IJPAC
© Global Research Publications

Vol. 14 • Nos. 1-2 • January-June, 2019
pp. 43-47

Determination of energy band gap and specific heat of armchair and zigzag single wall carbon nanotubes by quantum treatments

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ABSTRACT: The energy band gap of armchair and zigzag single wall carbon nanotubes have been calculated as a function of diameter using the Schrödinger-Poisson equation.The results are compared with available experimental and theoretical data.In addition to the energy band gap, electron density per unit surface and the specific heat at room temperature and at the Debye temperature as a function of diameter for both type of nanotubes are also evaluated. A comparison of our evaluated specific heat for carbon nanotubes at room temperature reveals a satisfactory agreement with the theoretical data.

Key words: Carbon nanotubes, energy band gap, specific heat

Introduction

Nanomaterials of carbon of different dimensionalities like carbon nanotubes, fullerenes, etc. have been a subject of interest over two decades due to their growing interest in various nanoscale electronic devices [1-2]. Graphene, the two dimensional flat monolayer of carbon atoms packed into a honeycomb lattice is the least addition to this family owing to the recent progress in experimental and theoretical techniques [3-8]. Because of its sophisticated low dimension electronic properties and substantial applications,it has attracted the attention of a big scientific community in recent times to explore it in various aspects [9-12]. Graphene nanoribbons/ nanotubes are also called half metallic materials recently playing a promising role in spintronics applications. For the purposes of device applications, two categories of nanotubes: one with armchair edges and the other with zigzag edges are receiving the most interest.

In the present work, we have reported a comprehensive theoretical study of band gap, electron density per surface and specific heat of one dimensional nanostructure materials namely; the carbon nanotubes, at room temperature and Debye temperature. In this study, we have taken armchair and zigzag carbon nanotubes. The calculations are based on the quantum mechanical treatment through the solution of Schrodinger-Poisson problem. On the experimental side the only experimental measurement for band gap for armchair was carried out by Wildöer et al. [12,21]. Theoretically, the calculations for band energies include the only determination of Draesselhaus et al. [1]. Moreover, for the calculations for specific heat at room temperature, Saxena et al. [13] derived the results which were noted in satisfactory agreement with our evaluations. With the help of specific heat of CNTs, we can also study the other thermal properties such as thermal conductivity, thermal resistivity etc. Whereas, the thermal conductivity is equal to the product of the specific heat, square of the phonon group velocity and the phonon relaxation time [14-15].

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Theoretical

Carbon nanotubesare made of translational lattice indices [L,M].[L,M] type of nanotubes are in general, called armchair nanotubes whereas [L,0] types are called zigzag nanotubes. The diameter of carbon nanotube d_{CNT} is given by the equation [16]

$$d_{CNT} = \frac{a}{\pi}\left[L^2 + M^2 + LM\right]^{\frac{1}{2}} \quad (1)$$

where a is honeycomb lattice parameter and its value is 2.46 A°. The electron density per unit lengthin CNT is given by the equation [17-18]

$$N_e = \int_0^R dr \int_0^{2\pi r} n(r,s)ds \qquad (2)$$

with

$$n(r,s) = \sum_{m=0}^{\infty} |\psi_m(s)|^2 \, \delta(r-R)|_{Em}^{\infty} \; g(E,E_m), f(E,E_F)dE \qquad (3)$$

Where $f(E,E_F)$ is Fermi statistics and $g(E,E_m)$ is the contribution of subband energy E_m to one dimensional density of state. The δ function is used to localize the charge over the nanotubes surface. The value of $\Psi_m(s)$the corresponding angular Eigen function is calculated from Schrödinger equation with periodic boundary conditions (see for instance Refs. [17-18] for detailed description)

$$-\frac{\hbar^2}{2m_e}\frac{d^2\Psi_m(s)}{ds^2} + V(s)\Psi_m(s) = E_m\Psi_m(s) \qquad (4)$$

From equations 2-4, we have obtained the electron density per unit surface as

$$N = \left[\frac{4}{\hbar\pi d_{CNT}}\right][2m_e k_B T]^{\frac{1}{2}} e^{\left(\frac{E_F - E_m}{k_B T}\right)} \qquad (5)$$

According to the thermodynamic principles, each electron is associated with kinetic energy $3/2k_BT$. Therefore, energy associated with N electrons is given by the equation

$$U = \frac{3}{2}k_B T N \qquad (6)$$

The specific heat per unit surface of CNT is evaluated by $C_V=|dU/dT|$.

$$C_V = \left[\left\{\frac{6}{\hbar\pi d_{CNT}}\right\}\{2m_e\}^{\frac{1}{2}}\{k_B\}^{\frac{3}{2}}\right]\left[\frac{3}{2}(T)^{\frac{1}{2}}e^{\left(\frac{E_F-E_m}{k_BT}\right)} - \left\{\frac{E_F-E_m}{k_BT}\right\}\{T\}^{\frac{1}{2}}e^{\left(\frac{E_F-E_m}{k_BT}\right)}\right] (7)$$

