



Electronic and Vibrational studies of Single Wall Carbon Nanotubes inside Boron nitride Nanotubes

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ABSTRACT

This work focuses on Raman spectra and band gap calculations of single-walled carbon nanotube (SWCNT) inside single-walled boron nitride nanotube (SWBNNT). The diameter and chirality effects are discussed. The spectral moment's method was shown to be a powerful tool for determining vibrational spectra (infrared absorption, Raman scattering and inelastic neutron-scattering spectra) of harmonic systems. The calculations of vibrational properties of double-walled hybrid nanostructures SWCNT inside SWBNNT (SWCNT@SWBNNT) are performed in the framework of the force constants model, using the spectral moment's method (SMM). The electronic density of states and the band structures of our systems was investigated. This study can provide benchmark to understand the experimental data of SWCNT@SWBNNT nanotubes.

Key words: Electronic, Carbon, Boron Nitride, Raman spectra, Nanotube, SMM

1. INTRODUCTION

The discovery of nanomaterials such as fullerenes [1], carbon nanotubes [2] and boron nitride nanotubes [3] prevails over science and technology at nanoscale levels and becomes a hot topic for researchers and industrialists. Multi-walled carbon nanotubes (MWCNTs) have been firstly synthesized by Iijima et al. in 1991 [2] and single walled carbon nanotubes (SWCNTs) in 1993 [4]. Considering their special structures, and their different applications, carbon nanotubes (CNTs) have gained the attention of many experimental, theoretical, and computational research groups, in particular due to the possibility for many applications. In fact, CNTs showed a number of exceptional and promising properties, as for instance, high mechanical stability, unique optical and electronic characteristics, high chemical stability or efficient thermal conductivity [5,6,7]. Following discovery of CNTs, it was speculated that other materials could possibly form similar nanostructures. The viable candidate was Boron Nitride Nanotubes

(BNNTs). BNNTs were firstly theoretically predicted to be stable in 1994 [8] and then experimentally synthesized by arc-discharge in 1995 as multiwall nanotubes (MWBNNNTs) [3] and as single wall nanotubes (SWBNNTs) in 1996 [9]. BNNTs are isoelectronic to CNTs and similarly possess high mechanical strength [10] and excellent chemical and thermal stabilities [11]. BNNTs have the same atomic structure as CNTs, however, the BNNTs properties are very different: CNT can be metallic or semiconducting whereas BNNT is an electrical insulator with a band gap between 5.0 and 6.0 eV independent to tube chirality and diameter [9,12,13].

One of the most powerful tools to investigate nanostructures vibrational, optical and electronic properties is Raman spectroscopy. Vibrational Raman spectroscopy has been shown to play a major role in CNTs [14,15,16,17] and in BNNTs [18,19,20]. Raman spectra of CNTs and BNNTs show a strong line located in the 1570-1600 cm^{-1} range [21] and in the 1360-1380 cm^{-1} range [22,23,24,25,26]. Raman spectra of SCNTs and SBNNTs are dominated by the so called radial breathing mode (RBM) below 500 cm^{-1} and by the tangential modes (TM) between 1200 and 1600 cm^{-1} [27,28,29]. The thermal treatment of fullerene inside BNNTs (C60@BNNT) at 1200 °C in argon triggers drastic transformations of the guest molecules which polymerize and coalesce into carbon nanotubes inside boron nitride nanotubes thus forming a hybrid nanostructure CNT@BNNT [30,44]. It's found that the electronic properties of SWNTs is determined by their chirality (n,m), which defines the manner which a graphene sheet is rolled up to form SWNTs. The (n,n) armchair SWNTs are metallic, whereas the (n,0) zigzag and (n,m) chiral tubes are metallic or quasi-metallic with a very narrow band gap for $mod(n-m,3)=0$, and semiconducting for $mod(n-m,3) \neq 0$ [32]. Comparing to CNTs, the BNNTs nanotubes have a weak electric conductivity and exhibit an insulators nature with a wide band gap (4.5~5.5 eV), which are predicted to be practically independent of the diameter and chirality indexes (n,m) [8,33].

