Phonons, elastic and mechanical properties in (10,10) Nanotube using Force Constant Model

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ABSTRACT

The use of the Force Constant model to reveal the phonon dispersion relation of a single-wall carbon nanotube (SWNT) with chirality (10, 10) is adopted. The qualitative features of the dispersion curve are discussed in detail. Further, from the low wave vector transfer region of the dispersion curve longitudinal acoustic velocity (v_{LA} = 16 Km/s) and transverse acoustic sound velocity (v_{TA}= 8 Km/s) have been accessed. A novel method is adopted to evaluate the elastic constants. Additionally, Young modulus, Bulk modulus, Shear modulus, and Poisson's ratio of SWNT have been computed. The numerical value of Young's Modulus is 270.7 GPa and Bulk Modulus is 180.5 GPa. Our results explicitly show that armchair (10, 10) SWNT is mechanically stable. Furthermore, the phonon density of states successfully explains the origin of many phonons branched in the dispersion curve.

Keywords: Carbon Nanotube, Phonon dispersion, Force Constant Model, Elastic constants, Mechanical properties

1. Introduction

For over three decades, scientists have shown keen interest in studying carbon nanotube (CNT) because of their exceptional mechanical and electronic properties [1-4]. These properties have been extensively explored, along with these the phonon properties of CNT are also miraculous. The properties include unique 1D behavior, radial breathing mode, the twist acoustic mode, and 1D phonon subbands [2].

Recently, vibrational dynamics of CNT have also drawn considerable attention, in which Raman spectroscopy has been widely used to characterize the dynamic behavior of CNT's [5-7]. These approaches incorporate phonons in isolated nanotubes whereas most SWNT self-assembles into bundles. The zone folding technique studied the passage of phonon dispersion from a 2D graphene to 1D CNT [8, 9]. But this technique was not able to describe all modes. The continuum-atomistic approach [10], tight binding approach [11], and ab initio method [12] have been used to display phonon relation.

There are two different routes to evaluate this nanostructural material's mechanical and elastic properties, namely, experimental [13, 14] and theoretical computational techniques [15, 16]. Theoretical works by researchers incorporate an improved 3D finite element (FE) model proposed by Lu et al [17], Bernoulli–Euler beam bending theory [18] of Govindjee and Sackman, and the model of Liang et al [19], which is based on anisotropic elasticity and classical lamination theory. All these investigations reveal that CNT has extraordinary high stiffness and axial strength [20].

Experimental techniques at the nanoscale are very costly and this has encouraged many of the researchers to perform simulation techniques for CNT for exploring their vibrational, elastic, and mechanical properties. With this in mind, the Force Constant Model [6] has been used to study the phonon dispersion relation of (10, 10) SWCNT. In this paper, simulation is performed using CNT Phonon Nanohub Simulator [21]. Our main focus is on the low wave vector transfer regime of the curves, from this region elastic constant and mechanical properties have also been derived. Along with this, the results of the density of states have also been reported. It must be stressed that the results of vibrational dynamics, elastic and thermal properties are in good agreement with the available data.

2. Theory

2.1 Structure of CNT

CNT are cylindrical carbon molecules composed of sp^2 bond and are characterized by a pair of integers (n, m), corresponding to a Chiral vector $C_h = na_1 + ma_2$ on the graphite plane, where a_1 and a_2 are unit vectors for the honeycomb lattice of the graphene sheet [5]. A single layer of a graphite crystal is rolled up in such a way that the start and the end of the vector join to form the circumstantial circle of an SWNT. Illustrating the twist of a tube by the chiral angle, which varies between 0 and 30°, is expressed as
$\theta = tan^{-1}[\sqrt{3}m/(m+2n)]$.

The chiral vector or the chiral angle defines the basic structure of SWNT: armchair nanotubes (n = m, θ> 30), zigzag nanotubes (m= 0, θ = 0) and chiral nanotubes (n =m, 0 < θ< 30) [19]. The nanotube diameter is given by $d_t = C_h/\pi = \sqrt{3}a_{cc}(m^2 + nm + n^2)^{1/2}/\pi$ where a_{CC} is the nearest-neighbor C-C distance (1.421 Å in graphite [22]).

2.2 Force Constant Model

Phononic band structures in the force constant model are evaluated by neglecting the anharmonic contribution to energy. Hence, using this consideration near the equilibrium, the structure of CNT is approximated by the sum of pairwise harmonic potentials between atoms.

CNT builds its structure by the conformal mapping of the graphite sheet onto a cylindrical surface. In CNT the radius is of the order of nm, and since the curvature is very minute so short-range atomic interactions correspond to graphite [6]. A force constant tensor from the constituent atoms by taking fourth-neighbor in-plane and out-of-plane interactions are developed. Using the force constants, a 6N * 6N dynamical matrix is developed. Diagonalization of the matrix results in the formation of phonon energy dispersion relations.

3. Results and Discussion

3.1 Phonon Dispersion Relation for (10, 10) CNT

A complete understanding of phonon dispersion is remarkably required to know about the CNT properties. The dispersion behavior of (10, 10) armchair CNT is shown in Fig. 1.

