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Modeling of Single Wall Carbon Nanotube as a Nanopipe During Molecule Passage

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Abstract: Single Wall Carbon Nano-Tubes (SWNT) have novel mechanical properties. Therefore, they are nominated for many applications. Their ability to transfer molecules has been observed and one of SWNT applications which is going to be developed is storing and transformation of fuel molecules in fuel cells for power generation. In this study the passage of a hydrogen molecule through a SWNT and their interactions were studied by a combination of analytical and Finite Element methods. It was seen that molecule passage causes transient vibrations in SWNT due to van der Waals interactions and SWNT attracts and absorbs hydrogen molecule. As the SWNT diameter increases the applied attraction force reduces. Thus, it is possible to use large diameter SWNTs as a Nano-Pipe and SWNTs with small diameter as a Nano-Pump.

Key words: Single Wall Carbon Nanotubes (SWNT), van der waals interactions, fuel cell

INTRODUCTION

Since carbon naono-tubes discovery in 1991, due to their novel mechanical and electrical characteristics, they have been subjected to many theoretical and experimental studies. They have high stiffness, axial strength and flexibility, which nominate them for various applications. Single Wall Carbon Nano-Tubes (SWNT) are considered as rolled graphite sheets with hexagonal lattices, which forms seamless cylinders, by various researches such as; Jiang *et al*. (2003), Budyka *et al*. (2005), Gates and Hinkley (2003) and Cotfas (2005).

The previous studies by Qian *et al*. (2002), showed that bucky balls are attracted into the SWNTs. This study proposes an application for SWNTs as super high ways for mass transfer. For this reason, one of SWNT's potential applications is storing and transferring fuel molecules like hydrogen and methane in fuel cells for energy generation. In present study, the passage of a single hydrogen molecule with an initial velocity through a SWNT is considered. To study the SWNT and passing hydrogen molecule interactions, conventional analytic equation calculating van der Waals forces was used and Finite Element method was employed to derive SWNT responses. For simplicity it is assumed that SWNT is fixed at its both ends, the molecule axis is aligned with SWNT axis and it inters into the SWNT in its center point.

SWNT MODELING

SWNTs are modeled either as a space frame structures or continuum shells by Valavala and Odegard (2005), Odegard *et al*. (2003), Tserpes and Papanikos (2005), Odegard *et al*. (2002), Lau *et al*. (2004) and Leamy (2005). In space frame model, the inter-atomic interactions between carbon atoms in a carbon lattice are considered as structural beam elements. To show the bonding interaction Modified Morse Potential was hired and to consider non bonding interactions, Lennard-Jones Potential was used. In this way, a space frame model is generated in the shape of hexagonal carbon lattice which consists of twelve members. To simplify the modeling and reducing analysis time and expenses, effective elements in the shape of carbon lattice shape has been developed based on equality of deformation energy stored in both models. In this way, the effective Young modulus and diameter of the effective space frame model has been calculated as $E_{effective}$ = 6 TP_a and $d_{effective}$ = 0.1448 nm (Fig. 1-4).

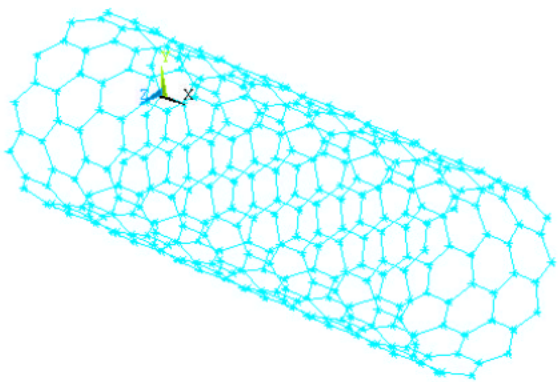

Fig. 1: A SWNT is considered as a space frame model

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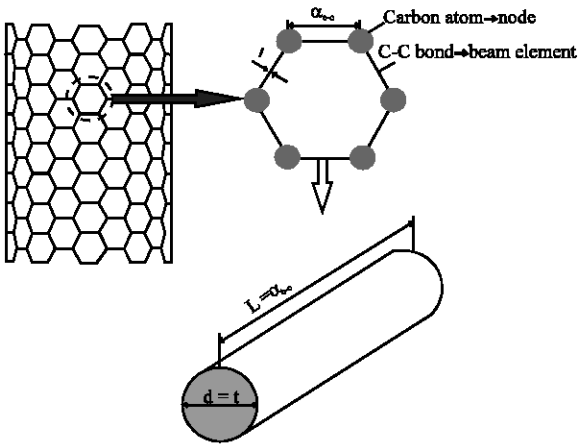

