VIBRATIONAL STUDY OF AN EMBEDDED DOUBLE-SHELL FULLERENE

K. Behfar

Department of Mechanical Engineering, University of Alberta, Edmonton, Alberta T6G 2G8, Canada.
Email: kbehfar@ualberta.ca

There are several methods for the analysis of nanostructures. These methods lie in the context of molecular simulations and continuum-based models. There exist two major categories of molecular simulation methods: ab initio and classical molecular dynamics. Despite existing computational power, even molecular dynamics computations are still restricted to the analysis of systems with maximum 10^6-10^8 atoms for a few nanoseconds. The simulation of larger systems has to be left to continuum methods. The nano continuum methods have successfully been used for the analysis of mechanical behaviors of nanostructures. In this regard, Yoon et al. [1] have published a brief report on the vibration of MWNTs that focuses on resonant frequencies and the associated vibrational modes. In addition, the authors have already investigated vibrational analysis of an embedded multi-layered graphene sheet and obtained the resonant frequencies and corresponding mode shapes [2], also have recently rendered a method to determine bending modulus of a multi-layered sheet using a geometrically-based analytical approach [3].

In this article, modeling of the motion of an embedded double-shell fullerene with interlayer van der Waals interaction is investigated and some explicit and general formulae are derived. Based on the proposed model, the vibrational analysis of the double-shell fullerene embedded in an elastic medium is performed and the natural frequencies are determined. For modeling the motion and specifying the natural frequencies, the embedded double-shell fullerene is assumed to be isotropic. Also, the elasticity generated by the bonds is assumed to be isotropically distributed over the fullerene surface. The deflections of neighboring spherical shells are coupled through the van der Waals interaction. For small deflection of the spherical shells, it is assumed that the interaction pressure at any point between them linearly depends on the difference of their deflections. The equations of motion for a double-shell fullerene are:

$$1L\begin{cases} f_1(u_1, v_1, w_1) = \rho R_1^2 \sin\varphi\, \ddot{u}_1 \\ f_2(u_1, v_1, w_1) = \rho R_1^2 \sin\varphi\, \ddot{v}_1 \\ f_3(u_1, v_1, w_1) + [C(w_2 - w_1)] R_1^2 \sin\varphi = \rho R_1^2 \sin\varphi\, \ddot{w}_1 \end{cases} \quad \& \quad 2L\begin{cases} f_1(u_2, v_2, w_2) = \rho R_2^2 \sin\varphi\, \ddot{u}_2 \\ f_2(u_2, v_2, w_2) = \rho R_2^2 \sin\varphi\, \ddot{v}_2 \\ f_3(u_2, v_2, w_2) + [-C'w_2 - C(w_2 - w_1)] R_2^2 \sin\varphi = \rho R_2^2 \sin\varphi\, \ddot{w}_2 \end{cases}$$

The foregoing equations of motion are resulted from equations of motion for each spherical shell briefly demonstrated by the functions f_1, f_2, f_3 where $u, v \text{ and } w$ are the deflections in the directions of $\varphi, \theta \text{ and } r$ in a regular spherical shell with radius R, respectively. ρ is the density per unit area and $C \text{ and } C'$ are the carbon-carbon van der Waals interaction coefficients which yield the inter-atomic pressure when multiplied by the difference of deflections [2]. The lowest natural frequencies of the fullerene $C_{60} @ C_{240}$ based on the elastic properties adopted from reference [4] are calculated as, $\omega 1 = 7.197\ THz$, $\omega 2 = 16.755\ THz$, which are in agreement with results in [1,2].

Reference

[1] J. Yoon, C.Q. Ru, and A. Mioduchowski, "*Vibration of an embedded multiwall carbon nanotube,*" Composites Science and Technology **63**, 1533-1542, 2003

[2] K. Behfar and R. Naghdabadi, "*Nanoscale vibrational analysis of a multi-layered graphene sheet embedded in an elastic medium,"* Composites Science and Technology **65**/7-8, 1159-1164, 2005.

[3] K. Behfar, P. Seifi, R. Naghdabadi, and J. Ghanbari, "*An analytical approach to determination of bending modulus of a multi-layered graphene sheet,"* Journal of Thin Solid Films **496**, 475-480, 2006.

[4] V.M. Levin, "*Elastic modules of solid C60: measurement and relationship with nanostructure,"* Journal of Physics and Chemistry of Solids **61**, 1017-1024, 2000.

Keywords: vibration, fullerene