International Journal of Chemical, Materials and Biomolecular Sciences
ISSN: 2415-6620
Vol:8, No:1, 2014

Simulation of Hydrogenated Boron Nitride Nanotube's Mechanical Properties for Radiation Shielding Applications

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***Abstract*—**Radiation shielding is an obstacle in long duration space exploration. Boron Nitride Nanotubes (BNNTs) have attracted attention as an additive to radiation shielding material due to B^{10}'s large neutron capture cross section. The B^{10} has an effective neutron capture cross section suitable for low energy neutrons ranging from 10^{-5} to 10^{4} eV and hydrogen is effective at slowing down high energy neutrons. Hydrogenated BNNTs are potentially an ideal nanofiller for radiation shielding composites. We use Molecular Dynamics (MD) Simulation via Material Studios Accelrys 6.0 to model the Young's Modulus of Hydrogenated BNNTs. An extrapolation technique was employed to determine the Young's Modulus due to the deformation of the nanostructure at its theoretical density. A linear regression was used to extrapolate the data to the theoretical density of 2.62g/cm^3. Simulation data shows that the hydrogenated BNNTs will experience a 11% decrease in the Young's Modulus for (6,6) BNNTs and 8.5% decrease for (8,8) BNNTs compared to non-hydrogenated BNNT's. Hydrogenated BNNTs are a viable option as a nanofiller for radiation shielding nanocomposite materials for long range and long duration space exploration.

***Keywords*—**Boron Nitride Nanotube, Radiation Shielding, Young Modulus, Atomistic Modeling.

I. Introduction

FOR the last decade, there has been increased focus in developing materials for radiation shielding to protect the astronauts, space structures and equipment from space radiation. Space radiation is composed ionizing radiation and non-ionizing radiation [1]. There are three main types of ionizing radiation: Solar Particle Events (SPE), Galactic Cosmic Rays (GCR), and Secondary Neutrons. Solar particle events are high energy electrons, protons, and heavy particles that are generated mainly from solar events such as solar flares. GCRs are particles ranging from a single proton to heavy nuclei of particles and originate from outside our solar system. Secondary neutrons are produced by interaction of GCRs and SPEs with matter [1]. It has become necessary that a shielding solution be developed that is lightweight, cost effective and durable to insure the safety of astronauts and success of long duration missions.

Boron Nitride Nanotubes (BNNTs) have become an attractive nanomaterial for this application. BNNTs are similar in structure to Carbon Nanotubes (CNTs) but the carbon atoms are replace with boron and nitrogen atoms, with almost identical lattice parameters, bond angles, and bond spacing [2]. The structural similarities of BNNTs and CNTs lead researchers to believe that these two structures have similar mechanical properties. CNTs have become a focal point for enhancing the mechanical properties of composite materials because of their superb mechanical properties. Boron is the key element associated with the radiation shielding characteristics of BNNT's because of B^{10}'s large neutron capture cross section, making it effective at capturing harmful neutrons [1]. Single-walled BNNTs have a band gap of 5.0 to 6.0eV (semiconducting range) [2]-[4]. BNNT's also offer better thermal conductivity and chemical stability, which are beneficial in the fabrication of radiation shielded suits and composites [5]-[8]. These properties have made BNNT's a good choice for applications in radiation shielding material in the structure of space craft and organic photovoltaic packaging material [9]-[10].

In the past it was very difficult to fabricate large amounts of high quality BNNTs. Most of the draw backs were due to the high synthesis temperatures and toxic precursor gases required to manufacture highly crystalline, low impurity, low defect BNNTs. Recently, the National Aeronautics and Space Administration (NASA) developed a new synthesis method that addresses the challenges mentioned above. The method is called the pressure vapor condenser (PVC) method and this breakthrough has made BNNTs a viable solution to create radiation shielding nanocomposites.