Fig. 2: Definition of space frame model representing SWNT

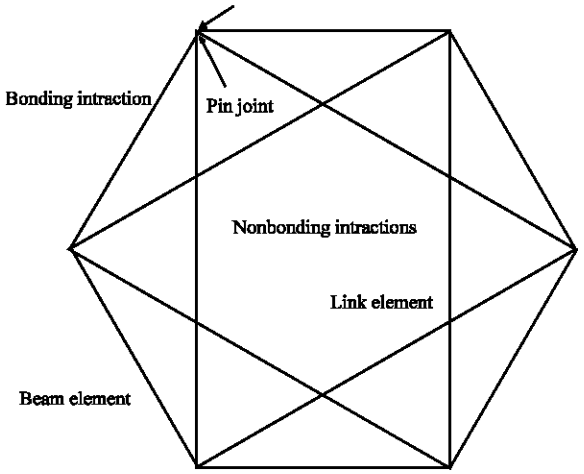

Fig. 3: Bonding and none bonding interactions in a carbon lattice

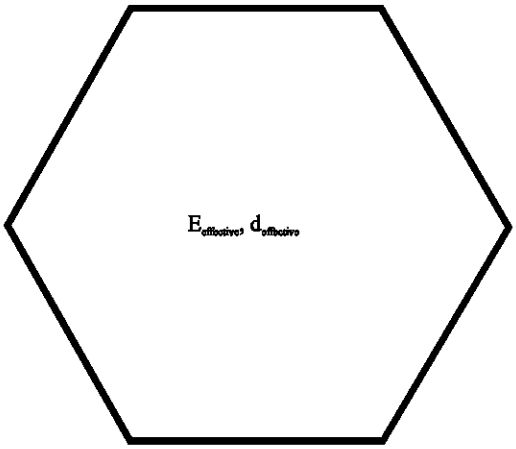

Fig. 4: Developed space frame elements with effective mechanical properties

MOLECULE PASSAGE SIMULATION

When a molecule passes through a SWNT, there is no concept as internal pressure like macroscopic environment. Because in macroscopic point of view, the definition of pressure is applied force on a surface divided by surface size, but it is not possible to determine the concept of internal surface for such this application because there is no certain description for SWNT thickness.

When a particle passes through a SWNT the van der Waals interactions between SWNT atoms and the particle are generated. In order to consider SWNT and passing particle behaviors during particle passage, following assumption were made:

- The particles are interring with initial velocity in axial direction and center point of SWNT only.
- The SWNT behavior is elastic:
- All carbon atoms, in SWCNT which are positioned in a circumferential ring have the same displacement.

Dequenes *et al.* (2004) showed that the amount of interactions can be obtained by Lennard-Jones equation, describing the nature of the interactions which can be attractive or repulsive by:

$$\phi_{ij} = \frac{C_{12}}{r_{ij}^{12}} - \frac{C_6}{r_{ij}^{6}} \quad (1)$$

which C_6 and C_{12} are attractive and repulsive van der Waals constants, respectively and r_{ij} is interactive atoms' distance.

By differentiating Eq. 1 with respect to interactive atoms' distance, the applied force is calculated (Fig. 5):

$$F = -\frac{d\phi}{dr_{ij}} \Rightarrow F = \frac{12C_{12}}{r_{ij}^{13}} - \frac{6C_6}{r_{ij}^{7}}$$
$$r_{ij} = \sqrt{R_{NT}^2 + d_i^2} \quad (2)$$

Where R_{NT} is SWNT's radius. Levesque *et al.* (2002) presented the van der Waals constants for C-H interactions as followings:

$$C_6 = 79.857949 \frac{kcal.\mathring{A}^6}{mole}$$
$$C_{12} = 29108.222 \frac{kcal.\mathring{A}^{12}}{mole} \quad (3)$$

