matrix material is modeledas continuum, the nanotube is approximated in the same manner. Once the modelingis done the two different models of CNT/BNNT and Matrix is assembled in somemodeling software in such a way that they can react as a single unit. Further, the boundary condition is applied with one end fixed on one side, and an axial force of about 5000nN is applied on both matrix and nanotube in opposite direction to fixed face. The parameters for analysis are:

Table 1: Parameter of the analysis

Length of matrix and nanotube	100nm
Thickness of nanotube	0.4nm
The outer diameter of nanotube	5nm
The inner diameter of nanotube	4.6nm
Hexagonal side length	11nm

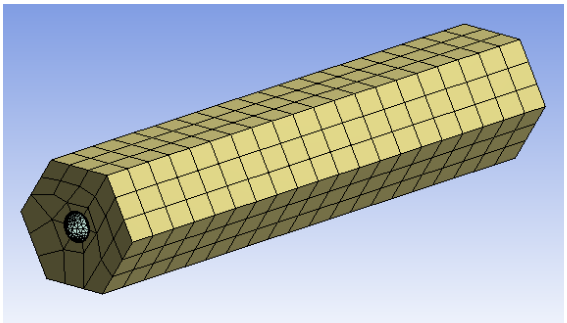

Fig 2. Finite element mesh modal

2. Rule of Mixtures

A simple rule of mixture can be established based on the strength of materials theory. These rules of mixture can be applied to verify the numerical results for the effective Young’s moduli in the nanotube axial direction. More general theories and extended results, in the context of fiber-reinforced composites.

a) CNT/BNNT through the length of RVE

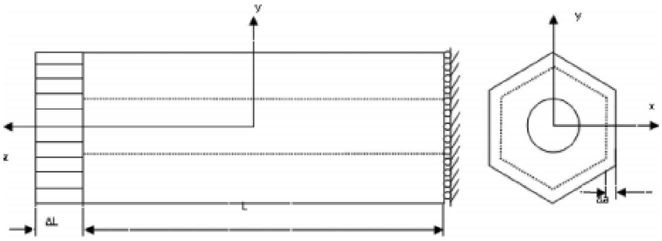

Fig 3: CNT/BNNT through the length of RVE

This is the case when the CNT/BNNT is relatively long with large aspect ratio, and therefore a segment can be modeled using an RVE. The simplified Strength ofmaterials models based on hexagonal RVEs is used in the present study for estimatingthe Young's modulus in the CNT/BNNT direction. For hexagonal RVE, the volume fraction of the CNT/BNNT is defined by

$$V^t = \frac{\pi(r_0^2 - r_i^2)}{\sqrt[3]{\frac{3a^2}{2}} - \pi r_i^2}$$

The effective Young's modulus Ez in the axial direction is found to be:

$$E_z = E^t V^t + E^m(1 - V^t)$$

Where, Et is the Young's modulus of the CNT/BNNT and Em is the Young's modulus of the matrix.

b) CNT/BNNT through half of the length of RVE

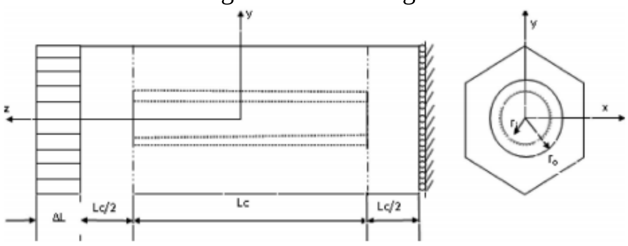

Fig 4: CNT/BNNT through half of the length of RVE

The two hemispherical end caps of the nanotube have been ignored in this derivation. Since the center part is a special case of the above figure, its Young's modulus isfound to be

$$E^e = E^t V^t + E^m(1 - V^t)$$

Using the above equation in which the volume fraction of the nanotube given by and is computed based on the centerpart of the RVE only.

$$\frac{1}{E_z} = \frac{1}{E^m}\left(\frac{L_e}{L}\right) + \frac{1}{E^e}\left(\frac{L_e}{L}\right)\left(\frac{A}{A_e}\right)$$

Where A is the area of hexagon minus area of cylinder this equations will beapplied to compare the FEM results.

