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Analysis of Fullerene as a Building Block for Nano Machines Used in Cancer Cell Dissociation

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***Abstract*— Accurate prediction of static and dynamic response of nano structures is one of the important interests of scientists in the last decade. Recently, application of the nano machines is increased in recognizing and disassembling cancerous cells and injecting them into the bloodstream of cancer suffers. Nano machines could also be used to build molecular support structures for strengthening bones and muscle tissues by reassembling nearby tissues. These applications make it necessary to analyze the components of nano machines, precisely. For this reason, Molecular Dynamic Method and some experimental methods are implemented in this area. Nano bearing as an important part of nano machine has been analyzed statically and dynamically in several studies. In this paper, a Fullerene which is one of the most important parts of nano bearings is simulated by a spherical super element whose deformations and natural frequency are calculated. The Fullerene is considered to be the C60 which is properly similar with a 66 surface-node spherical super element. Also the mechanical properties of the fullerene and boundary conditions of the nano ball bearing under loading are introduced and deformation and natural frequency of a fullerene under extensive load is presented with two different strategies, super element and conventional elements. Compatible findings of these two methods validate and confirm the results. Findings indicate that applying 1 super element for the simulation of the fullerene leads to same results as implementing 154764 conventional elements.**

Keywords-Fullerene, Nano ball bearing, Spherical super element, Deformation, Nano machine, Cell

I. INTRODUCTION

Since the nano technology had a revolutionary impact on computing, medicine and nanoscale engineering [1], a large number of studies have been done to emerge it as a practical and useful technology. During the improvement step of this science, discovery of fullerene in 1985 [2] encouraged the scientists to implement this material with specific properties in terms of electrochemistry, gas-absorption, optical and mechanics [2] in their theoretical and experimental investigations. Several studies have been done to introduce different properties of the fullerene. F. Cecchet investigated structural and electrochemical characteristics of monolayer fullerene. [3] T. Ogasawara, Y. Ishida and T. Kasai focused their studies on mechanical properties of carbon fiber/fullerene dispersed epoxy composites [2]. Vibration and electronic properties of fullerene are presented by I. Olejniczak [4]. Some other researches are concentrated on optimizing the properties of fullerene.

Compressive mechanical properties of Si-C60 are presented by H. Shen [5]. T. Tokunaga, K. Kaneko, K. Sato and Z. Horita investigated the microstructure and mechanical properties of aluminum-fullerene composite fabricated by high pressure torsion. Some other studies introduced other kinds of fullerene like C44, C50, C76, C80, C84, C90, C94, C120, C180 and C540 [6-9].

Application of fullerene in nano bearing has been presented in some researches. An atomistic study of fullerene nano ball bearing is done by J. W.Kong and H. J. Hwang [1]. Ultra-low friction fullerene ball bearing is simulated by X. Li and W. Wang [10]. These studies show the importance of fullerene in producing rotational motion in nano scale engineering. As mentioned, most of researches are focused on frictional simulation of fullerene in the nano ball bearing, for this reason, in this paper a fullerene is simulated by a 66 Surface-Node spherical super element whose deformation and natural frequency are obtained and findings are validated by results of several conventional elements used in ANSYS. Also, mechanical properties and boundary conditions are presented that describe the working condition of a C60 in the nano ball bearing.

II. FULLERENE (C60)

The C60 fullerene consists of 60 atoms of carbon which construct a spherical network because of the covalence forces between each two atoms. The van der waals force which is one of the molecular forces surrounds the C60 and these forces give some mechanical properties to C60 like Modulus of Elasticity and Poisson's Ratio. These properties have been studied for different kinds of nanotubes [11]. In Fig. 1, the variation of the modulus of elasticity with respect to the outermost tube diameter is shown [11]. It can be seen that when the tube diameter is larger than 1nm, the modulus of elasticity is approximately constant. Also Fig. 2 shows the relationship between the shear modulus and the outermost tube diameter [11]. As it is shown, the variation of the shear modulus is almost zero when the outermost tube diameter is larger than 1nm [11]. If we consider the carbon nanotube as a rolled graphene sheet, it can be concluded from Fig. 1 and Fig.2 that when the diameter of nanotube is larger than 1nm, rolling does not change mechanical properties such as the modulus of elasticity and the Poisson's ratio. In a similar manner, we can estimate the mechanical properties of fullerene which change with respect to the diameter and will be approximately constant when the diameter is larger than 1nm.