All symbols in this equation have their usual values such as Boltzman constant k_B=1.38 x 10^{-23}J/K and effective mass of electron m_e=7.55 x 10^{-31} kg. The Debye temperature for carbon is taken as T=1860 K. The value of E_m, angular energy level is calculated by equation [17-18]

$$E_m = \frac{|3m+1||V_{PP}|a_{cc}}{d_{CNT}} \qquad (8)$$

where V_{PP}(= -2.379eV),the nearest neighbour interaction potential is evaluated byBrenner-Tersoff data.a_{cc}, the carbon- carbon bond length of 1.42 A° for carbon graphite [10]is taken in the present calculations. Specifically, the density of states derived from the first order expansion of the graphene two-dimensional band structure near the corners of the Brillouin zone [19-20] which leads to:

$$E_g = 2E_0 = \frac{|V_{pp}|}{2R}a_{cc} \quad \text{at } m=0 \qquad (9)$$

Results and discussion

In the present work, we have evaluated the energy band gap, electron density per surface and specific heat at room temperature and Debye temperature as a function of diameter for armchair and zigzag carbon nanotubes at interaction potential -2.379 eV, employing the quantum mechanical principals.These parameters for carbon nanotubes depend only on the diameter. The numeric values of our calculations are presented in table 1-2.A comparison of the presently evaluated band gap for L=M,CNTs,with the experimental data of Wildöer et al. [12]

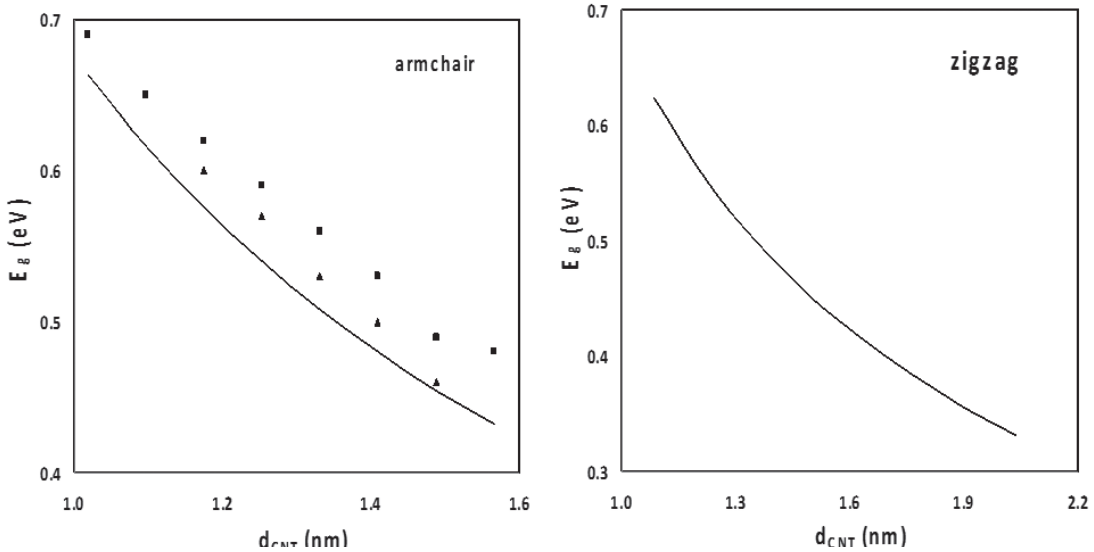

Figure 1: The energy band gap Egprofiles as a function of diameters dCNTof CNTalong with the theoretical data: ▲- ref.[1] andexperimental data ■- ref.[12].

shows a uniform deviation varying up to 10%higher than our calculated values. This is the only data for L=M type semiconductor measured by Scanning Tunnelling Microscope(STM) within experimental accuracy of 0.05 to 0.10 eV. The theoretical data of Dresselhaus et al. [1] for the same CNTs also revealed the same trend within 7% with our calculations,however, agree well with the experimental data [12].In case of M=0, zigzag CNTs the trend of our results is the same as for L=M. The evaluated electron density per unit surface as a function of diameter of CNTs,when energy level is below than Fermi energy level,is depicted in

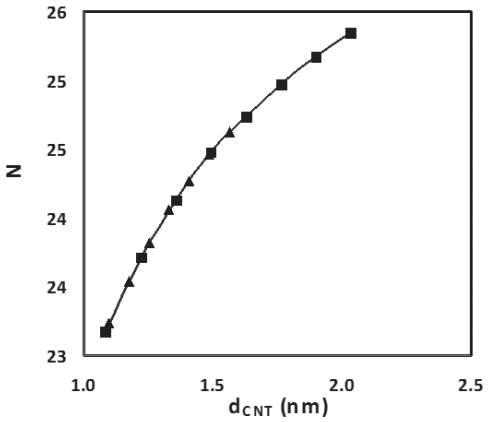

Figure 2: Variation of electron density per unit surface as a function of diameter of CNTs. Solid line with solid triangle represents the armchair CNT and line with solid rectangle represents the zigzag CNT.

and show a systematic behaviour as expected. The evaluated electron density per unit surface for zigzag CNT is however, maximum 3% lower than the armchair. However, to the best of our knowledge, there is no experimental/ theoretical data available for comparison of our data for electron density for CNTs.