IV. Results and Discussion

The above model is imported to Ansys, and a static structural analysis is performed.The boundary condition is set, as one end fixed and another end with force in an axialdirection opposite to the fixed face. Then the model is assigned with the properties ofthe material, and CNT/BNNT and analysis are carried out, and the result is plotted down.The results for effect on Poisson'sratio are shown in Fig. 5for the variation in diameter for matrix materials; Polyethylene and poly carbonate. The obtained results shows that the CNT based nano-composites are having higher value of Poison's ratio compare to BNNT based nano-composites. The Poison's ratio varies in the range of 0.23 to 0.35 for the Polyethylene matrix material. And for the Polycarbonate matrix material Poison's ratio varies in the range of 0.29 to 0.43. The variation in diameter is considered in the range of 03 nm to 07 nm.

As seen in Fig. 6 for the variation in length for matrix materials; Polyethylene and poly carbonate. The obtained results shows that the CNT based nano-composites are having higher value of Poison's ratio compare to BNNT based nano-composites. The Poison's ratio varies in the range of 0.26 to 0.38 for the Polyethylene matrix material. And for the Polycarbonate matrix material Poison's ratio varies in the range of 0.34 to 0.45. The variation in length is considered in the range of 60 nm to 140 nm.

As seen in Fig. 7 for the variation in diameter for matrix materials; Polyethylene and poly carbonate. The obtained results shows that the Polycarbonate is having higher young's modulus than the polyethylene based BNNT/CNT reinforced composite. It can also be seen that the Young's modulus increases with increases in diameter. The Young's modulus varies in range of 5E+09 pa to 9.3E+9 pa for Polycarbonate matrix material. And for the Polyethylene the Young's modulus varies in range of 2.8E+09 pa to 4.5E+09 pa. The variation in diameter is considered in the range of 2.6 nm to 6.6 nm.

As seen in Fig. 8 for the variation in length for matrix materials; Polyethylene and poly carbonate. The obtained results shows that the Polycarbonate is having higher young's modulus than the polyethylene based BNNT/CNT reinforced composite. It can also be seen that the Young's modulus decreases with increases in length. The Young's modulus varies in range of 7.5E+9 pa to 1.50E+10 pa for Polycarbonate matrix material. And for the Polyethylene the Young's modulus varies in range of 4.50E+09 pa to 7.50E+09 pa. The variation in length is considered in the range of 60 nm to 140 nm.