III. Element Design

Consider a hollow sphere with inner and outer radius r1 and r2, respectively. This sphere is divided to several parts by some equatorial and meridian orbits which nodes are placed in each intersection of these orbits [12-15]. The number of nodes in each super element is considered to be $2(N\times2^N+2)$ which N is an arbitrary integer. The number of nodes that are placed in both inner and outer surface must be almost 60, so the best selection for N is 4 that leads to 66 nodes for each surface and 132 nodes totally. This super element consists of 16 meridian and 6 equatorial orbits in each surface. These 66 nodes can show the characteristics of carbon atoms in fullerene, so static and dynamic analysis of this super element can predict the structural behavior of fullerene. In the following, the interpolation functions are presented and by using these functions, deformation and natural frequencies of the fullerene under concentrated loads are illustrated.

IV. Local Coordinates

Three independent coordinates (r, φ, θ) that are called general coordinates can define and characterize the spherical super element. For simplifying the calculations, three other independent coordinates are defined as x, y and z that are related to r, φ and θ as;

$$x=\frac{2r-(r_2+r_1)}{r_2-r_1}, y=\frac{2\varphi}{\pi}-1, z=\frac{\theta}{\pi}-1 \quad (1)$$

and are named local coordinates. According to the domains of general coordinates;

$$r_1<r<r_2, \qquad 0<\varphi<\pi, \qquad 0<\theta<2\pi \quad (2)$$

the domains of local coordinates are defined as;

$$-1<x,y,z<1 \quad (3)$$

Using the local coordinates, the interpolation functions will be generated which are shown in (11).

V. Deformation Analysis

The mechanical systems can be analyzed statically by the following equation;

$$F=KX \quad (4)$$

which K is the stiffness matrix and is defined as;

$$K=\int_V B^T DB dv \quad (5)$$

that B, D, F and X are strain-interpolation, material property, force and displacement matrices, respectively.

VI. Natural Frequencies

The motion of a mechanical system is defined by the following equation;

$$M\ddot{X}+C\dot{X}+KX=0 \quad (6)$$

which C vanishes in undamped systems. Considering the motion of the system in only one of mode shapes, the simple harmonic motion with respect to the natural frequency ωi will be resulted, therefore the displacement vector could be expressed as;

$$X=A_i\cos(\omega_i t) \quad (7)$$

that A_i is the amplitude vector. [14-15]

Substituting (7) in (6) leads to;

$$(-M\omega_i^2+K)Q_i=0 \quad (8)$$

The determinant coefficient matrix must be zero for finding nontrivial answers for the equation 8 [14-15];

$$|-M\omega_i^2+K|=0 \quad (9)$$

Solving this equation leads to eigenvalues of the matrix $(M^{-1}\times K)$ which are the square of natural frequencies [14-15].

In (8), M is Mass matrix and defined as;

$$M=\int_V \rho N^T N\, dv \quad (10)$$

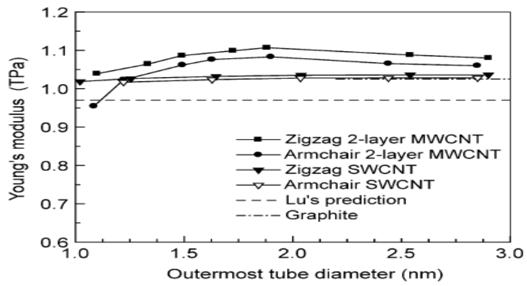

Figure 1. The effects of tube diameter and tube chirality on Young's moduli of two-layer MWCNT. [11-13]

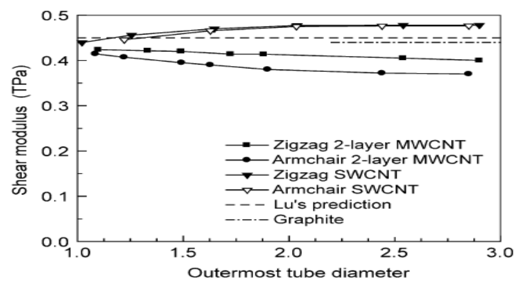

Figure 2. The effects of tube diameter and tube chirality on shear modulus. [11-13]

