

VARIATION OF ANISOTROPIC ELASTIC MODULI AT THE END-CAPPED REGION OF AN ARMCHAIR TYPE SINGLE WALLED CARBON NANOTUBE

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Introduction

Both ends-open type Single Walled Carbon Nanotubes (SWCNTs) are studied extensively during the past two decades by many researchers and their mechanical properties, such as elastic moduli, are well known by now.

Both or one end-capped carbon nanotubes which are considered in this study have the end-caps which are half fullerene structures. In this paper, the variations of the anisotropic elastic moduli at the end-capped region of one-end-capped (5, 5) armchair carbon nanotube is reported. In another study by authors of this paper, mechanical properties, mainly the anisotropic elastic moduli, of C₆₀ fullerenes (buckyballs) are also found by considering the behaviour of carbon-carbon bonds and those results are also used here. Since this is an ongoing research work, the variations of elastic moduli at the end-capped regions of carbon nanotubes of other chiralities are currently under the investigation and not reported here.

Material properties and geometry

The nanomechanics model used in this study is based on inter-atomic forces which hold the carbon atoms together by forming inter-atomic covalent bonds which are assumed to act as linear springs.

The Morse potential is taken to represent the energy in the bond and the inter-atomic forces are derived from it. The inter-atomic forces and the geometry of atomic structure are the main factors that affect the mechanical properties of a material. The elastic law for carbon-carbon (C-C) bond can be written as $f=k\Delta$, where f is the bond force, k is the bond stiffness and Δ is the relative displacement of a C-C bond from its equilibrium position. At the equilibrium position, the C-C bond length, a_{cc} , is taken to be 0.1421 nm (Dresselhaus *et al.*, 1995). The C-C bond stiffness has been reported to fall between 326 nN/nm and 831 nN/nm (Meo *et al.*, 2006).

In this study, a half of a C₆₀ fullerene structure is used to end-cap a single walled (5, 5) armchair nanotube at one end and the other end of the nanotube is kept open. 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 currently a hot research area and for this study it is taken to be one hexagonal unit cell length of the tube. The geometrical arrangement of this one end capped carbon nanostructure is schematically shown in Fig.1.

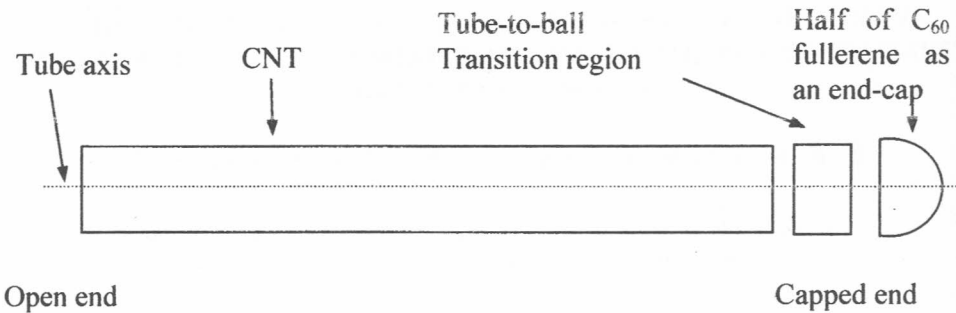


Fig. 1. Schematic representation of the exploded view of an end-capped carbon nanotube (CNT) structure

Results

For an equilibrating loading system applied to the nanostructure shown in Fig. 1, the bond forces are calculated and these bond forces are used to obtain the elastic moduli at the end-capped region of the nanostructure. The anisotropic elastic moduli of

different regions, which are shown in Fig.1, obtained from this study are reported in Table 1. Equatorial and meridional direction elastic properties of C₆₀ fullerenes are used as hoop and tube axis direction elastic properties of half of C₆₀ fullerene end-caps.

Table 1. Anisotropic elastic moduli of different regions near the end-capped region of an armchair carbon nanotube (CNT)

Region	Elastic Modulus/TPa	
	Tube axis-direction	Hoop-direction
CNT ^a	1.398	1.484
Middle of tube to ball Transition	1.372	1.370
Half of C ₆₀ fullerene end-cap ^b	1.358	0.870

^aFrom available literature, ^bTube axis and hoop directions are meridional and equatorial directions of C₆₀ fullerenes respectively.

Conclusions

From the results given in Table 1, it can be observed that the anisotropic elastic moduli of the CNT drop gradually when approaching the end-cap from CNT side. The tube axis-direction elastic moduli of CNT and that of C₆₀ fullerene are well within the reported limits by many researchers and experimental and theoretical studies about the elastic moduli in the

tube-ball transition region are not to be found yet in the literature. Hence the findings of this study on the anisotropic elastic moduli of the tube-ball transition region of an end-capped armchair carbon nanotube could be used as a guideline for experimental and theoretical studies in that region. It is also important to know the elastic

properties and the load transfer mechanisms in that region when end-capped CNTs are to be used in composites as a reinforcing element and also in medicine as a drug delivery agent.

References

Dresselhaus, M.S, Dresselhaus, G., Saito, R. (1995), Physics of Carbon Nanotubes, Carbon, 33, pp 883-891

Meo, M., Rossi, M. (2006), Prediction of Young's modulus of single walled carbon nanotubes by molecular dynamic based FE modelling, Composites Science and Technology, 66, pp 1597-1605