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PHONON PROPERTIES OF BORON NITRIDE NANOSHEET

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Abstract:

The exceptional properties of Boron Nitrides (BN) nanotube have attracted the attention of the researchers in past few years. BN nanotubes can be considered as insulating materialand are highly resistive to oxidation. In air BN nanotubes are stable up to at least 700˚C while highly crystalline and low defective BN nanotubes show stability up to 900˚C. High density nano electronic devices demands a nano material with good thermal conductivityand BN nanotube is among the best options as its thermal conductivity is high. BN nanotube show lot of other excellent properties like non cytotoxicity and ability of stable interaction with bio molecules make it more suitable for biological applications. The BN nanotubes have received considerable attraction on account of their unusual properties, which differ significantly from bulk counterpart. The possibilities for technological applications of BN nanotubes have motivated the researchers for study of properties and applications of these nanotubes. Therefore, these properties must be evaluated accurately and comprehensively to predict the possible behavior and potential of BN nanotubes for device applications. In crystalline materials, the scattering of mobile charge carriers occurs due to the fluctuating potential arising from lattice vibrations. Physically these lattice vibrations are attributed to the phonons, which signify the importance of phonon calculation. The crystal structure and inter-atomic interactions are also well described by phonon spectrum. The calculations for phonon spectrum of BN nanotubes are yet to explore completely. Furthermore, these calculations lead to investigate other physical properties like entropy, specific heat capacity, Debye temperature and so on.The BN nanotube is basically a cylindrical structure formed by rolling h-BN sheet and it can be classified into two categories chiral nanotube and achiral nanotube depending upon chiral angle. The achiral nanotube can be further classified as zigzag nanotube and armchair nanotube. The understanding of the dynamical properties of h-BN sheet is necessary. Therefore, in this work a short range force constant model has been used to study the phonons in sheet of zigzag BN nanotube by considering the interatomic interactions up to 2^{nd}nearest neighbor. The calculated results are compared and analyzed with available results.

Introduction:

The recent discovery of carbon nanotubes and then non carbon materials having layered structure capable of forming nanotubes has inspired many researches for theoretical and experimental investigations. There have also been several activities in exploring the attractive physical properties of these nanomaterials lke, fullerenes and single wall carbon nanotubes (SWCNT) and boron nitride nanotubes (BNNT) etc (praprti et al 2004). At present single wall nanotubes are getting attention, as they are best candidates for future nanoscale devices due to their structural and electronics properties (Dresselhous, 1996). Other outstanding properties are one-dimensional conduction, electric field induced electron emission [Tans 1998, Kim 2000] and unique capillary behavior [Pederson 1992, Ijima 1991]. Furthermore boron nitride nanotubes are chemically more inert than the carbon nanotubes and can also act as insulators, hence they may also serve as insulating and protective shields for encapsulating metallic clusters and nanorods. Non cytotoxicity and capability of stable interaction with biomolecules make it more suitable for biological applications (Ansari et al., 2016). A nanotube exhibits various unpredicted and very appealing electronic properties, like they may be moderate gap semiconductors or insulators, depending on their chirality, which is defined by the orientation of hexagons w.r.t. nanotube axis [Hamada 1992]. The possibilities for technological applications of BNNTs motivated the development of various methods of their fabrication like laser ablation, arc discharge and chemical vapor deposition techniques. But the complete and detailed vibrational spectra are still scared in literature. The careful study of BN nanostructure is necessary for proper description and prediction of phonons and elastic structure. It is therefore, the detailed phonon properties of h-BN, zigzag nanotubes have been presented in this work.

In the present study we have computed the phonon band structure hexagonal BN sheet and single walled (5, 0) BN nanotube using De Launay force constant model. The primitive cell of h-BN is assumed to be consisting of two atoms (one B and one N) placed alternatively. The first and second neighbor interactions have been considered explicitly to calculate the central and angular force constants. These results are then used to derive the phonon dispersion relations for (5, 0) nano sheet of BN.

Structure and Symmetry Properties of Zigzag Nanotube:

Nanotubes are usually classified on the basis of their angle of chirality, which can be defined as the angle between the circumference and the nearest zigzag structure. For Zigzag nanotube the angle of chirality is equal to zero as shown in figure 1. As nanotube is formed by rolling of the h-BN sheet therefore its structure can

be understood in terms of real space unit vectors of the sheet. The unit cell of zigzag (n, 0) BN nanotube consists of four atomic rings in parallel planes perpendicular to the axis. There are two pairs of rings each consists of planes with n number of nitrogen and n number of boron atoms.

It is found that unit cell of (n, 0) zigzag nanotube possesses n-fold rotation axis and rotation angle is $2\pi/n$. In addition, n vertical reflection symmetry planes can be found. Thus unit cell of zigzag nanotube transforms under C_{nv} symmetry group (Wirtz 2003). The 6N phonon modes make over according to the following irreducible representation.

$$\Gamma_{6N}^{zig} = \Gamma_{6N}^{zig}.\Gamma_v = 4A_1 + 2A_2 + 4B_1 + 2B_2 + \sum_{j=1}^{n-1} 6E_j$$

Where $\Gamma_a^{zig} = 2\left(A_1 + B_1 + \sum_{j=1}^{n-1} E_j\right)$

and $\Gamma_v = A_1 + E_1$.