$$N_1 = \frac{1}{128}(\cos(4\pi z))(1+\cos(4\pi z))(1+\cos(2\pi z))(1-\cos(\pi z))(\cos(2\pi y))(1+\cos(2\pi y))(1-\cos(\pi y))\left(1-\sin\left(\frac{1}{2}\pi y\right)\right)(1-x)$$

$$N_2 = \frac{1}{128}(\cos(4\pi z))(1+\cos(4\pi z))(1+\cos(2\pi z))(1-\cos(\pi z))(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_3 = \frac{1}{128}(\sin(4\pi z))(1+\sin(4\pi z))\left(1+\sin\left(2\pi z+\frac{1}{4}\pi\right)\right)\left(1-\sin\left(\pi z+\frac{3}{8}\pi\right)\right)(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_4 = -\frac{1}{128}(\cos(4\pi z))(1-\cos(4\pi z))(1+\sin(2\pi z))\left(1-\sin\left(\pi z+\frac{1}{4}\pi\right)\right)(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_5 = -\frac{1}{128}(\sin(4\pi z))(1-\sin(4\pi z))\left(1-\cos\left(2\pi z+\frac{1}{4}\pi\right)\right)\left(1-\sin\left(\pi z+\frac{1}{8}\pi\right)\right)(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_6 = \frac{1}{128}(\cos(4\pi z))(1+\cos(4\pi z))(1-\cos(2\pi z))(1-\sin(\pi z))(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_7 = \frac{1}{128}(\sin(4\pi z))(1+\sin(4\pi z))\left(1-\sin\left(2\pi z+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\pi z+\frac{3}{8}\pi\right)\right)(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_8 = -\frac{1}{128}(\cos(4\pi z))(1-\cos(4\pi z))(1-\sin(2\pi z))\left(1+\cos\left(\pi z+\frac{1}{4}\pi\right)\right)(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_9 = -\frac{1}{128}(\sin(4\pi z))(1-\sin(4\pi z))\left(1+\cos\left(2\pi z+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\pi z+\frac{1}{8}\pi\right)\right)(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_{10} = \frac{1}{128}(\cos(4\pi z))(1+\cos(4\pi z))(1+\cos(2\pi z))(1+\cos(\pi z))(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_{11} = \frac{1}{128}(\sin(4\pi z))(1+\sin(4\pi z))\left(1+\sin\left(2\pi z+\frac{1}{4}\pi\right)\right)\left(1+\sin\left(\pi z+\frac{3}{8}\pi\right)\right)(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_{12} = -\frac{1}{128}(\cos(4\pi z))(1-\cos(4\pi z))(1+\sin(2\pi z))\left(1+\sin\left(\pi z+\frac{1}{4}\pi\right)\right)(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$N_{13} = -\frac{1}{128}(\sin(4\pi z))(1-\sin(4\pi z))\left(1-\cos\left(2\pi z+\frac{1}{4}\pi\right)\right)\left(1+\sin\left(\pi z+\frac{1}{8}\pi\right)\right)(\sin(2\pi y))(1+\sin(2\pi y))\left(1-\sin\left(\pi y+\frac{1}{4}\pi\right)\right)\left(1+\cos\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1-x)$$

$$\vdots$$

$$N_{132} = -\frac{1}{128}(\cos(4\pi z))(1+\cos(4\pi z))(1+\cos(2\pi z))(1-\cos(\pi z))\left(\cos\left(2\pi y+\frac{3}{8}\pi\right)\right)\left(1-\cos\left(2\pi y+\frac{3}{8}\pi\right)\right)\left(1+\cos\left(\pi y+\frac{3}{8}\pi\right)\right)\left(1+\sin\left(\frac{1}{2}\pi y+\frac{3}{8}\pi\right)\right)(1+x) \quad (11)$$

VII. EXAMPLE 1

In this example, a fullerene under two concentrated loads is investigated. Consider a fullerene with inner radius r1=0.16 nm and outer radius r2=0.5 nm with Poisson's ratio $\nu = .159$ and modulus of elasticity $E = 1.05$ TPa that is subjected to two concentrated radial forces of magnitude $f_r = 2.55\times10^{-3}$ nN which are exerted to the North and South poles of outer surface of the fullerene in the r-direction. (Properties of the fullerene are shown in Table 1.)

