# Nonresonant Raman Spectrum Of Boron Doped Single Walled Carbon Nanotubes

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**Abstract:** In the present work, We use a force constant model to study the vibrationnel modes of boron doped single walled carbon nanotubes. This model is used to calculate the nonresonant Raman spectra of these nanomaterials in the framework of bond-polarisation theory by using either direct diagonalisation of the dynamical matrix or the spectral moments method. The effect of substitution of carbon by boron atoms shows that the higher Raman frequency region is dominated by a broad bond whereas the lower one is characterized by a shift of radial bonds.

## I. Inrtoduction

Since the discovery by Iijima in 1991[1], single-wall carbon nanotubes(SWCNTs) have attracted a lot of attention in the physical and industrial societies.This new forms of carbon such as (SWCNTs) have been attracting considerable interest for a number of years. It has been experimentally shown that boron and nitrogen can be doped SWCNTs, forming a boron carbide and carbon nitride structure.In this work, we interest to the $BC_3$ nanotubes (BCNTs). The (BCNTs) have been studied both theoretically and experimentally due to its unique physical properties.The principal aim of researchers nowadays is to investigate how such features can be controlled for a wide range of practical applications such as integration of carbon nanotubes for logic circuits [2]. Some research groups predicted theoretically that carbon nitride films present superhard mechanical properties and more interesting electronic behavior in comparison with pure carbon films [4,5]. In our case, we want to study if there is any relation between the morphology of the tubes and the way boron is incorporated and the concentration in nanotubes. We will then study their vibrational and structural features in order to control their physical properties.In our work the theoretical study on the vibrationnel and electronic properties of highly boron substituted (SWCNTs),we use the spectral moments method in the framework of the bond-polarization theory to calculate polarized non-resonant Raman of these systems.

## II. Models And Method

The SWCNTs nanotube structure can be obtained from graphene sheet by rolling it up along the straight line connecting two lattice points into a seamless cylinder in such a way that the two points coincide [6].The tube can be specified by integers (n,m) that define the translation vector between the two points. Alternatively, the tube can be described by its diameter D and the chiral angle $\theta$ which is the angle between the tube circumference and the nearest zigzag of carbon-carbon bonds.The tube is called achiral for \theta=0 (zigzag) and \theta=30(armchair) and chiral for 0< \theta <30.

The SWCNT C-C and C-B intratube interactions are described by using the same force constants set that the one used in our calculation of the Raman spectrum of isolated SWCBNTs nanotubes. The moments method was initially developed by different authors for studying electronic properties in solid-state physics. A few years ago, the spectral moments method (SMM) was shown to be a powerful tool for determining infrared absorption, Raman scattering, and inelastic neutron scattering spectra of harmonic systems [7].Our calculations are based on this method. Recently, this method was used to calculate polarized nonresonant Raman spectra of chiral and achiral SWCNT's as a function of their diameter and length, in the framework of the bond-polarization theory, successfully [10].Using a force constants model in which the interatomic force constants up to the fourth-nearest neighbor interaction are fitted to experimental data, many calculations of phonon have been performed for graphite and carbon nanotubes [11]. These approaches are very fast and allow a good understanding of phonon in carbon nanotubes. The same approach was developed recently by Xiao et al for phonons in Boron nitride [9] and $BC_3$ [9] nanotubes.

## III. RESULTS AND DISCUSSION

In this section we report the results of calculated Raman spectra for infinite boron doped SWNTs. Our calculations are performed by applying periodic conditions for units cells. We consider the Z direction as the nanotube axis direction, the Y direction as the light propagation direction, and a carbon atom is the long X axis of the nanotube reference frame.

 

In the Z, ZX and XY polarization geometries, where the letters indicate the polarization direction of the (incident, scattered) light.

**Table 1**: Force-constant parameters for C-C, B-C and B-B in units of $10^4$ dyn/cm. Here the subscripts r, ti, and to refer to radial, transverse in plane, and transverse out of plane, respectively.

| Radial | Tangential | |
|---|---|---|
| $\phi_r^{1(C-C)} = 32.0$ | $\phi_{ti}^{1(C-C)} = 23.0$ | $\phi_{lo}^{1(C-C)} = 8.5$ |
| $\phi_r^{1(B-C)} = 28.0$ | $\phi_{ti}^{1(B-C)} = 18.0$ | $\phi_{lo}^{1(B-C)} = 5.8$ |
| $\phi_r^{2(C-C)} = 8.00$ | $\phi_{ti}^{2(C-C)} = -3.0$ | $\phi_{lo}^{2(C-C)} = -0.3$ |
| $\phi_r^{2(B-C)} = 5.0$ | $\phi_{ti}^{2(B-C)} = -3.5$ | $\phi_{lo}^{2(B-C)} = -0.40$ |
| $\phi_r^{2(B-B)} = 7.0$ | $\phi_{ti}^{2(B-B)} = -2.8$ | $\phi_{lo}^{2(B-B)} = -0.25$ |
| $\phi_r^{3(C-C)} = 2.5$ | $\phi_{ti}^{3(C-C)} = -5.0$ | $\phi_{lo}^{3(C-C)} = 0.3$ |
| $\phi_r^{3(B-B)} = 1.0$ | $\phi_{ti}^{3(B-B)} = -3.5$ | $\phi_{lo}^{3(B-B)} = 0.7$ |
| $\phi_r^{2(C-C)} = 0.88$ | $\phi_{ti}^{2(C-C)} = -0.32$ | $\phi_{lo}^{2(C-C)} = -0.04$ |
| $\phi_r^{3(B-C)} = 2.0$ | $\phi_{ti}^{3(B-C)} = -4.5$ | $\phi_{lo}^{3(C-C)} = 0.5$ |
| $\phi_r^{4(C-C)} = -1.9$ | $\phi_{ti}^{4(C-C)} = 2.0$ | $\phi_{lo}^{4(C-C)} = -0.55$ |
| $\phi_r^{4(B-C)} = -1.8$ | $\phi_{ti}^{4(B-C)} = 1.0$ | $\phi_{lo}^{4(B-C)} = -0.22$ |