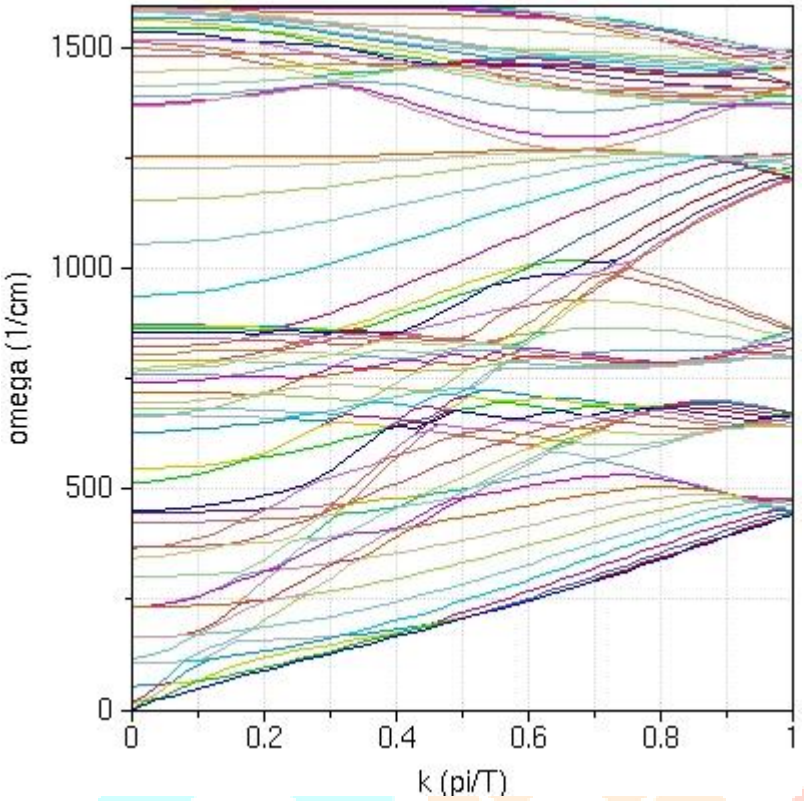

Fig.1 Phonon dispersion curve of (10, 10) CNT

For an (n, n) armchair there are 6N branches, as N=2n, (N is the number of hexagons per unit cell of CNT), so there are 12n branches in the nanotube unit cell. Hence in (10, 10) CNT, there are 120 branches. Among these branches, only 66 phonon branches are distinct. Out of 66, 54 are double degenerate and 12 are non-degenerate [6]. CNT is the cylindrical arrangement of 2D graphene sheets in one-dimensional projection. This structural change introduces the additional quantization arising from electron confinement around the CNT circumference.

The phonon dispersion curve, originating from the Γ point on the Brillouin zone in the long-wavelength limit has four acoustic branches. The first is the longitudinal acoustic mode (LA), corresponding to atomic displacement occurring in the direction of the nanotube axis, this branch has the highest group velocity. The lowest energy mode near the k=0 point is two degenerate transverse acoustic mode branches (TA), which have atomic displacement perpendicular to the nanotube axis. The LA mode has only an in-plane component, whereas the TA mode comprises of in-plane and out-of-plane component. The result of the phonon dispersion curve obtained is well supported by the results of Dresselhaus [5]. Slopes of the acoustic branches around the Γ point $(dw/dk)_{k=0}$ give their relevant sound velocities. These velocities are reported in Table 1 and are found to be in good agreement with the available data [6]. The fourth acoustic branch 'twist mode' corresponds to the torsion of the tube around its axis.

Further, Fig. 1 shows that the dispersion curve comprises several optical branches along with these acoustic branches. The optical branches include longitudinal, transverse, and twisting motions to various degrees. These branches arise due to atomic motion within the unit cell which may oppose each other and some of these branches also occur in degenerate pairs [23].

No phononic bandgap is observed in CNTs with the index n-m equal to a multiple of 3. Hence, armchair CNT with (n, n) chirality has no phononic bandgap. This spectacular feature is exhibited in Fig. 1 for (10, 10) CNT.

3.2 Density of States

The Density of states determined using the simulation method is shown in Fig. 2. The shape of the density of states depends on dimensionality. Spikes in the density of states of SWNT have been reported, these are called Van Hove Singularities and manifest the confinement properties in a direction perpendicular to the tube axis. A large amount of sharp structure in the density of states reflects the many phonon branches as shown in Fig.1. Phonon density of states for the (10, 10) nanotube Is in excellent agreement with the earlier reported results [5].

