Research note

Static and vibrational analysis of fullerene using a newly designed spherical super element

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Abstract

Accurate prediction of static and dynamic response of nano structures under external excitations has been one of the interests of scientists in the last decade. Several applications of nano machines make it necessary to analyze their components, such as nano bearing, precisely. In this paper, the static and vibrational behavior of a fullerene as a sensitive part of nano bearing under external forces is simulated by a newly designed spherical super element.

This super element is designed in such a way that the user can select as many numbers of nodes as desired, so that it can be implemented in different desired precisions. In this study, a 228-node super element, which is similar to a hollow sphere (114 nodes on each inner and outer surface), is used, and the formulation of shape functions are introduced. Also, the mechanical properties of fullerene and the boundary conditions of nano ball bearings are presented. Two strategies are utilized to validate the results; the super element and conventional elements. Findings indicate that applying one super element for simulation of the fullerene leads to the same results as implementing 154764 conventional elements.

Infinitesimal relative errors show the accuracy of calculations and shape functions of the super element.

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1. Introduction

Since nano technology has had a revolutionary impact on computing, medicine and nanoscale engineering [1], a large number of studies have been done to introduce it as a practical technology [2–8]. During the improvement step of this science, the discovery of fullerene and its derivatives in 1985 [9,10] encouraged scientists to implement these systems with specific properties, in terms of electrochemistry, gas absorption, optics and mechanics [9], in their theoretical and experimental research. Several studies have been done to introduce different properties of fullerene. In this regard, Cecchet et al. investigated the structural and electrochemical characteristics of monolayer fullerene [11]. Some other studies are focused on the mechanical properties of fullerene [12] and its effects on dispersed epoxy composites [9]. Vacik, Huo and their co-workers introduced structural, biological and tribiological properties of fullerene [13,14]. Furthermore, the vibration and electronic properties of fullerene are presented by Olejniczak et al. [15]. Some other research concentrated on optimizing the properties of fullerene. In this regard, the compressive mechanical properties of Si–C 60 are presented by Shen, which indicates the relationship between temperature and strain in fullerences and shows that within a range of 300–1100 K, temperature has little effect on their mechanical properties [16]. Atomistic studies of fullerene have been done by Yakobson and Sonsonde [17]. The Density Functional Theory (DFT) is used to analyze the structural and electronic properties of fullerene as a HIV-1 protease inhibitor [18]. Zagorodny and his co-workers concentrated their studies on structural analysis and property improvements of the fullerene using a theoretical approach called molecular design to analyze a way to connect linker molecules to the node molecules, in order to improve the mechanical and dielectric properties of C 60 [19]. Choi and his colleagues used Scaled Quantum Mechanical (SQM) calculations for vibrational assignment of all 46 fundamentals of C 60 [20]. Some other studies introduced other kinds of fullerene, like C 44, C 50, C 76, C 80, C 84, C 90, C 120, C 180 and C 540, and identified them theoretically [10,21].
Application of fullerene in nano bearing has been presented in some research. Legoas et al. implemented the molecular dynamic method for analysis of ultra-lubricated systems based on fullerene C$_{60}$ molecules, and introduced the energetically stable configuration of a C$_{60}$ monolayer deposited over a graphite surface [22]. An atomistic study of a fullerene nano ball bearing was done by Kang and Hwang [1]. They evaluated the ultimate pressure of fullerene, using classical molecular dynamics, and revealed that the bulk modulus and ultimate pressure of K–C$_{60}$ are higher than those of C$_{60}$.

Ultra-low friction fullerene ball bearing is simulated by Li and Yang [23]. They implemented direct molecular dynamic simulations for molecular ball bearings composed of fullerene molecules and multi-walled carbon nanotubes, and indicated that fullerene ball bearings have extremely low friction and energy dissipation. However, the deformation analysis and natural frequencies of fullerene used in nano ball bearings are not well addressed in literature.