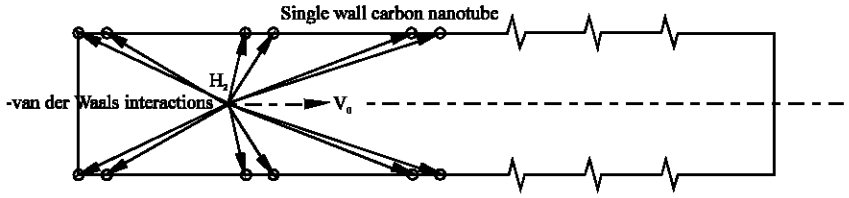

Fig. 5: van der Waals interaction between SWNT and passing molecule

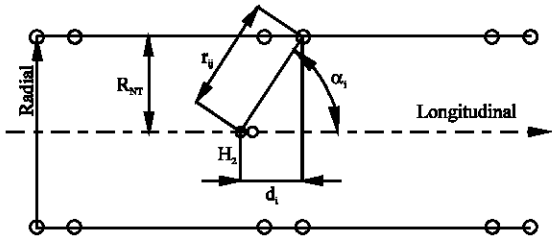

Fig. 6: Degrading interaction forces into longitudinal and radial directions

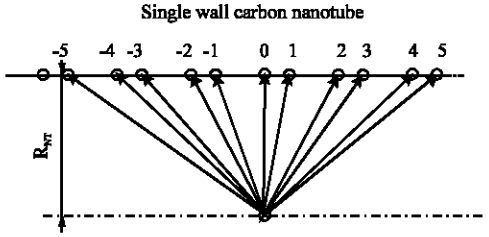

Fig. 7: Numbering system of SWNT carbon atom rings employed in this study to show the van der Waals interactions pattern acting on SWNT rings

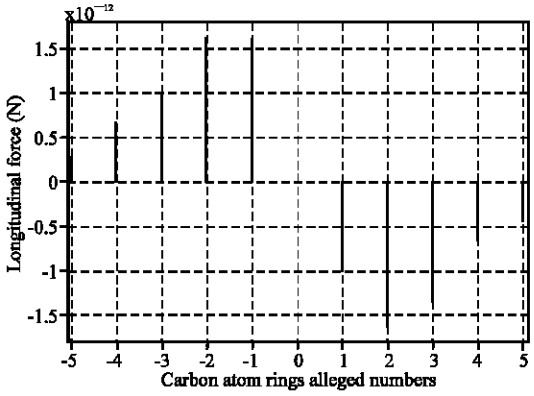

Fig. 8: Longitudinal van der waals force pattern acting on SWNT rings

The interaction force is degraded in to two directions; SWNT longitudinal and Radial directions by (Fig. 6):

$$\alpha_i = \text{Arctg}(\frac{R_{NT}}{d_i}) \quad (4)$$

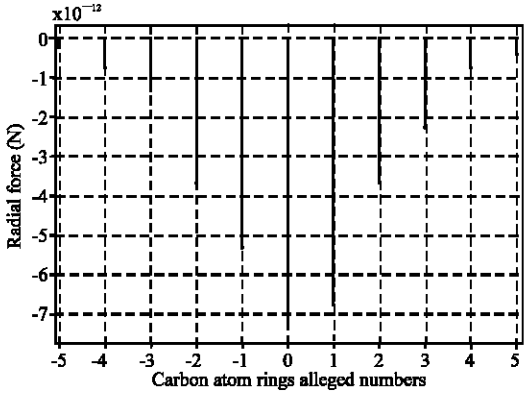

Fig. 9: Radial van der Waals force pattern acting on SWNT rings

$$F_L = \sum_{i=1}^{n}[(\frac{12C_{12}}{r_{ij}^{13}} - \frac{6C_6}{r_{ij}^{7}})].N.\text{Cos}\alpha_i$$
$$F_R = \sum_{i=1}^{n}[(\frac{12C_{12}}{r_{ij}^{13}} - \frac{6C_6}{r_{ij}^{7}})].N.\text{Sin}\alpha_i \quad (5)$$

Where F_L is longitudinal part of forces, F_R is radial part of force, N is the number of atoms per a SWNT ring and n is the number of considered rings identifying the SWNT length. In this way it is possible to calculate and obtain the amount of interaction forces between passing hydrogen atom and SWNT in two directions as well as their pattern. For a R_{NT} = 0.47 nm longitudinal and radial force patterns are calculated. The obtained pattern shows that, when the molecule is situated in a carbon ring, in radial direction, SWNT's after passage area is under tension whereas SWNT's before passage area is under compression. In longitudinal direction, the SWNT is only under tension (Fig. 7-9).

Combination of these deformations in affected region is similar to Fig. 10, which has a lot of similarities to one of SWNT's natural mode shapes (Fig. 11). This means that the transient response of SWNT due to hydrogen molecule passage is dominated by this natural mode shape (Fig. 12 and 13).