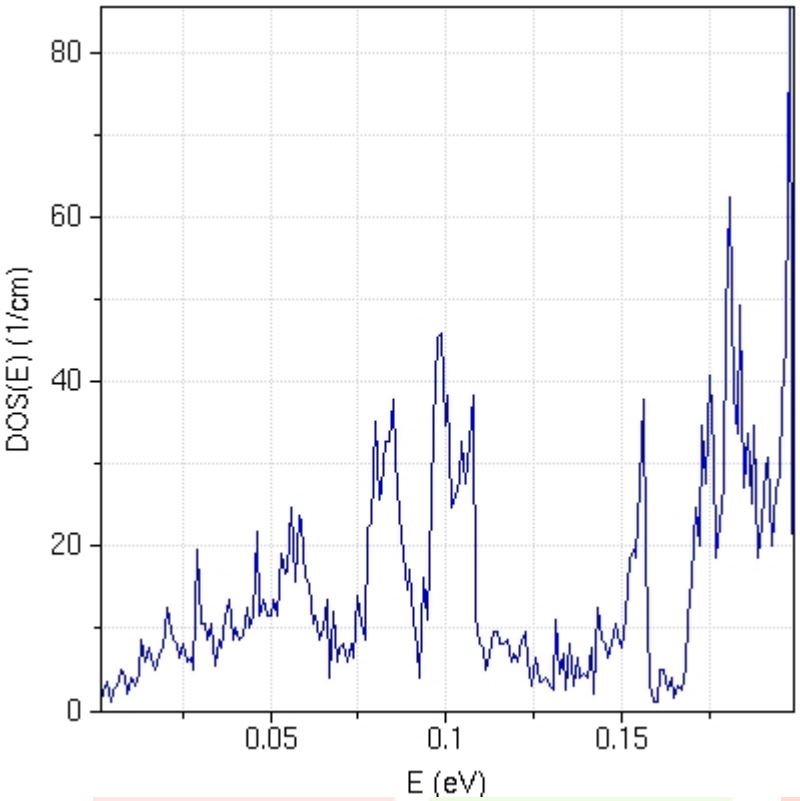

Fig. 2 Density of States of (10, 10) CNT

3.3 Elastic and Mechanical properties

Long-wavelength limit of phonon energy dispersion curve for a hexagon close-packed lattice of (10, 10) CNT has been utilized to determine elastic and mechanical properties. The elastic constants are calculated by the second derivative of energy of strained nanotube. Using the relation $C_{ij} = \rho v^2$, where v is the respective velocity and ρ is the density of Nanotube and has been taken as 1337Kg/m^3 [7], the elastic constants C_{11}, C_{33}, and C_{44} have been determined. Apart from these the other elastic constants obtained by using the relation between them for the hexagonal lattice [15] are also tabulated in Table 1. The computed elastic constants are positive and satisfy Born-Huang criteria suggesting mechanical stability. From the tabulated values, it is found that most of the elastic constants are in agreement with the available data [15]. A small deviation in some elastic constants may be attributed to the small value of mass density used.

v_{LA} (Km/s)	v_{TA} (Km/s)	C_{11} (GPa)	C_{44} (GPa)	C_{66} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{33} (GPa)
16	8	342	85	114	114	85	373
20.35[a]	9.42[a]	424.3[b]	112.0[b]	166.4[b]	104.2[b]	93.4[b]	463.1[b]

[a] [6], [b][15]

Table 1. Velocities and Elastic Constants of (10, 10) CNT

Furthermore, the calculated mechanical properties Young's Modulus Y, Bulk Modulus B and, Shear Modulus G are also reported in Table 2. The expressions [15] used are given by

$$B = [2(C_{11} + C_{12}) + 4C_{13} + C_{33}]/9 \quad (1)$$

$$G = [C_{11} + C_{12} + 2C_{33} - 4C_{13} + 12(C_{44} + C_{66})]/30 \quad (2)$$

$$Y = 9BG/(3B + G) \quad (3)$$

These values are evaluated using the elastic constants C_{ij}mentioned in Table 1.

From the examination of numbers in Table 2, we can conclude that (10, 10) CNT is strong and has tensile strength. This strength results from the covalent sp^2 bonds formed between the individual carbon atom. Finally, from the knowledge of bulk modulus and shear modulus, the value of Poisson ratio is evaluated using the expression.

$$v = (3B - 2G)/2(3B - G) \quad (4)$$

For most materials, the radial dimension is reduced, when it is axially elongated. The ratio of reduction in radial dimension to the axial elongation defines the Poisson ratio. The value of the Poisson ratio evaluated from Eq.(4) is also incorporated into Table 2. Table 2 also summarizes the available results [15] for support of calculated values.

B (GPa)	G (GPa)	Y (GPa)	v
180.5	108.3	270.7	0.375
210.4[b]	147.4[b]	358.5[b]	0.340[b]

[b][15]

Table 2. Mechanical Properties of (10, 10) CNT

4. Conclusions

Based on the above study, it can be concluded the Force constant model enables us to explore the complete features of the phonon dispersion curve of armchair (10, 10) SWNT. The density of states study demonstrated Van Hove singularities in 1D CNT. A detailed study of sound velocities, elastic constants, Young's Modulus, Shear modulus, Bulk Modulus, and the Poisson ratio has been made. The results obtained show good matching with published results. Young modulus and shear modulus values reveal that CNT possesses ultimate tensile strength, making it a promising material to be used in nanoscale engineering.

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