MATHEMATICAL MODELING FOR SINGLE-WALLED CARBON NANOTUBES (SWCNTS) BASED ON MAGNETO-ELECTRO-ELASTIC BEAM MODEL

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Introduction

Carbon nanotubes (CNTS) have addressed extensively growing attentions from a wide range of scientific fields ever since its first discovery by Iijima [1]. Recent studies showed that carbon nanotubes behave as ballistic quantum conductors with long phase-coherence lengths for the charge carriers [2]. Magnetoelectronic properties of finite double-walled carbon nanotubes, whose structure belongs to D5h, are studied by the tight-binding model [3].

The main objective of the present study is to propose a theoretical approach to investigate the wave propagation of single-walled nanotubes made of carbon or other materials such as BC3 or Boron nitride. The theoretical approaches are derived from a simplified one-dimensional theory of linear magneto-electro-elasticity, and a newly invented governing equation indicating the triple effects of magnetization, electricity and elasticity for modeling the innovative properties of nanotube is obtained in this paper. On the basis of the magneto-electro-elastic simple beam model for nanotubes, the dispersive characteristics of the wave propagation in single-walled carbon nanotubes are further examined.

Mathematical Modeling

Kirchhoff hypothesis

B-1. Plane section which is initially normal to the longitudinal axis of the beam remain plane and normal during flexure.

B-2. The beam has both geometric and material property symmetry about the neutral surface (i.e. the beam is symmetrically arranged along the x-axis).

B-3. The material is linearly magneto-electro-elastic with no shear coupling.

B-4. The only stress components present are T_{11} and T_{13}.

B-5. The in-plane electric effect and magnetic effect are ignored, i.e., $D_1 = D_2 \equiv 0$ and $B_1 = B_2 \equiv 0$, only transverse electric field $E_z \equiv E_3$ and $H_z \equiv H_3$ are considered in the present study. [4][5]

Constitutive equation

$$T = -Yz\frac{\partial^2 w}{\partial x^2} + e\frac{\partial \phi}{\partial z} + q\frac{\partial \psi}{\partial z},$$

$$D = -ez\frac{\partial^2 w}{\partial x^2} - \varepsilon\frac{\partial \phi}{\partial z} - d\frac{\partial \psi}{\partial z},$$

$$B = -qz\frac{\partial^2 w}{\partial x^2} - d\frac{\partial \phi}{\partial z} - \mu\frac{\partial \psi}{\partial z},$$

Gaussian's Laws

$$\frac{\partial D}{\partial z} = -e\frac{\partial^2 w}{\partial x^2} - \varepsilon\frac{\partial^2 \phi}{\partial z^2} - d\frac{\partial^2 \psi}{\partial z^2} = 0,$$

$$\frac{\partial B}{\partial z} = -q\frac{\partial^2 w}{\partial x^2} - d\frac{\partial^2 \phi}{\partial z^2} - \mu\frac{\partial^2 \psi}{\partial z^2} = 0,$$

Exact solutions for electric and magnetic fields

$$\frac{\partial \phi}{\partial z} = -\frac{\Delta_1}{\Delta} z\frac{\partial^2 w}{\partial x^2},$$

$$\frac{\partial \psi}{\partial z} = -\frac{\Delta_2}{\Delta} z\frac{\partial^2 w}{\partial x^2}.$$

Governing equation

$$\left(Y + EE + MM\right)\cdot I\frac{\partial^4 w(x,t)}{\partial x^4} + \rho A\frac{\partial^2 w(x,t)}{\partial t^2} = q(x,t)$$

where $EE \equiv e\frac{\Delta_1}{\Delta}$ and $MM \equiv q\frac{\Delta_2}{\Delta}$ are defined as the effective rigidities due to the presence of electricity and magnetism in the nanotube, respectively.

Flexural wave and dispersion equation

The dispersion equation is given by $k^4 - \frac{1}{c_0^2}\cdot\omega^2 = 0$, with c_0 being defined as

$$c_0 \equiv \sqrt{\frac{(Y+EE+MM)\cdot I}{\sqrt{\rho A}}}.$$

Numerical Results and Discussions

For the convenience of numerical computation, the parameters of material and geometry are taken (Pantano et al., 2003) as follows throughout the whole discussion except for those specified otherwise,

Young's modulus: $Y \equiv 1.1\ \mathrm{TPa}$,
mass density: $\rho \equiv 1.3\times10^3\ \mathrm{kg/m^3}$,
nanotube length: $L = 45\ \mathrm{nm}$,
outside diameter: $d_{out} = 3\ \mathrm{nm}$,
inside diameter: $d_{in} = 2.32\ \mathrm{nm}$.

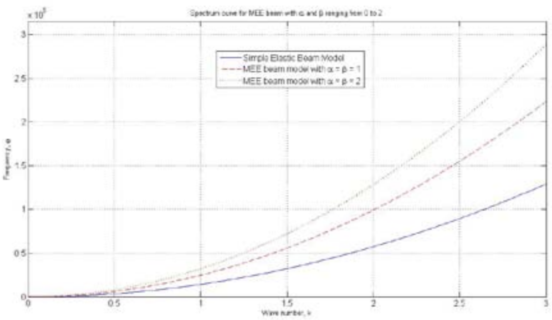

Fig.1 Spectrum curves for MEE beam model

Figure 1 and Figure 2 show the changes of spectrum and dispersion curve for SWNTs with respect to pure elastic, piezoelectric, and magneto-electro-elastic single beam models. It can be seen from these two figures that both frequencies and phase velocities increase with the non-dimensional parameters α and β, that is, the existences of electricity and magnetism would effectively enforce the rigidity of the nanotube as a beam.

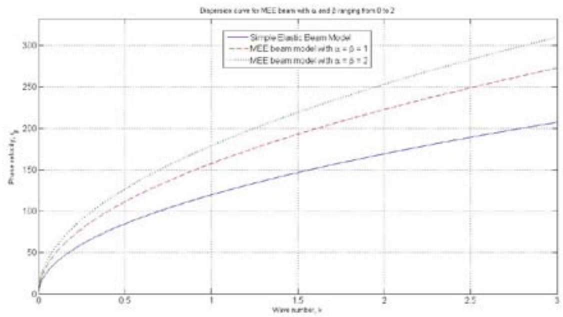

Fig.2 Dispersion curves for MEE beam model

Conclusions

In this paper, governing equation for the wave propagation of a single-walled nanotube can be derived. Spectrum and dispersion curves for the SWCNT based on the proposed methodology are examined; it is found that both frequencies and phase velocities increase with the electric- and magnetic-related parameters. It can be concluded that the consideration of piezoelectricity and piezomagnetism actually enhances the rigidity of the nanotube.

References

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