Using Molecular Mechanics principals, the interactions of three SWNTs with different diameters has

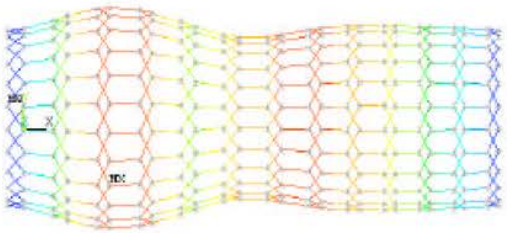

Fig. 10: Combination of radial and longitudinal deformation of SWNT during molecule passage

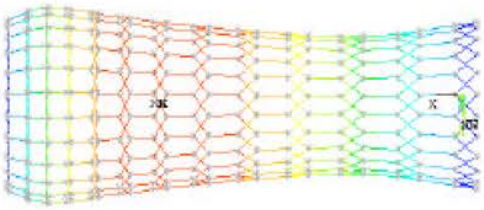

Fig. 11: Dominating SWNT natural mode shape during molecule passage

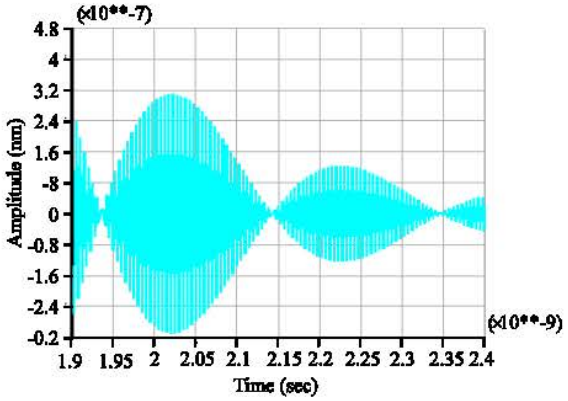

Fig. 12: Transient radial vibration of a certain ring of the SWNT, due to passage of a hydrogen molecule

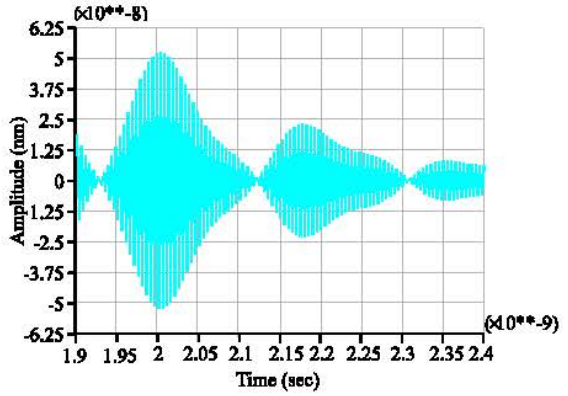

Fig. 13: Transient longitudinal vibration of a certain ring of the SWNT, due to passage of a hydrogen molecule

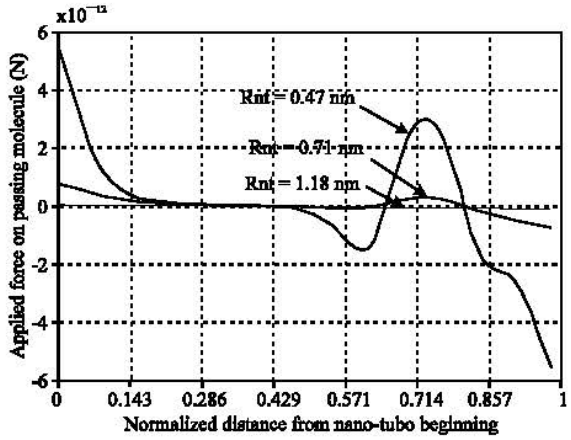

Fig. 14: Van der Waals force applied on a hydrogen molecule during its passage through three SWNTs with different diameters

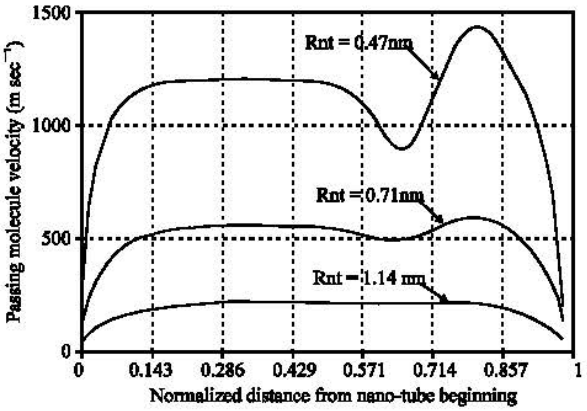

Fig. 15: Hydrogen molecule passage speed through three SWNTs with different diameters