II. Simulation Details

Materials Studios 6.0 by Accelrys was used to perform the Molecular Dynamics (MD) Simulation. A universal force field was used, inside of the CASTEP module which uses Density Functional Theory (DFT) to calculate the various parameters of the system. The simulation process consists of five steps:

1. Construction of a BNNT and a Periodic Box,
2. Loading of the BNNT with hydrogen
3. Geometry optimization
4. Calculation of Elastic Constants
5. Calculation of Mechanical Properties.

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Once the construction of the BNNT and periodic box has been completed, we begin to load the BNNT with Hydrogen. Covalently bonded hydrogen was attached to the Boron and Nitrogen atoms within the BNNT creating a fully hydrogenated structure as was described by Tanskanen et al. [11]. Two configurations of Hydrogenated BNNTs (HBNNTs) were constructed. In the first structure, hydrogen is attached externally to Boron and Nitrogen. The second configuration attaches hydrogen externally to Boron and internally to Nitrogen. These two configurations were chosen because they were shown to be the most energetically favorable structures of HBNNTs [11]. Also, two different size nanotubes were simulated, (6,6) and (8,8) armchair nanotubes. Nanotubes are in the armchair configuration when the integers (n,m) in the chiral vector R= na_1+ma_2 are the same value [12].

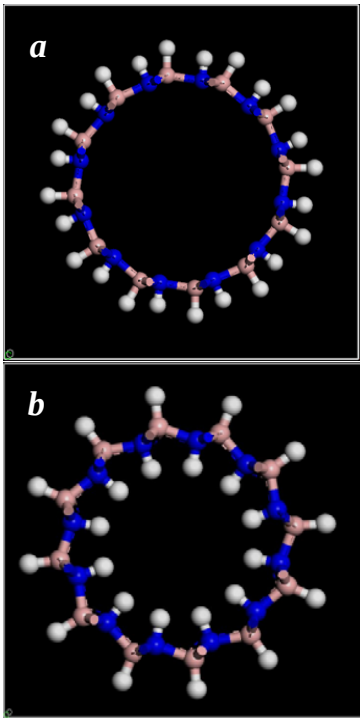

Fig. 1 (a) HBNNT with Hydrogen externally bonded (b) HBNNT with Hydrogen externally bonded on Boron and internally bonded on Nitrogen

Next, geometry optimization is performed on the HBNNTs using DFT, and the hybridized functional (Becke, 3-Parameter, Lee Yang (B3LYP)) [11]. Linear extrapolation was performed to correct the distortion experienced by the nanotubes at the theoretical density, ~2.62g/cm^3. Thus, four larger periodic boxes were constructed to lower the overall density of the system and a linear regression method was used to extrapolate the Young's Modulus to the theoretical density of the BNNTs [13].

Lastly, the elastic constants are calculated using DFT with a general gradient approximation (GGA) and the Perdew Wang 91 (PW91) functional set [12]. Then, the Material Studios software analyzes the elastic constant and calculates the Young's modulus for the BNNT systems.

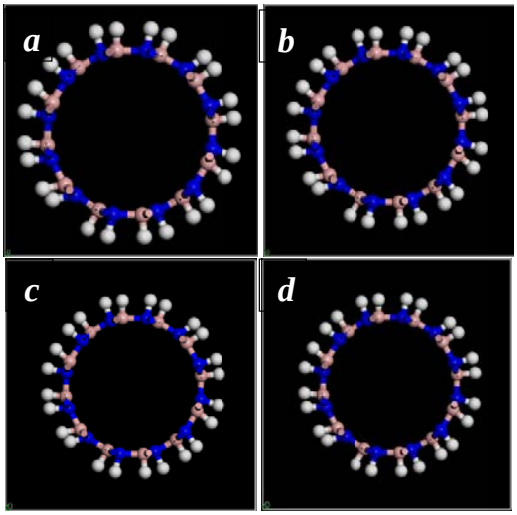

Fig. 2 Depicting the increased lattice size parameters from a-d of (6,6) BNNT, 12.3 Å , 13.5 Å, 14.8 Å, 16.2 Å