The objective of this study is to simulate fullerene by a new spherical super element. In this paper, deformation, stress and natural frequencies of fullerene are obtained, and findings are validated by results of several conventional elements. In this paper, two strategies are applied to find the deformation, stress and natural frequencies of fullerene; the super element and conventional elements. In Section 2, the element design and shape function generation of the super element are briefly described to show how this new element is designed. Deformation and vibrational analysis is formulated in Section 3 to represent how conventional elements could be implemented in the Finite Element Method to investigate the static and dynamic response of fullerene in different excitations. In Section 4, the mechanical properties of fullerene are surveyed and it is indicated how property parameters used in FEM formulation are evaluated. A numerical example is presented in Section 5 to illustrate how the static and dynamic behavior of fullerene used in nano ball bearings could be estimated by the super element. Section 6 presents conclusions and deductions.

### 2. Element design

There are different techniques available from the literature (e.g. [19,22,23]) for property determination and simulating the fullerene. In this paper, a newly designed spherical super element proposed in [24] is adopted for the structural analysis of fullerene. Details of the generation of this element can be found in [24]. Major formulas and definitions are provided in the following.

In this super element, the number of equatorial and meridian orbits on each inner and outer surface are $2^{N-1} + 1$ and $2^N - 1$, respectively, where $N$ is an arbitrary positive integer (Figure 1). Nodes are placed at the intersections of these orbits, so the total number of nodes in each super element would be $2^N(2^{N-1} - 1) + 2$ [24]. There is a shape function corresponding to each node which must satisfy three essential conditions:

1. They must be continuous;
2. They must be differentiable;
3. The shape function corresponding to each node must be 1 at that node and vanish at other nodes.

By considering these conditions, the following shape functions will be generated:

$$N_{i,j,p} = \frac{1}{2^{N-1}} \cos \left[ \frac{2^{N-2} \theta - (j - 1) \pi}{2^{N-1}} \right] \times \left\{ \begin{array}{l} 1 + \cos \left[ \frac{2^{N-2} \theta - (j - 1) \pi}{2^{N-1}} \right] \\ 1 + \cos \left[ \frac{2^{N-3} \theta - (j - 1) \pi}{2^{N-1}} \right] \\ \vdots \\ 1 + \cos \left[ \frac{2 \theta - (j - 1) \pi}{2^{N-1}} \right] \\ \end{array} \right\}$$

$$1 \leq i \leq 2^{N-1} + 1, \quad 1 \leq j \leq 2^N$$

Figure 1: (a) Spherical coordinates. Numbering of orbits when $N = 3$. (b) Half-meridian orbits. (c) Equatorial orbits.
3. Deformation and vibrational analysis

To investigate the static and vibrational behavior of C₆₀, the equilibrium equation and the equation of motion are applied. The equilibrium equation of a system can be defined as:

\[ \{ F \} = [K] \{ X \}, \]

where \( K \) is the stiffness matrix and is defined as:

\[ K = \int_B B^T D B dV. \]

In which \( F \) and \( X \) are force and displacement vectors, respectively. Moreover, \( D \) and \( B \) are material property and strain-interpolation matrices and could be evaluated as:

\[ D = \frac{E}{1 + \nu} \begin{bmatrix} m & v & 0 & 0 & 0 \\ v & m & 0 & 0 & 0 \\ 0 & 0 & m & 0 & 0 \\ 0 & 0 & 0 & n & 0 \\ 0 & 0 & 0 & 0 & n \end{bmatrix}, \]

\[ B = LN, \]

where \( N \) is interpolation function matrix and \( L \) is a derivative matrix, which is defined in spherical coordinates as follows:

\[ L = \begin{bmatrix} \frac{1}{r} & 0 & 0 \\ 0 & \frac{1}{r} & 0 \\ 0 & 0 & \frac{1}{r} \end{bmatrix}, \]

\[ [L] = \begin{bmatrix} \frac{1}{r} & 0 & 0 \\ 0 & \frac{1}{r} & 0 \\ 0 & 0 & \frac{1}{r} \end{bmatrix}. \]

Based on Eq. (2), the deformation could be calculated by the following equation:

\[ \{ \epsilon \} = \{ X \} \cdot \{ D \}. \]