been calculated. It is observed that in the iterance point of the SWNT, a great attractive force is applied on the hydrogen atom. While the SWNT diameter is smaller, the attractive force is greater. In the first half of the SWNT the hydrogen passage velocity becomes stable because attractive and repulsive forces neutralize each other. In the beginning of the second half, there is a repulsive and attractive force which acting on passing hydrogen which their result is an increase in passing molecule velocity When the molecule reaches to the end of SWNT, due to an attracting force absorbing hydrogen molecule into the SWNT, it velocity decreases rapidly. It is observed that when SWNT's diameter is large enough, the exit speed of hydrogen molecule is nearly equal to its iterance speed while in relatively small diameter SWNTs, the exiting speed of hydrogen is greater then its entering speed (Fig. 14 and 15).

CONCLUSIONS

As the SWNT was considered as an elastic material, its deformation due to flow of hydrogen atoms can be demonstrated by super position of several one atom-passages resulted deformations. The interactions between passing molecule and SWNT cause a vibration in it. As the deformation shape of SWNT is very similar to one of its natural mode shapes, the SWNT respond in governed by its frequency and transient analysis by FEA confirmed it. As mentioned before, when the SWNT diameter is smaller, its attractive force on passing molecule is greater. Therefore it is possible to use a SWNT with a small diameter as a Nano-pump system and a SWNT with a large diameter as a Nano-piping system. In this way, it is possible to form a piping system consisting storage tank, pumps, pipes and flow controls introduced by Grujicic *et al.* (2005) in nano-scale.

REFERENCES

Budyka, M.F., T.S. Zybina A.G. Ryabenko, S.H. Lin and A.M. Mebel, 2005. Bond lengths and diameter of armchair single wall carbon nanotubes. Chem. Phys. Lett., 407: 266-271.

Cotfas, N., 2005. An alternate mathematical model for single wall carbon nanotubes. J. Geometry Phys., 55: 123-134.

Dequenes, M., Z. Tang and N.R. Aluru, 2004. Static and dynamic analysis of carbon nanotube-based switches. Trans. ASME., 126: 230-237.

Gates, T.S. and J.A. Hinkley, 2003. Computational materials: Modeling and simulation of nanostructured materials and systems, NASA/TM-2003-212163.

Grujicic, M., G. Cao, B. Pandurangan and W.N. Roy, 2005. Finite element analysis-based design of a fluid-flow control valve. Mater. Sci. Eng., 117: 53-61.

Jiang, H., P. Zhang, B. Liu, Y. Huang, P.H. Geubelle, H. Gao and K.C. Hwang, 2003. The Effect of nanotube radius on the constitutive model for carbon nanotubes. Comput. Mater. Sci., 28: 429-442.

Lau, K.T., M. Chipara, H.Y. Ling and D. Hui, 2004. On the effective elastic moduli of carbon nanotubes for nanocomposite structures. Composites, 35: 95-101.

Leamy, M.J., 2005. Dynamic finite element modeling of carbon nanotubes using an intrinsic formulation. IDETC/CIE 2005, DETC2005-844482.

Levesque, D., A. Gicquel, F.L. Darkin and S.B. Kayiran, 2002. Monte carlo simulation of hyrogen storage in carbon nanotubes. J. Phys. Condens. Matter., 14: 9285-9293.

Odegard, G.M., T.S. Gates, Lee, M. Nicholson and K.E. Wise, 2002. Equivalent continuum modeling of nano-structured materials. Comp. Sci. Technol., 62: 1869-1880.

Odegard, G.M., T.S. Gates, K.E. Wise, C. Park and E.J. Siochi, 2003. Constitutive modeling of nanotube-reinforced polymer composites. Comp. Sci. Technol., 63: 1671-1687.

Qian, D., G.J. Wagner, W.K. Liu, M.F. Yu and R.S. Ruoff, 2002. Mechanics of carbon nanotubes. Applied Mech. Rev., 55: 495-533.

Tserpes, K.I. and P. Papanikos, 2005. Finite element modeling of single walled carbon nanotubes. Composites, 36: 468-477.

Valavala, P.K. and G.M. Odegard, 2005. Modeling techniques for determination of mechanical properties of polymer nanocomposites. Rev. Adv. Mater. Sci., 9: 34-44.