In this work, we study the vibrational spectroscopy of SWCNT@SWBNNT using SMM to calculate the Raman spectra of hybrid nanostructure CNT@BNNT as a function of their diameters and chiralities. We present the calculated Raman spectra in the breathing-like Mode (BLM), intermediate-like mode (ILM) and tangential-like mode (TLM) ranges. By using the tight bending model, the electronic density of states and the band structures of (10,10)@(15,15)(armchair SWCNT@armchair SWBNNT) and (17,0)@(26,0)(zigzag SWCNT@zigzag SWBNNT) were calculated.

2. MODELS AND METHOD

Many papers have described the structures of an ideal infinitely long SWCNT [5], [34] and SWBNNT [34]. The diameter of a (n,m) nanotube is given by $D = \frac{a}{\pi} \sqrt{m^2 + n^2 + mn}$ where $a=0.142$ nm and $a=0.1435$ nm is the nearest-neighbor for C-C and B-N distance respectively. The previous relations allow us to derive all the possible (k,l) outer tubes for a specific (n,m) innertube, which lead to (n,m) SWCNT@(k,l)SWBNNT. From minimum energy calculations, the interwall distance of the stable structures is about 0.35 nm for the armchair (n,n)@(n+5,n+5) structure and from 0.33 to 0.36 nm for the zigzag (n,0)@(n+9,0) structures, respectively. This distance is consistent with the experimental values [30] and which is consistent with the theoretical values [35], [36]. The relation between the diameters of the inner (D_i) and the outer (D_o) tubes is $D_o = D_i + 2d$.

The intratube interactions are described by using a force constants model and previously used in our calculations of the Raman spectrum of isolated SBNNTs [37] and SCNTs [38]. Van der Waals interaction between the inner SWCNT and the outer SWBNNT is described by the Lennard-Jones potential is given by the following expression:

$$U_{LJ}(r_{ij}) = \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] \quad (1)$$

Where: ϵ_{ij} and σ_{ij} are the energy and length parameters in LJ potentials, and r_{ij} denotes the distance between the centers of particle i and particle j. The parameter ϵ_{ij} of boron, nitrogen and carbon atom is 0.004116 eV, 0.006281 eV and 0.002635 eV, and σ_{ij} is 0.3453 nm, 0.3365 nm and 0.3369 nm, respectively [39], [40]. The parameters ϵ_{ij} and σ_{ij} between different particles are calculated by the following Lorentz-Berthelot rules $\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}$ and $\sigma_{ij} = (\sigma_i + \sigma_j)/2$.

The Raman efficiency of modes is calculated according to the bond-polarizability (BP) model [41]. For each bond are assigned a longitudinal polarizability, α_l , and a polarization perpendicular to the bond, α_p . Thus, the polarizability contribution $\pi_{ij}(r)$ of a particular bond \vec{r} is:

$$\pi_{ij}(r) = \frac{1}{3}(\alpha_l + \alpha_p)\delta_{ij} + (\alpha_l - \alpha_p)\left(\hat{r}_i \hat{r}_j - \frac{1}{3}\delta_{ij}\right) \quad (2)$$

Where: i and j relate to the cartesian components (x,y,z) and \vec{r} is the unit vector along the vector \vec{r} connecting two atoms which are covalently bonded. The parameters l and p indicate the longitudinal and perpendicular bond polarizability respectively. In this approximation, one can assume that the bond polarizability

parameters are depending on the bond lengths r only. The derivatives $\pi_{ij,k}^n$ are given by:

$$\begin{aligned} \pi_{\alpha\beta,\gamma}^n &= \sum \frac{1}{3}(\alpha'_l + 2\alpha'_p)\delta_{\alpha\beta} \hat{r}_\gamma \\ &+ (\alpha'_l - \alpha'_p)\left(\hat{r}_\alpha \hat{r}_\beta - \frac{1}{3}\delta_{\alpha\beta}\right) \hat{r}_\gamma \quad (3) \\ &+ \frac{\alpha_l - \alpha_p}{r}(\delta_{\alpha\gamma} \hat{r}_\beta + \delta_{\beta\gamma} \hat{r}_\alpha - 2\hat{r}_\alpha \hat{r}_\beta \hat{r}_\gamma) \end{aligned}$$

Where: $\alpha' = \left(\frac{d\alpha}{dr}\right)_{r=r_0}$ and r_0 is the equilibrium bond distance.