These modes are transforming according to $\Gamma_1 = A_1 + E_1 + E_2$ and/or Γ_v are Raman and/or IR active respectively. Four of the 6N phonon modes are those which transform as Γ_v and $\Gamma_{R_z} = A_2$ have vanishing frequencies that is acoustical modes. Consequently, out of 6N phonon modes the symmetries and numbers of optically active phonon modes in zigzag BN nanotubes are given by.

$$\Gamma_{Raman}^{zig} = 3A_1 + 5E_1 + 6E_2$$

For zigzag tube 14 phonon modes are Raman active modes having 3 with A_1 symmetry, 5 with E_1 symmetry and 6 with E_2 symmetry while 8 are IR active modes having 3 with A_1 symmetry, 5 with E_1 symmetry.

$$\Gamma_{IR}^{zig} = 3A_1 + 5E_1$$

Note that the numbers of Raman and IR active phonon modes found for zigzag BN nanotubes are almost twice than that of zigzag Carbon nanotube.

Methodology:

In de Launey angular force constant model non central interaction of the reference atom and its neighbors is considered. The non central force is combination of central and angular forces. The non central restoring force acting on atom 'o' due to atom 'i' is given by,

$$F_i = -\alpha'\left(s_0 - s_i\right) - (\alpha - \alpha')\left[\hat{\zeta}_i X\left(s_0 - s_i\right)\right] X \hat{\zeta}_i$$

The solutions of the above equation of motion is assumed to be plane wave with an angular frequency ω, amplitude A and propagation vector k.

This determinant equation is the secular determinant, which determines the angular frequencies of the normal mode of vibration. Secular determinant is of the form as given below.

$$\left[D_{ij}(q) - M\omega^2 I\right] = 0$$

Where D_{ij} are the elements of the dynamical matrix and I is the unit matrix.

The unit cell of two-dimensional sheet contains only two independent atoms, hence we get a dynamical matrix (4x4), whose solutions results in two acoustic and two optical modes. By solving (4x4) dynamical matrix the force constants has been obtained. The nanotube is formed by folding two dimensional sheet two dimensional sheet so the derived force constants are then used to find the phonon relations of BN (5, 0) nanotube.

The area of unit cell of two dimensional sheet of BN Nanotube is defined by two vectors a_1 and a_2. The number of hexagons per unit cell N can be calculated by dividing area of the nanotube unit cell divided by area of hexagon and is obtained as a function of n and m as

$$N = \frac{|C_h X T|}{|a_1 X a_2|} = \frac{2(m^2+n^2+nm)}{d_r} = \frac{2L^2}{a^2 d_r}$$

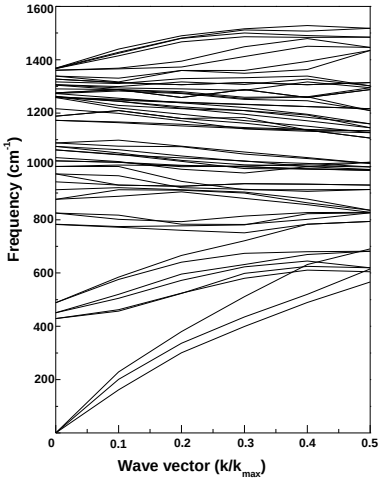
Where d_r is the GCD (greatest common divisor) of (2m+n) and (2n+m). It is also to be noted that each hexagon contains two atoms hence there are 2N atoms in each unit cell of the BN nanotube.

Therefore, in case of (5, 0) nanotubes there are twenty independent atoms in the unit cell, and hence, we have twenty sub lattices leading to a 60x60 dynamical matrix. The (60x60) dynamical matrix is diagonalized at different points along the symmetry direction [k 0 0] using FORTRAN programming.

Results and Discussion:

For zigzag (5, 0) nanotube there are twenty independent atoms in the unit cell, which results in sixty phonon modes right through the Brillouin zone out of which few modes may degenerate at the zone centre and zone boundary. The obtained (60x60) dynamical matrix is diagonalized at different points along the symmetry direction [k 0 0]. A curve is plotted for obtained frequencies at different points and is called phonon dispersion relation shown in figure 2. At zone centre, 36 phonon frequencies have been observed out of which 24 are doubly degenerate while 12 phonon frequencies are non degenerate, which is in accordance with the symmetry

properties of BN nanotubes. For zigzag nanotube 14 phonon modes are found Raman active while 8 phonon modes are observed which are IR active. In our present calculations radial breathing mode (RBM) for an isolated (5,0) BN nanotube appears at 429 cm^{-1} which seems to be higher when compared with radial breathing mode of (17,0) BN nanotube as it is 148 cm^{-1}. The higher value of RBM is due to the small radius of (5,0) BN Nanotube. It is acknowledged that the magnitude of RBM show dependence on the diameter as well as chirality of the nanotubes (Fakrach et al., 2009). It suffers an up-shift with the decrease in diameter of nanotube for the same configuration. Also magnitude of RBM is higher for the tubes of zigzag configuration (Akdim et al., 2003). So both these factors lower radius and zigzag configuration causes higher value of the RBM. Three acoustic modes are obtained in this work. The fourth acoustic modes were expected to be observed as it is reported for other nanotubes of larger radius. The fourth mode is considered to be due to movement of the atoms around the axis but as the radius of tube decreases to such value so that radial dimension becomes comparable to inter atomic dimension such movements becomes less probable.



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