

## Elastic Moduli Variation near the End-Capped Region of a Zigzag Type Single Walled Carbon Nanotube

K.R.B Herath<sup>1</sup> and J.P. Karunarathna<sup>1,2</sup>

<sup>1</sup>*Department of Civil Engineering, Faculty of Engineering, University of Peradeniya*

<sup>2</sup>*Central Engineering Consultancy Bureau, Colombo*

One end-capped zigzag type single walled carbon nanotubes (SWCNTs), which are considered in this study, have end-caps which are half C<sub>60</sub> fullerenes (half buckyballs). In the (9, 0) zigzag type SWCNT considered in this study, one end is capped and the other end is kept open. The variation of the anisotropic elastic moduli near the end-capped region of (9, 0) zigzag type SWCNTs is reported in this paper.

The length of the nanotube section is considered to be much larger than the diameters of both buckyball and nanotube. The tube-to-ball transition region is taken to be one hexagonal unit cell length of the nanotube.

For an equilibrating loading system applied to the nanostructure, the bond forces are calculated and these bond forces are used to obtain the elastic moduli at the end-capped region. The anisotropic elastic moduli of different regions, obtained from this study are reported below.

**Table 1.** Anisotropic elastic moduli of different regions near the end-capped region of a (9, 0) zigzag carbon nanotube (CNT)

Region	Elastic Modulus/TPa	
	Tube axis-direction	Hoop-direction
(9,0) zigzag carbon nanotube	1.411	1.411
Middle of tube-to-ball Transition	1.405	1.392
Half of C <sub>60</sub> fullerene end-cap	0.870	1.358

It is important to know the elastic properties and the load transfer mechanisms near the end-capped regions of CNTs when such nanostructures are to be used in composites as reinforcing elements and also in medicine as drug delivery agents.