The usual method to calculate the Raman spectrum consists of direct diagonalization of the dynamical matrix of the system. However when the system contains a large number of atoms, the dynamical matrix is very large and its diagonalization fails or requires a long computing time. By contrast, the SMM allows the Raman spectrum of very large harmonic systems to be directly computed without any diagonalization of the dynamical matrix. To calculate the electronic density of states and the band structures of our (SCNT@SBNT) systems. The total Hamiltonian matrix is obtained from the Hamiltonian matrices of the inner (first neighbour C-C interactions) and outer (first neighbour B-N interactions) tubes. The interactions between the tubes (C-N and C-B) are described by a hopping parameter $\gamma_1 = 0$, 35eV [42], whose a cut-off distance is 3.45Å. In our calculations, we neglected the effects of tube curvature.

3. RESULTS AND DISCUSSION

Three geometrical configurations are considered: in the ZZ configuration, both incident and scattered polarizations are along the Z axis and, for ZX (XY) configurations, the incident and scattered polarizations are along the Z(X) and X(Y) axes respectively. First, we focus on the Raman spectra of infinite isolated SWCNT@SWBNNT double-walled hybrid nanostructures. These SWCNT@SWBNNT are identified as (n,0)@(n+9,0) zigzag@zigzag hybrid systems. Infinite tubes have been obtained by applying periodic conditions on the unit cells of the two single walled nanotubes. In order to illustrate our results, the calculated ZZ, ZX and YX Raman spectra of (17,0)@(26,0) SWCNT@SWBNNT are shown in the Breathing Like-Mode (BLM) (Figure 1, left), intermediate (ILM) (Figure 1, middle) and Tangential Like-Mode (TLM) (Figure 1, right) ranges, respectively.

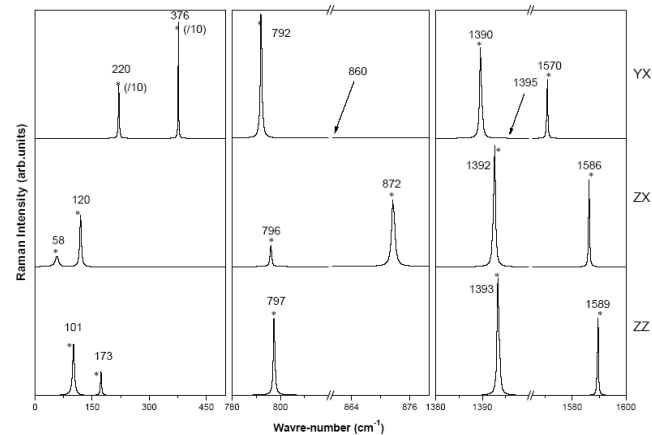


Figure 1: Calculated ZZ, ZX and YX polarized Raman spectra of zigzag SWCNT@SBNNT: (17,0)@(26,0). Spectra are displayed in the BLM (left), intermediate (Middle) and TLM (right) regions. The stars give the position of the active modes of carbon and boron nitride isolated tubes

For each polarized ZZ, ZX and YX Raman spectra of the figure 1, the BLM range show two modes associated to the breathing-like modes in SWCNTs@SWBNNT. A systematic wavenumber up-shift (1 to 3 cm^{-1}) of these modes with respect to SWCNTs and SBNNTs (symbol) is indicated, such slight up-shift are induced by the effect of van der Waals interactions: For example, in the case of the (17,0)@(26,0) SWCNT@SBNNT, they are centered at 58 (E_{1g}), 120 (E_{1g}), 101 (A_{1g}), 173 (A_{1g}), 220 (E_{2g}), and 376 cm^{-1} (E_{2g}). These lines result from the in-phase and counter-phase coupled motions of the breathing modes of the inner and outer tubes. In the intermediate region, we observe that the ZX and YX polarized spectra show two peaks, and only one for the ZZ polarization. They are associated with the in-phase and counter-phase coupled motions of the intermediate modes of the inner and outer tubes. A small up-shift of 1 to 2 cm^{-1} in the wavenumber of the active Raman modes is found in SWCNT@SBNNTs compared with the wavenumber of the intermediate modes in isolated tubes.