To calculate the stress vector, the relationship between stress and strain vectors is used as follows:

\[ \sigma = \{ \epsilon \} \cdot \{ B \}. \]

\[ \{ \epsilon \} \text{ is the strain vector and could be calculated as:} \]

\[ \{ \epsilon \} = \begin{bmatrix} \epsilon_r \\ \epsilon_\varphi \\ \epsilon_{\theta} \\ \tau_{r\varphi} \\ \tau_{r\theta} \\ \tau_{\varphi\theta} \end{bmatrix}. \]

\[ \{ \sigma \} \text{ is the stress vector and could be calculated as:} \]

\[ \{ \sigma \} = \begin{bmatrix} \sigma_r \\ \sigma_\varphi \\ \sigma_{\theta} \\ \tau_{r\varphi} \\ \tau_{r\theta} \\ \tau_{\varphi\theta} \end{bmatrix}. \]

In vibrational analysis of a system, mass ([\( M \)], damping ([\( C \)]) and stiffness matrices are used to write the equation of motion as:

\[ [M] \ddot{\{ X \}} + [C] \dot{\{ X \}} + [K] \{ X \} = 0, \]

where \( \{ X \}, \{ \dot{X} \} \) and \( \{ \ddot{X} \} \) represent position, velocity and acceleration vectors of the system, respectively, and \( [C] \) vanishes in undamped systems. By imposing harmonic vibration, eigenvalues are calculated from the mass and stiffness matrices. Natural frequencies of the system are obtained from the eigenvalues.

4. Mechanical properties of fullerene

To investigate the static and vibrational behavior of the fullerene, mechanical properties, such as modulus of elasticity...
Figure 3: Effects of tube diameter and tube chirality on Young's moduli of CNTs [25].

Figure 4: Effects of tube diameter and tube chirality on shear modulus [25].

and the Poisson ratio of this system, must be estimated. These properties are studied for different kinds of nanotube [25]. Figures 3 and 4 show variations of the modulus of elasticity and shear modulus versus the outermost tube diameter [25]. It should be noted that when the tube diameter is larger than 1 nm, the modulus of elasticity and shear moduli are approximately constant and their variations are almost zero. If we consider the carbon nanotube as a rolled graphene sheet, it can be concluded from Figures 3 and 4 that when the diameter of the nanotube is larger than 1 nm, bending does not change the mechanical properties [25]. In a similar manner, we can estimate the mechanical properties of fullerene, which change versus the diameter, and are approximately constant when the diameter is larger than 1 nm.

5. Example

In this example, a fullerene which is implemented in a nano ball bearing is statically and dynamically investigated. As shown in Figure 5, a fullerene in a nano ball bearing has special boundary conditions. Two nano tubes surround it, so the rotational movement is transferred from the inner nano tube to the outer nano tube by fullerenes.

To simulate the boundary conditions, consider a fullerene, with inner radius \( r_1 = 0.16 \) nm and outer radius \( r_2 = 0.5 \) nm, with Poisson’s ratio \( \nu = 0.159 \) and modulus of elasticity \( E = 1.05 \) TPa, which is subjected to two concentrated radial forces that are exerted on the North and South poles of the outer surface of the fullerene in a \( r \)-direction (properties of fullerene are shown in Table 1). Normal forces, which are exerted on the fullerene versus the rotational velocity of a nano ball bearing, are investigated by the molecular dynamic method [18]. Figure 6 shows that the magnitude of this force is \( f_r = 2.55 \times 10^{-3} \) nN.

To find the deformation of fullerene under external forces, a designed super element is implemented. By selecting \( N = 4 \) (positive integer), a 228-node element (Figure 7) would be generated whose shape functions are introduced in Eq. (13). The shape functions of this super element could be used to generate the stiffness and mass matrices for static and vibrational analysis.

| Table 1: The properties of fullerene. |
|-----|-----|-----|-----|-----|-----|
| \( R_1 (\text{nm}) \) | \( R_2 (\text{nm}) \) | \( E (\text{TPa}) \) | \( N \) | \( G (\text{TPa}) \) | \( \text{Density} (\text{kg/m}^3) \) |
| 0.16 | 0.5 | 1.05 | 0.159 | 0.44 | 1650 |

Figure 5: (a) A nano ball bearing which is consisted of several C\(_{60}\) and nanotubes [23]. (b) Simulated boundary conditions of a fullerene in a nano ball bearing.
Figure 6: Variations of average normal force versus rotation velocity for molecular bearings [23].