TABLE I
PHYSICAL CHARACTERISTICS OF THE UNIT CELLS USED FOR (6,6) BNNTS WITH HYDROGEN

(6,6) BNNT with Hydrogen				
Run #	1	2	3	4
Diameter of BNNT (Å)	8.14	8.14	8.14	8.14
Lattice size (A=B, C)	12.3, 24.595	13.5,24.595	14.8, 24.595	16.2, 24.595
Density (g/cm^3)	1.383	1.148	0.955	0.797
(8,8) BNNT with Hydrogen				
Run #	1	2	3	4
Diameter of BNNT (Å)	10.85	10.85	10.85	10.85
Lattice size (A=B, C)	15.5, 24.595	17.0,24.595	18.6, 24.595	20.5, 24.595
Density (g/cm^3)	1.525	1.329	1.190	1.103

III. Results and Discussion

The young's modulus for bnnt and the two configurations of HBNNTs were determined using the extrapolation technique (Figs. 3 and 4). Table II shows predicted values of E where theoretical density of 2.28 g/cm3 and 2.62 g/cm3 were used for BNNT and HBNNT, respectively. In case of (6,6) nanotubes, addition of Hydrogen to the structure of tube resulted in 11.6 percent decrease in Young's modulus (for both configurations) while for (8,8) nanotubes smaller decrease is observed with 10 percent for the external Hydrogen configuration and 7 percent for Hydrogen on the external side of B and the internal side of N configuration. Therefore, it is expected that by introducing Hydrogen to the structure of nanotubes, the Young`s modulus value will decrease by the average of 8.5 percent.

TABLE II
PREDICTED YOUNG`S MODULUS FOR (6,6) AND (8,8) BNNTS AND HBNNTS

BNNTs Type	6,6	8,8
External Hydrogen Only	733	715
Hydrogen on External B and Internal N	732	736
No Hydrogen	830	795

Interestingly, the changes of Young`s modulus for Hydrogen on the external side of B and the internal side of N for both (6,6) and (8,8) nanotubes is very close (11 and 10 percent, respectively) while for the external Hydrogen configuration, changes in E for (8,8) is smaller than (6,6) tubes. Even though further investigation is needed, addition of Hydrogen on only external sites has been demonstrated to have less effect on Young`s modulus of nanotubes with larger diameter. The relationship between tube diameter and the effect of introducing Hydrogen on Young`s modulus may be explained through atomic interactions between Hydrogen and B and N atoms. In the smaller tube, e.g.(6,6) with 0.814 nm diameter, the distances between atoms are so small that changing the position of Hydrogen from the outside to the inside of the tube might not affect the total interaction between the three types of atoms. On the other hand, the larger (8,8) Nanotubes (diameter of 1.085 nm) shows a dependence on the configuration of the hydrogen which is probably due to the increased distance between the atoms, resulting in a decreased disturbance on the overall system.

Although, based on presented results, addition of Hydrogen reduces the elastic modulus of BNNTs and degrades mechanical properties, HBNNTs still offer a unique and interesting combination of strength and shielding capability. Researchers have long tried to improve the mechanical strength of carbon composite by adding Carbon Nanotubes, but the results are not as promising as was expected. Addition of Carbon nanotubes into composites has introduced new challenges such as dispersion of nanotubes throughout the composite, nanotube agglomeration, interface interaction between nanotube and matrix, a limit on the maximum percentage of Carbon nanotubes that can be incorporated into the composite and many others. Therefore, HBNNTs can be interesting candidates for space application, considering that they possess a combination of properties including improved radiation shielding properties, high Young`s modulus (+ 700 GPa comparing to 150 GPa for carbon fiber) and light weight. Once fabrication challenges are solved and good quality composites are made using HBNNTs, addition of Boron Nitride nanotubes are expected to increase the mechanical strength of carbon fiber nanocomposite while improving chemical and thermal stability [6], [10], [14].