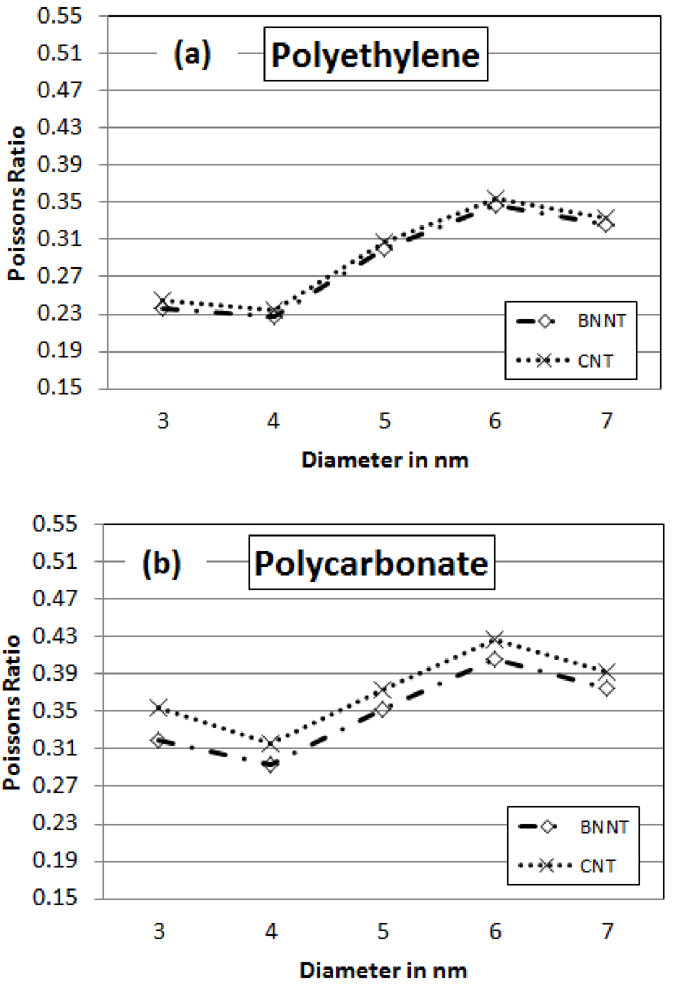

Fig 5: Variation in Poison's ratio against diameter of nanotubes (CNTs and BNNTs) (a) Polyethylene matrix, and (b) Polycarbonate matrix

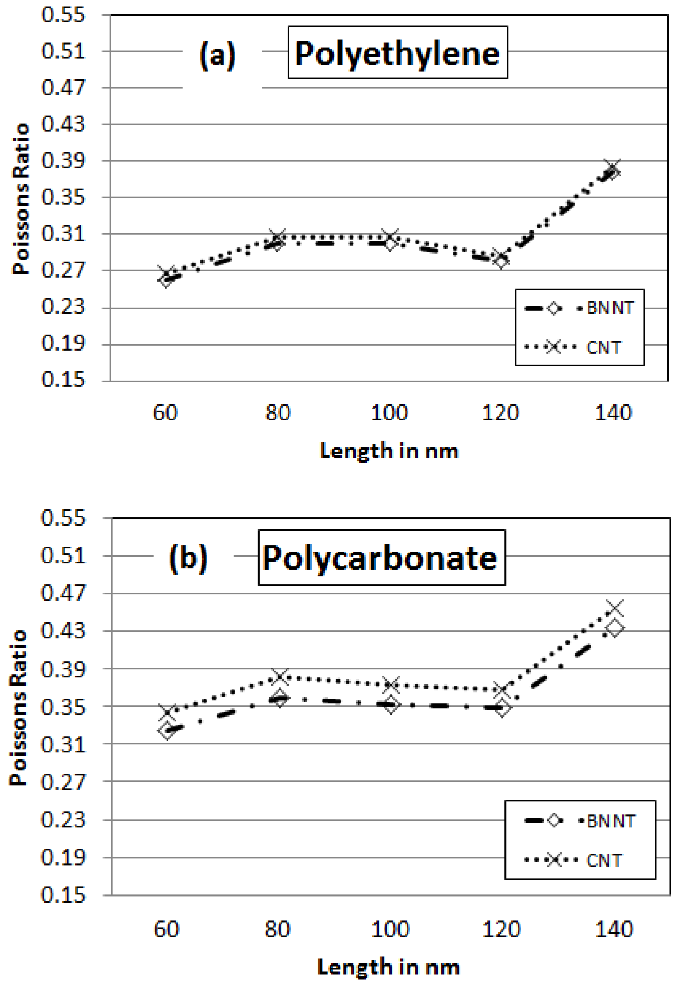

Fig 6: Variation in Poison's ratio against length of nanotubes (CNTs and BNNTs) (a) Polyethylene matrix, and (b) Polycarbonate matrix.