This example is desired to find the deformation of the C60 where the force is applied and to obtain the natural frequency of the Fullerene. A 132-node super element is implemented to simulate the fullerene for finding the deformation and natural frequencies which has 66 nodes in each inner and outer surface. For validating the results of the super element, several conventional elements are implemented. Comparable results of these two methods can validate the interpolation functions of super element.

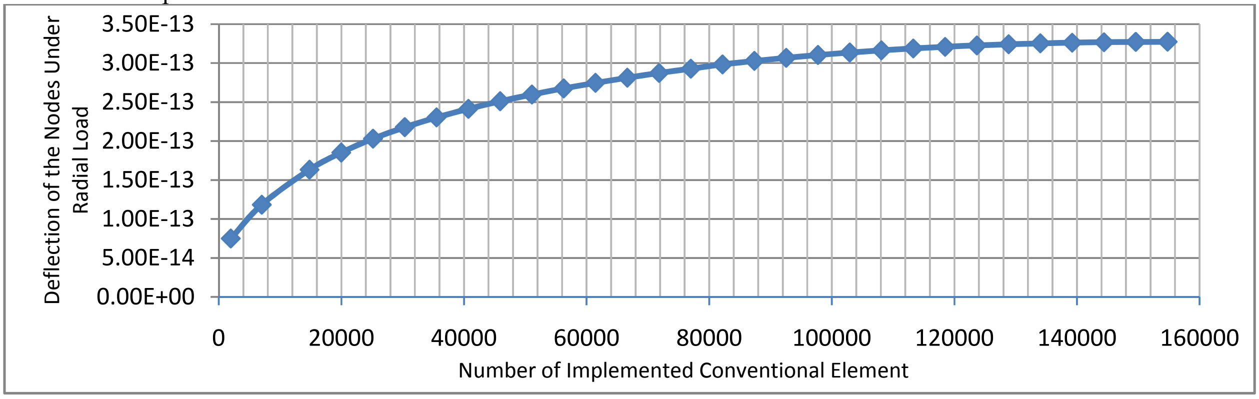

Figure 3. Convergence of the results of conventional brick element into the result of super element in finding the deformation of the Fullerene under concentrated radial loads

TABLE I. PROPERTIES OF THE FULLERENE (C60)

R1 (nm)	R2 (nm)	E (TPa)	ν	G (TPa)	Density (Kg/m3)
0.16	0.5	1.05	0.159	0.44	1650

TABLE II. DEFORMATION OF THE FULLERENE UNDER CONCENTRATED RADIAL FORCES IN EXAMPLE 1

	Method		**Relative Error**
	ANSYS(154764)	**Super element**	
Deflection of the Fullerene Under 2 concentrated Radial forces	3.2724 E-13	3.2731 E-13	0.021%

TABLE III. COMPARISON OF NATURAL FREQUENCY OF TORSIONAL MODE OBTAINED FROM SUPER ELEMENT AND CONVENTIONAL BRICK ELEMENT

Mode Shape	**Natural Frequency**		**Relative Error**
	ANSYS (19548)	**Super element (1)**	
Radial	8.790 E12	8.712 E12	0.9%

VIII. REMARKS

A. *Remark 1*

As it is shown in the example, the results of super element in prediction of the static response of fullerene is similar to the findings of 154764 conventional elements, this similarity shows the accuracy of the interpolation functions.

B. *Remark 2*

It should be noted that two radial forces of magnitude $f_r = 2.55\times10^{-3}$ nN can cause a deformation of magnitude 3.2731 E-13 in fullerene. This infinitesimal magnitude of deformation shows the importance of accurate calculation of K and M matrices to predict the deformation of fullerene. The introduced super element can generate the K and M matrices properly.

IX. CONCLUSION

In this paper, static and dynamic behavior of a fullerene is predicted by a spherical super element. This super element with 66 nodes in each inner and outer surface is properly designed to simulate the C60. There is a node on each North and South Pole of the sphere and others are distributed on the surface which are available to be exerted to several forces or other boundary conditions. Shape functions are generated to satisfy the essential conditions for each interpolation function. Also distribution of nodes on surface of the super element shows the similarity between this element and fullerene. In addition, mechanical properties of the fullerene are extracted from studies that are done about the CNT. Implementing this 132-node spherical super element to predict the behavior of a nano structure leads to comparable results with findings of several conventional elements. Accurate prediction of static and dynamic behavior of C60 by this element shows the eligibility of it to be used for analyzing the nano structures such as nano ball bearings.

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