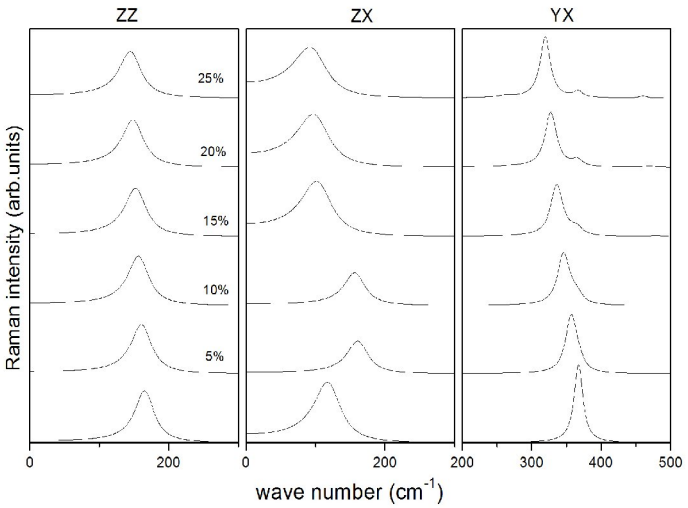


FIG.1: The ZZ, ZX and YX Raman spectra, in RBM region, calculated for a (10,10) SWCNT for 0%, 5%,10%,15%,20% and 25% boron doped rate.

We consider an (10,10) armchair boron doped SWCNT model. The system structure is obtained by substituting boron by carbon in the $BC_3$ nanotube. The ZZ, ZX and YX Raman spectra of the infinite SWBCNT are displayed in the radial breathing modes (RBM) and the tangential modes (TM) regions as function of six values og the doping rate: 0%, 5%, 10%, 15%, 20% and 25%.The extreme 0% and 25% values are corresponding to the Raman spectra of the purely infinite SWCNT and the $BC_3$ nanotube respectively.

In the RBM region (fig.1), the Raman response for the SWCNT is calculated around 165cm$^{-1}$ ($A_{1g}$), 122 cm$^{-1}$ ($E_{1g}$), 367cm$^{-1}$ ($E_{2g}$) for ZZ, ZX, YX configurations, respectively. Whereas, the radial modes of the $BC_3$ nanotube are located at $A_{1g}$ 145, $E_{1g}$ 90, $E_{2g}$ 318 cm$^{-1}$. One can see that the frequencies of radial modes are depending on the doped rate. A general downshift of A1g and E2g peaks is observed when the boron doping rate decreases with significant variations (20-40cm$^{-1}$). Concerning $E_{1g}$ mode, an upshift is observed for doping rate lower than 12.5% followed by a downshift for higher one with a significant variations (40-60cm$^{-1}$). The additional weak modes observed in YX configuration come from degenerate modes in the region.

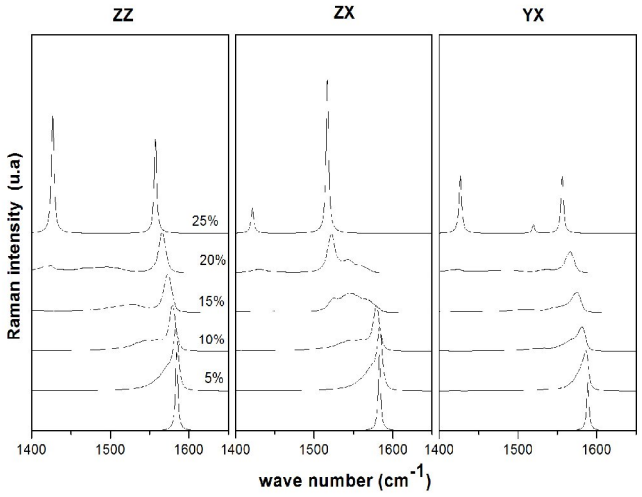


FIG.2: : The ZZ, ZX and YX Raman spectra, in TM region, calculated for a (10,10) SWCNT for 0%, 5%,10%,15%,20% and 25% boron doped rate.

In the TM region (fig.2), one can see that the mode frequencies decrease when the doping rate goes to the higher values. Moreover, the doped systems show a broad band in 1400-1550 cm$^{-1}$ range. As expected, this behaviour can be assigned to default modes observed in realistic SWCNT D band. In the case of $BC_3$ nanotube (25% of the doped rate), the Raman spectra are dominated by two peaks. This latter characterize the tangential modes associated to the B and C species in the $BC_3$ nanotube.

## IV. Conclusion

In conclusion, we have presented a force constant model for calculating the vibrational frequencies in the single walled BC3 nanotube and boron doped SWCNT. This model is used to calculate the Raman active modes of these systems. It is shown that the

frequencies of radial modes of SWCBNTs are dependent on the boron doping rate in the SWCNT. The tangential region is characterized by a broad band for doping rate between SWCNT and single wall BC3 nanotubes. This behavior is observed in experimental Raman spectra of SWCNT samples presenting defaults.

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