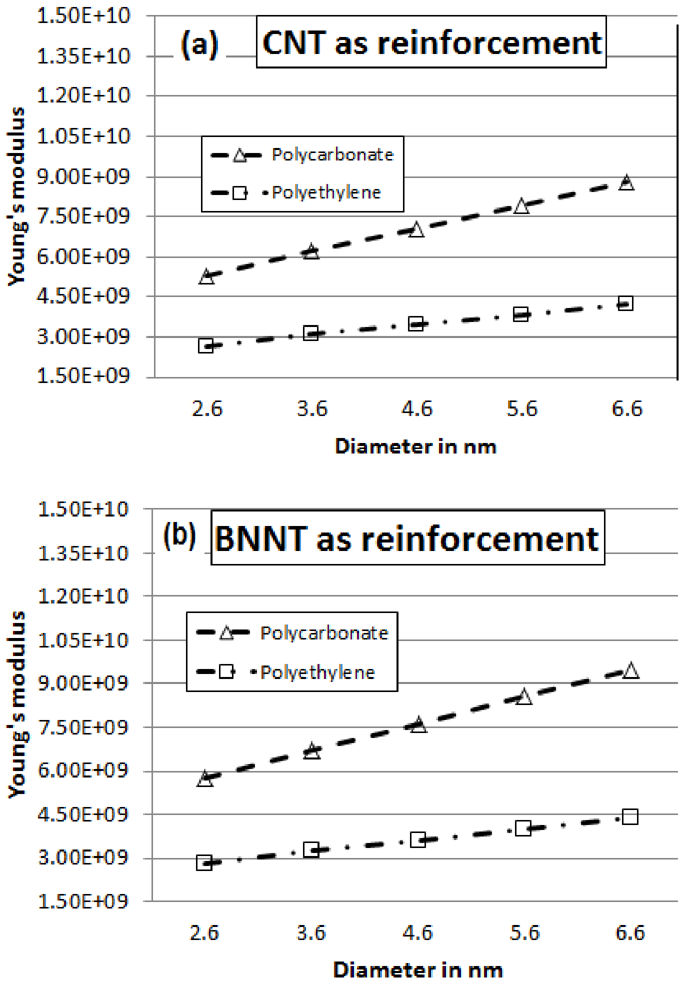

Fig 7: Variation in Young's modulus against diameter of nanotubes (CNTs and BNNTs) (a) CNT as reinforcement, and (b) BNNT as reinforcement.

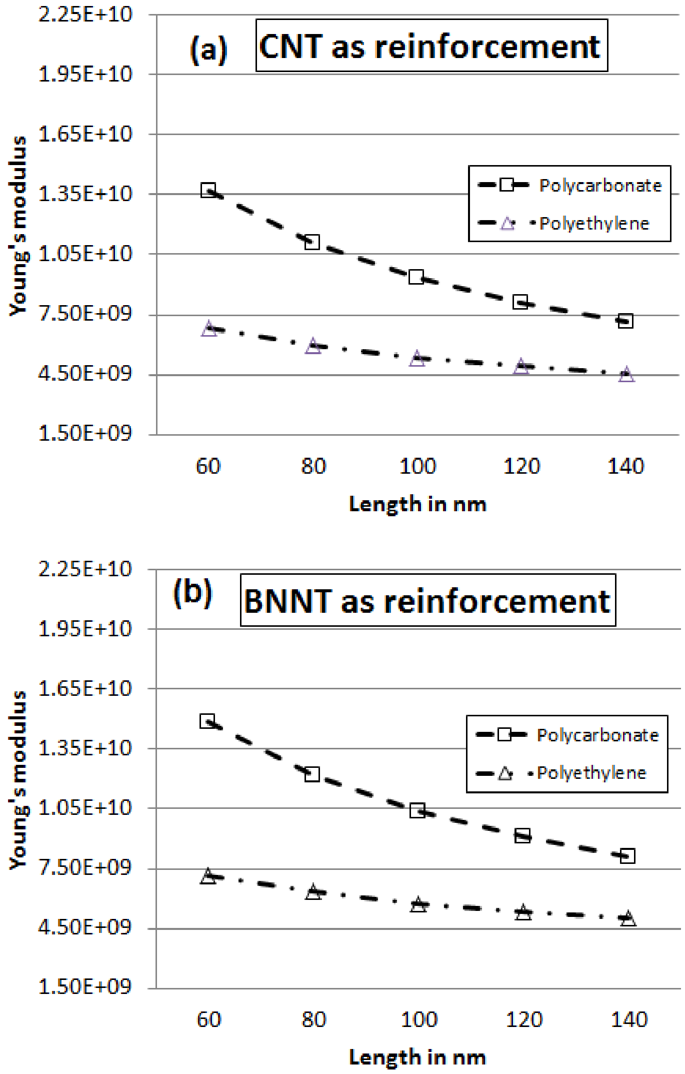

Fig 8: Variation in Young's modulus against length of nanotubes (CNTs and BNNTs) (a) CNT as reinforcement, and (b) BNNT as reinforcement.