In the TLM region, the illustrated spectra are characterized by two modes (1589 and 1393 cm^{-1}) associated with the in-phase and counter-phase coupled motions of the tangential modes (TMs) of the inner (SWCNT) and outer (SWBNNT) tubes. A slight up-shift of 1 to 2 cm^{-1} in the wavenumber of the active Raman modes is found in SWCNT@SBNNTs compared with the wavenumber of the Tangential modes in isolated tubes. Our results is in good agreement with experimental results on SWBNNT@SWCNTs hybrid system (Figure S6 in reference[43]).

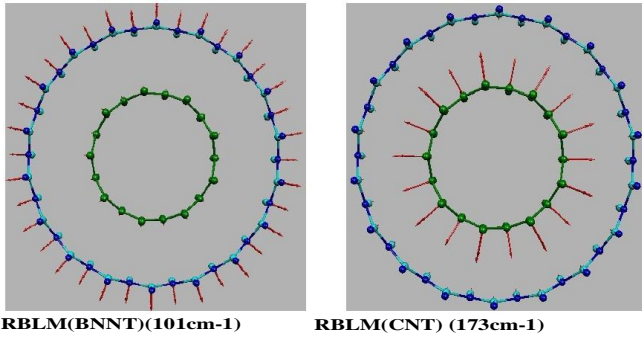


Figure 2: Atomic displacements of the active modes at 101 cm^{-1} and 173 cm^{-1} in ZZ polarised Raman spectra of SWCNT@SWBNNT.

To illustrate the diameter dependence of the Raman active modes in the low wavenumber range, figure 2 shows the diameter dependence of the specific BLMs and especially on the in-phase and counter-phase coupled motions of the RBMs of the inner and outer tubes. These modes are called RBLM1 (in-phase motions of both tubes) and RBLM2 (counter-phase vibrations of both tubes). For instance, they are, respectively, centered at 101 and 173 cm^{-1} in (17,0)@(26,0) zigzag@zigzag hybrid system. Their eigen displacement vectors obtained from the direct diagonalization of the dynamical matrix are displayed in Figure3.

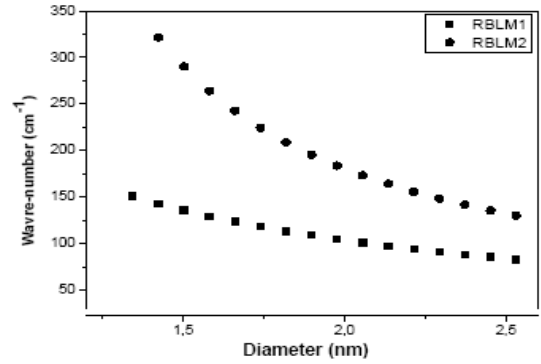


Figure 3: Diameter dependence on the wavenumber ZZ Raman active modes for zigzag SWCNT@SWBNNT in the low wavenumber region.

The dependence of the wavenumber of the RBLM mode as a function of tube diameter is described by an a/D scaling law with the a parameter depending on the mode symmetry (see Table 1). Where D is the outer nanotube diameter. The value of this a parameter is close to 195 and 605 nm cm^{-1} for the RBLM1 (SWBNNT) mode and RBLM2 (SWCNT) mode respectively (see table 1), independently of chirality. In comparison with carbon nanotubes for which a similar a/D trend has been obtained [27], the value of the a parameter is greater than that found in SWCNTs. In contrast, in comparison with boron nitride nanotubes for which a similar a/D trend has been obtained [20], [34], [28], [44], the value of the a parameter is consistent with that found in SWBNNTs.

TABLE CAPTIONS

Table 1: The a parameter for the a/D dependences of the modes as a function of the tube diameter D (nm cm^{-1}).

The parameters values in SWCNT@SWBNNT				
System	CNT		BNNT	
modes	RBLM	RBM	RBLM	RBM
$a(\text{nm.cm}^{-1})$	605	224[27]	195	190 [20]

The bands structures and the electronic density were calculated for one super-cell of (10,10)@(15,15) and (17,0)@(26,0) tubes. The periodic conditions are applied along the tube axis. We present the obtained results in the direction ΓM of the irreducible Brillouin zone of our systems. The obtained results for (10,10)@(15,15) and (17,0)@(26,0) are shown in figures 4 and 5 respectively.