On the other hand, we have evaluated the specific heat of carbon nanotubes at room temperature and Debye temperature. A comparison of our data with the only theoretical data of Saxena et al. [13] available at room temperature is shown the

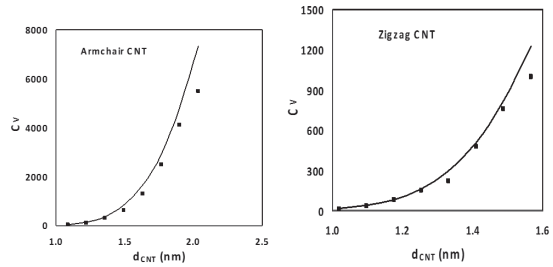

Figure 3:Variation of specific heat as a function of diameter of CNTs at room temperature along with the theoretical data ■- ref.[13].

Our calculated results for specific heat at room temperature show a satisfactory agreement with the theoretical data of Saxena et al. [13], however, a deviation at about 2nm diameter is noticed but lies in the composite error bars. Contrary to say that the specific heat for CNTs at room temperature increases exponentially with increasing the diameter.On the other hand, at Debye temperature, the behaviour of specific heat in

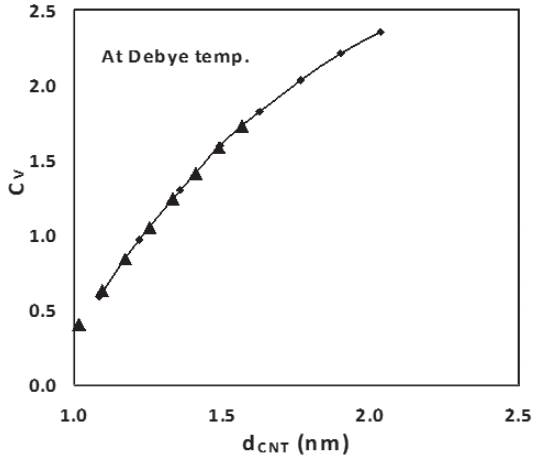

Figure 4: Variation of specific heat (10-4J/Kg-K)as a function of diameter of CNTs at Debye temperature. Solid line with solid triangle represents the armchair CNT and solid line with solid rectangle corresponds to the zigzag CNT

is almost opposite to the values as at room temperature.

Conclusion

For the first time, we have evaluated the energy band gap and the density of electrons per surface as a function of the diameters of armchair and zigzag carbon nanotubes employing the Schrödinger-Poisson equation. Specific heat for these CNTs was also evaluated at room temperature and the Debye temperature. The calculations were made corresponding to the different lattice indices of the crystalline carbon nanotubes. In case of energy band gap for armchair CNTs,a slightly deviation with the experimental and theoretical data was noticed while in case of specific heat at room temperature, a satisfactory agreement with the theoretical data was revealed. In conclusion, the present calculations peculate an idea for the calculations of thermal properties of importance for the carbon nanotubes. To check the accuracy and reliability of the present evaluations undoubtedly, further experimental and/or theoretical work is needed in this direction.

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Table 1:Energy bandgap, specific heat at room temperature and Debye temperature and electron density per unit surface (when angular energy level is below the Fermi level) with respect to the diameter of armchair CNTs.

Indices [L,M] (L=M) armchair	Diameter of CNT in nm	Energy Band Gap E_g (eV)	Specific heat at room temperature (J/Kg-K)	Specific heat at Debye temp. (θ_D) (10^{-4}J/Kg-K)	N (E_F>E_m)
(8 , 8)	1.085	0.624	32.597	0.589	23.175
(9 , 9)	1.221	0.554	125.558	0.965	23.708
(10 , 10)	1.357	0.498	361.722	1.302	24.130
(11 , 11)	1.493	0.452	850.643	1.599	24.473
(12 , 12)	1.628	0.416	1636.939	1.826	24.736
(13 , 13)	1.764	0.384	2914.219	2.029	24.968
(14 , 14)	1.898	0.356	4805.117	2.210	25.170
(15 , 15)	2.034	0.332	7322.595	2.352	25.340

Table 2:Energy band gap, specific heat at room temperature and Debye temperature and electron density per unit surface (when angular energy level is below the Fermi level) with respect to the diameter of zigzag CNTs.

Indices [L,0] Zigzag CNTs	Diameter of CNT in nm	Energy Band Gap E_g (eV)	Specific heat at room temp. (J/Kg-K)	Specific heat at Debye temp. (θ_D) (10^{-4}J/Kg-K)	N ($E_F > E_m$)
(13 , 0)	1.018	0.664	14.926	0.402	22.868
(14 , 0)	1.096	0.616	38.204	0.631	23.237
(15 , 0)	1.175	0.576	82.420	0.840	23.541
(16 , 0)	1.253	0.540	163.787	1.046	23.814
(17 , 0)	1.331	0.508	299.698	1.240	24.055
(18 , 0)	1.409	0.480	505.568	1.414	24.264
(19 , 0)	1.488	0.454	819.023	1.584	24.457
(20 , 0)	1.566	0.432	1224.621	1.724	24.619