Figure 7: Spherical super element, while $N = 4$.

\[ N_{2.1} = \frac{1}{128} (\sin (4\pi \lambda)) (1 + \sin (4\pi \lambda)) \]
\[ \times \left( 1 + \sin \left( 2\pi \lambda + \frac{\pi}{4} \right) \right) \left( 1 - \sin \left( \pi \lambda + \frac{3\pi}{8} \right) \right) \]
\[ \times (\sin (2\pi \xi)) (1 + \sin (2\pi \xi)) \left( 1 - \sin \left( \pi \xi + \frac{\pi}{4} \right) \right) \]
\[ \times \left( 1 + \cos \left( \frac{\pi}{2} \pi \xi + \frac{3\pi}{8} \right) \right) (1 - \eta) \]

\[ N_{2.3} = -\frac{1}{128} (\cos (4\pi \lambda)) (1 - \cos (4\pi \lambda)) (1 + \sin (2\pi \lambda)) \]
\[ \times \left( 1 - \sin \left( \pi \lambda + \frac{1}{4} \pi \right) \right) (\sin (2\pi \xi)) (1 + \sin (2\pi \xi)) \]
\[ \times \left( 1 + \sin \left( \pi \xi + \frac{1}{4} \pi \right) \right) \]
\[ \times \left( 1 + \cos \left( \frac{\pi}{2} \pi \xi + \frac{3\pi}{8} \right) \right) (1 - \eta) \]

\[ N_{2.4} = -\frac{1}{128} (\sin (4\pi \lambda)) (1 - \sin (4\pi \lambda)) \]
\[ \times \left( 1 + \cos \left( 2\pi \lambda + \frac{\pi}{4} \right) \right) \left( 1 + \cos \left( \pi \lambda + \frac{3\pi}{8} \right) \right) \]
\[ \times (\sin (2\pi \xi)) (1 + \sin (2\pi \xi)) \left( 1 - \sin \left( \pi \xi + \frac{\pi}{4} \right) \right) \]
\[ \times \left( 1 + \cos \left( \frac{\pi}{2} \pi \xi + \frac{3\pi}{8} \right) \right) (1 - \eta) \]
\[ N_{2.9.1} = \frac{1}{128} \cos (4\pi \lambda) (1 + \cos (4\pi \lambda)) (1 + \cos (2\pi \lambda)) \times (1 + \cos (\pi \lambda)) (\sin (2\pi \xi)) (1 + \sin (2\pi \xi)) \times \left( 1 - \sin \left( \frac{\pi \xi}{2} + \frac{1}{4} \right) \right) \times \left( 1 + \cos \left( \frac{1}{2} \pi \xi + \frac{3}{8} \pi \right) \right) (1 - \eta) \]

\[ N_{2.10.1} = \frac{1}{128} \sin (4\pi \lambda) (1 + \sin (4\pi \lambda)) \times \left( 1 + \sin \left( 2\pi \lambda + \frac{1}{4} \pi \right) \right) \left( 1 + \sin \left( \pi \lambda + \frac{3}{8} \pi \right) \right) \times (\sin (2\pi \xi)) (1 + \sin (2\pi \xi)) \left( 1 - \sin \left( \pi \xi + \frac{1}{4} \pi \right) \right) \times \left( 1 + \cos \left( \frac{1}{2} \pi \xi + \frac{3}{8} \pi \right) \right) (1 - \eta) \]

\[ N_{2.11.1} = \frac{1}{128} (\cos (4\pi \lambda)) (1 - \cos (4\pi \lambda)) (1 + \sin (2\pi \lambda)) \times \left( 1 - \cos \left( 2\pi \lambda + \frac{1}{4} \pi \right) \right) \left( 1 + \sin \left( \pi \lambda + \frac{3}{8} \pi \right) \right) \times (\sin (2\pi \xi)) (1 + \sin (2\pi \xi)) \left( 1 - \sin \left( \pi \xi + \frac{1}{4} \pi \right) \right) \times \left( 1 + \cos \left( \frac{1}{2} \pi \xi + \frac{3}{8} \pi \right) \right) (1 - \eta) \]