In Figure 4, we observe that the (10,10) armchair carbon tube is metallic with a zero gap energy. The (15,15) boron nitride tube present an insulator character with a wider band gap energy ~ 4.92 eV. For (10,10) @ (15,15) tube, a gap between valence and conduction bands which is about 50 meV is shown. This gap is of the same order as that obtained from graphene on four layers of h-BN substrate [45]. At around the Brillouin-zone corners, a low-energy band structure possesses nearly (10,10) carbon nanotube character. Such character indicating a weak interaction between the inner and outer tubes.

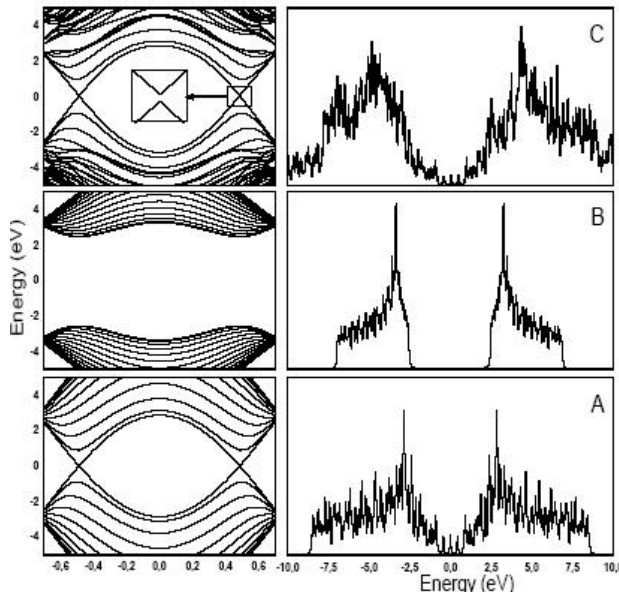


Figure 4: The bands structure and electronic density of states for (A) : (10,10) armchair carbon nanotube, (B) : (15,15) armchair boron nitride nanotube and (C) : (10,10)@(15,15) armchair SWCNT@SBNNT nanotube.

From figure 5, we observe that (17,0) zigzag carbon tube is semi-conductor with a small gap energy 0.2eV. Independently with the chirality, the (26,0) boron nitride tube exhibit the same character to the obtained one in (15,15) boron nitrid nanotube. A gap about 0.2 meV is shown in (17,0) @ (26,0) tube. Due to weak interaction between the inner and outer tubes, a low-energy band structure possesses a similar (17,0) carbon nanotube character in the Brillouin-zone corners.

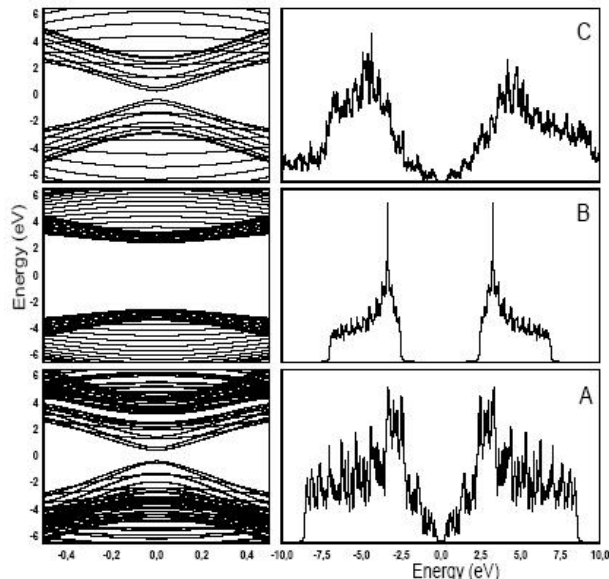


Fig.5: The bands structure and electronic density of states for (A) : (17,0) zigzag carbon nanotube, (B) : (26,0) zigzag boron nitride nanotube and (C) : (17,0)@(26,0) zigzag SWCNT@SBNNT nanotube.

4.CONCLUSION

In this work, we have calculated the Raman spectra of SWBNNT encapsulated inside SWCNT using the spectral moment's method. The dependence of the positions of the Raman-active modes in the low wavenumber range as a function of the encapsulated tube diameter is discussed. Our results show that the modes located in RBLM region are inversely proportional to the nanotube diameters for SWCNT@SWBNNT in 1.3- 2.7nm outer diameter range, which is in good agreement with previous theoretical results. The electronic density of states and the band structures of our systems are calculated. This results are useful in the interpretation of experimental data of SWCNT@SWBNNT.

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