V. Conclusion

The presented work is found to be important to estimate the mechanical properties of nanocomposites having CNT and BNNT as a one of the constituents. The Poisson's ratio obtained for the change in diameter is in range of 0.23 to 0.35 for polyethylene matrix material and 0.29 to 0.43 for poly carbonate matrix material. For change in Length the obtained value in range of 0.26 to 0.38 for polyethylene matrix material and 0.34 to 0.45 poly carbonate matrix material. The obtained results suggest that the polyethylene matrix material can be used for applications, where unidirectional strength is required (as the range of variation in Poisson's ratio is narrow compared to poly carbonate matrix material). But, for the overall strength of the nanocomposites materials, the poly carbonate matrix material provides good strength compare to poly ethylene materiax material. The Young's modulus forfor poly carbonate matrix material varies in the range of 5E+09 Pa to 9.3E+9 Pa and for the Polyethylene matrix material the Young's modulus varies in range of 2.8E+09 Pa to 4.5E+09 Pa.

References

[1] Sumio Iijima et al. Helical microtubules of graphitic carbon. nature, 354(6348):56-58, 1991.

[2] Nasreen G Chopra, RJ Luyken, K Cherrey, Vincent H Crespi, et al. Boron nitride nanotubes. Science, 269(5226):966, 1995.

[3] Shokoofeh Dolati, Abdolhossein Fereidoon, and Kazem Reza Kashyzadeh. A comparison study between boron nitride nanotubes and carbon nanotubes. Methods, 49:52, 2012.

[4] http://coecs.ou.edu/brian.p.grady/images/nanotube.jpg.

[5] Dong Qian, Wing Kam Liu, and Rodney S Ruo_. Mechanics of c60 in nanotubes. The Journal of Physical Chemistry B, 105(44):10753-10758,2001.

[6] Eric W Wong, Paul E Sheehan, and Charles M Lieber. Nanobeam mechanics: elasticity, strength, and toughness of nanorods and nanotubes. Science, 277(5334):1971-1975, 1997.

[7] Karl Sohlberg, Bobby G Sumpter, Robert E Tuzun, and Donald W Noid. Continuum methods of mechanics as a simplied approach to structural engineering of nanostructures. Nanotechnology, 9(1):30, 1998.

[8] Sanjay Govindjee and Jerome L Sackman. On the use of continuum mechanics to estimate the properties of nanotubes. Solid State Communications, 110(4):227-230, 1999.

[9] Xianlong Zhang, Liyuan Shen, HongWu, and Shaoyun Guo. Enhanced thermally conductivity and mechanical properties of polyethylene (pe)/boron nitride (bn) composites through multistage stretching extrusion. Composites Science and Technology, 89:24-28, 2013.

[10] Zeshuai Yuan, Zixing Lu, Mingyang Chen, Zhenyu Yang, and Fan Xie. Interfacial properties of carboxylic acid functionalized cnt/polyethylene composites: A molecular dynamics simulation study. Applied Surface Science, 351:1043-1052, 2015.

[11] Amanda L Tiano, Cheol Park, Joseph W Lee, Hoa H Luong, Luke J Gibbons, Sang-Hyon Chu, Samantha Applin, Peter Gnoo, Sharon Lowther, Hyun Jung Kim, et al. Boron nitride nanotube: Synthesis and applications. In SPIE Smart Structures and Materials+ Nondestructive Evaluation and Health Monitoring, pages 906006-906006. International Society for Optics and Photonics, 2014.

[12] Xiang Gao, Avraam I Isayev, and Chao Yi. Ultrasonic treatment of polycarbonate/carbon nanotubes composites. Polymer, 84:209-222, 2016.

[13] Mahmood M Shokrieh and Roham Rafiee. Prediction of mechanical properties of an embedded carbon nanotube in polymer matrix based on developing an equivalent long fiber. Mechanics research communications, 37(2):235-240, 2010.