\[ N_{2.12.1} = \frac{1}{128} (\cos (4\pi \lambda)) (1 + \cos (4\pi \lambda)) (1 - \cos (2\pi \lambda)) \times \left( 1 + \sin \left( \pi \lambda \right) \right) \left( 1 + \sin \left( 2\pi \xi \right) \right) (1 + \sin (2\pi \xi)) \times \left( 1 - \sin \left( \frac{\pi \xi}{2} + \frac{1}{4} \pi \right) \right) \times \left( 1 + \cos \left( \frac{1}{2} \pi \xi + \frac{3}{8} \pi \right) \right) (1 - \eta) \]

\[ N_{2.13.1} = \frac{1}{128} (\cos (4\pi \lambda)) (1 + \cos (4\pi \lambda)) \times \left( 1 + \sin \left( \pi \lambda \right) \right) \left( 1 + \sin \left( 2\pi \xi \right) \right) \times \left( 1 - \sin \left( \frac{\pi \xi}{2} + \frac{1}{4} \pi \right) \right) \times \left( 1 + \cos \left( \frac{1}{2} \pi \xi + \frac{3}{8} \pi \right) \right) (1 - \eta) \]

\[ N_{2.14.1} = \frac{1}{128} (\sin (4\pi \lambda)) (1 + \sin (4\pi \lambda)) \times \left( 1 - \sin \left( 2\pi \lambda + \frac{1}{4} \pi \right) \right) \left( 1 - \cos \left( \pi \lambda + \frac{3}{8} \pi \right) \right) \times (\sin (2\pi \xi)) (1 + \sin (2\pi \xi)) \left( 1 - \sin \left( \pi \xi + \frac{1}{4} \pi \right) \right) \times \left( 1 + \cos \left( \frac{1}{2} \pi \xi + \frac{3}{8} \pi \right) \right) (1 - \eta) \]

\[ N_{2.15.1} = -\frac{1}{128} (\cos (4\pi \lambda)) (1 - \cos (4\pi \lambda)) (1 - \sin (2\pi \lambda)) \times \left( 1 - \cos \left( \pi \lambda + \frac{1}{4} \pi \right) \right) \left( 1 - \sin \left( 2\pi \xi \right) \right) (1 + \sin (2\pi \xi)) \times \left( 1 - \sin \left( \pi \xi + \frac{1}{4} \pi \right) \right) \]

\[ \eta, \xi \text{ and } \lambda \text{ are the components of the local coordinates and are defined as:} \]

\[ \eta = \frac{2r - (r_2 + r_1)}{r_2 - r_1}, \quad \xi = \frac{2\varphi}{\pi} - 1, \quad \lambda = \frac{\theta}{\pi} - 1. \] (14)

Since there is no exact solution available for this case, the conventional model is made using a sufficient number of Brick elements (ANSYS) to validate the results of implementing the introduced super element. Figures 8 and 9 show the convergence of the results of applying a large number of elements in FEM to reach highly accurate results.

This example is designed to find the deformation and stress of the Fullerene using a 228-node spherical super element. Tables 2–4 indicate the results which are compared with the findings of the Finite Element Method. It should be noted that the results of applying one super element in the prediction of the static response of fullerene is similar to the findings of implementing 154,764 conventional brick elements with a very small relative error (0.01%–0.02%). This similarity
in results shows the accuracy of interpolation functions in calculating the infinitesimal deformation of fullerene under two crosscrisscross concentrated forces. The proposed super element could be used to analyze nano spherical structures such as fullerene and biological cells. Accurate prediction of the structural behavior of fullerene, such as deformation and natural frequencies, makes it feasible to design a nano ball bearing properly for implementation in nano machines that are mostly used in recognizing and disassembling cancerous cells and building molecular support structures for strengthening bones and muscle tissues.

6. Conclusion

Static and vibrational behavior of a fullerene under two crosscrisscross forces is predicted by a spherical super element. In this element, there is a node on each North and South Pole of the sphere, which is available for exertion on external excitations. Applying this element to predict the behavior of a fullerene implemented as a ball in nano ball bearing leads to results comparable with findings of implementing a large number of conventional elements in a limited time. It is perceived that forces of magnitude $2.55 \times 10^{-3}$ nN cause a deformation of magnitude $3.27 \times 10^{-13}$. The method reveals that the natural frequencies are in the range of 8–9 THz for a $C_{60}$.

References


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