IV. Conclusion

Using the extrapolation technique with the Material Studios software has shown that it is possible to predict Young's Modulus for BNNTs [13]. Results show an 11 % decrease in the Young's Modulus for the (6,6) HBNNTs and an 8.5 % decrease for the (8,8) HBNNTs . This would still result in an enhancement of the mechanical properties of the conventionally accepted and used carbon fiber composites. In conclusion, hydrogenated BNNTs are theoretically predicted to be a viable choice in radiation shielding nanocomposites.

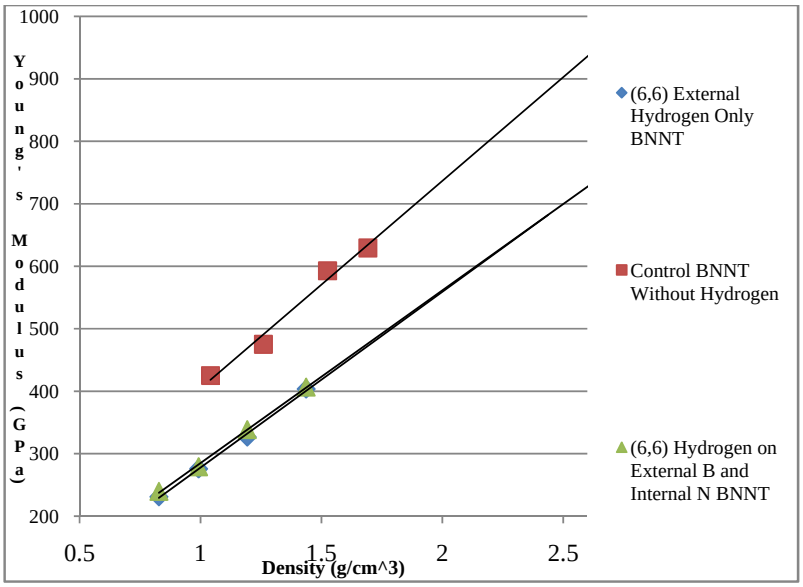

Fig. 3 Young's Modulus vs. Density for (6,6) BNNT w and w/o Hydrogen

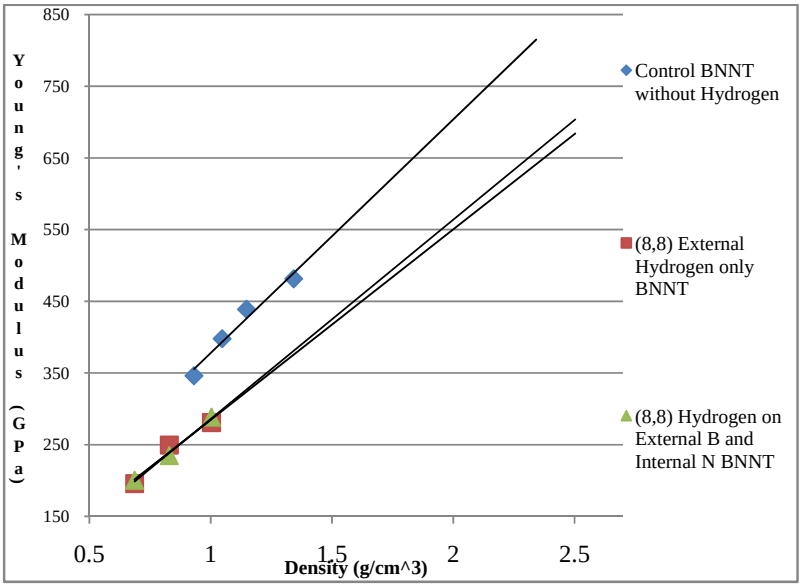

Fig. 4 Young's Modulus vs. Density for (8,8) BNNT w and w/o Hydrogen

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