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Electronic Structure of Atomically Resolved Carbon Nanotubes based on Nanotechnology

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Abstract—*The present paper reports the study of electronic structure of atomically resolved carbon nonatubes, based on nanotechnology. Carbon nanotube can be considered by as a graphitics one atom thick be rolled into a cylindrical tube whose radius be less than 1nm and diameler be 1. 4nm. Carbon nanotube is discovered in 1991. The remarkable electronic properties of these structures have attracted much attention. Their electronic conductivity has been predicted to depend sensitively on tube diameter, wrapping angle and helicity of the tube lattice. As we know that carbon nonatubes are molecular structures which contain graphite cylinders closed at either ends with caps containinng pentagonl rings. These are descenders of bucky balls, the soccer balls shaped molecules of 60 carbon atoms. Noriaski Hamada of NEC and M. S Dresselhaus of MIT calculated that if a raw of hexagon in a tube's along axis were straight the tube should be act as a metal and conduct electricity, and if a line of hexagons formed a helix, then tube should behave as a semiconductor and conduct electricity. In both cases, electricity is conducted by these structures. These parameters causing a shift from a metallic to a semicoducting state of carbon nanotubes. In other words, similar shaped molecules consisting of only one element that is carbon element may have very different and ballistic electronic behaviour. The electronic conductivity of this structure depends on its helicity, this helicity provides buckling and buckling provides bending. The bending phenomena in carbon nanotubes have been study experimentally and had indicated that under sever bending the buckling is usual way for nanotubes to reduce strain. The usual approach to the theoretical modelling of buckling phenomena has so far made use of classical potential. The electronic prperties of multiwalled and single walled carbon nanotubes have been proved experimentally, it has not yet been possible to relate these observations to the corresponding tstructure. Now we will study the result of scanning tunneling microscoroscopy and spectroscopy on individual single walled carbon nanotube from which atomically resolved images allow us to examine electronic properties as a function of tube diameter and bending angle. Here we will study and observe both metallic and semi conducing carbon nanotubes and find that their electronic properties depend on their bending angle. The band gaps of both the tubes is responsible for theoretical prediction as well as practical applications.*

1. INRODUCTION:-

Nanotechnology-

Nanotechnology is a field of applied science and technology covering a broad range of topics.

The main unifying theme is the control of matter on a scale smaller than one micrometer as well as the "well as the" fabrication of devices on this same scale. It is a highly multidisciplinary field, drawing from same fields such as colloidal science, device physics, and supramolecular chemistry. Much speculation exists as to what new science and technology might result from these lines of research[1].

Nanotechnology and nano science got started in the early 1980s with two major developments; the birth of cluster science and invention of scanning tunnelling microscope(STM).

This development led to discovery of fullerenes in 1985 and carbon nanotubes a few years later. Carbon nanotubes have recent received extensive attention due to their nanoscale dimension and outstanding materials properties such as ballistic electronic conduction, immunity from electro migration effects at high current densities, and transparent conduction.

As nano tube is fabricated it bends automatically due to its nano shape. Bending of nanotube provides buckling and this bucking is usual way for nanotube to reduce its strain. After that relaxed configuration is obtained. Now nano tube is ready for various purpuses. [2].

Carbon nanotubes:- When a graphene Sheet of one atom thick can be rolled into a tube then obtain helical tube is called carbon nano tube as shown in fig. 1[3]. As nanotube is fabricated it bends automatically due to its nano shape. Bending of nano tube provides buckling and this buckling is usual way for nanotube to reduce its strain. After that relaxed configurations is obtained. Now nano tube is ready for various purposes in the field of nano technology. Here we consider individual single walled carbon nanotube (SWCNT) for our re-search work [4].

Classification of nanotubes- Nanotubes can be classified on their basis of conductivity, chirality and layers.

(a) Basedon conductivity.
(i)Metallic (ii) Semiconducting

(b) Based on chirality.
(i) Zig-zag (ii) Armchair (iii) Chiral
(c) Based on layers.
(i) Single walled carbon nanotube (SWCN)
(ii) Muti walled carbon nanotube (MWCN)

Nano tube is mainly affected by its chirality (amount of twist in the tube). Twisting is found to transforms the tube from metallic nanotube to a semiconducting one with the band gap that varries with the twisting angle as shown in fig. 2.

Carbon nanotubes based on chirality are classified as zig-zag, armchair and chiral nanoatubes. Shape of these nanotubes are demonstrated in fig. 3. Carbon nanotubes are an outgrowth of the formation of carbon fullerene such as C_{60} Bucky ball molceules[5]. There are two kinds of nanotubes based on layers, these are single walled carbon nanotubes & multiwalled carbon nanotubes having one shell of carbon atoms in hexagonal arrangement. Single walled carbon nanotubes (SWCNT) is demonstrated in fig. 4 and multiwalled carbon nanotube(MWCNT) is demonstrated in fig. 5. Nanotechnology is a technology that uses carbon nanotubes material for various purposes in their field [6]. As nanotube is fabricated and studied by scanning tunnelling microscopy and spectroscopy after that its atomically resolved images are obtained. When we study these images, we find that its bending angle is the function of its electronic properties and diameter. After that we obtain conclusions of our work[7].

Steps for research work-As single walled carbon nanotube (SWCNT) is fabricated it bends automatically due to its nano shape. we have taken scanning tunnelling microscopy on nanotube from which atomically resolved images allowed us to examine electronic properties as a function that the electric indeed depend surely on its bending. The band gap of both types of tubes are consistent with theoretical prediction. This work is done for 25 to 30 single walled carbon nanotubes(SWCNT). After that we observe Van Hove singularities for confirmation of strongly one dimensional nature of conduction within nanotubes.

2. RESULT AND DISCUSSION:-

(a)Construction of carbon nanotube from graphene sheet:- As a graphene sheet of one atom thick can be rolled into a tube, then obtained helical tube is called carbon nanotube. Radius of this tube be less than 1nm and its diameter is 1. 4nm. when carbon nanotube is fabricated, it bends automatically due to its nano shape. In this tube two equivalent sites of the hexagonal lattice coincides[8]. This is demonstrated in fig. 6. The bending vector c that defines the relative location of two sites is specified by a pair of integers (n, m). Integers (n, m) is related with c to two unit vectors a_1 and a_2 as $c=na_1+na_2$. If n=m, then tube is called arm chair, where as m=0, then tube is called zig-zag. All other tubes are of chiral type and have a finite bending angle $\emptyset$ with $0^0<\emptyset<30^0$. To find the relation between electronic properties and its atomic structure, atomically resolved on images are required[9].

(b) Vector notation in carbon nanotubes:-When carbon nanotube is constructed, then it contains the following vectors. (a)Bending vector c. (b)Tube axis vector- T. (C)Solid vector-H. as demonstrated in fig. 6. A single graphene sheet rolling up along bending vector c then a nanotube indicated by indices(11, 7) is obtained. Bending vector along dotted lines be the zig zag or armchair. All other the bending angle related with chiral tubes with bending angle is specified relative to either the zig-zag direction θ or to armchair direction ($\emptyset = 30^0 - \theta$) Dashed line perpendicular to c and run in the direction of tube axis and indicated by T. The solid vector-H is perpendicular to the arm chair direction and specifies the direction of nearest neighbour hexagon rows indicated by the block dots. The angle between T and H is called chiral angle[10].

(c) Scanning Tunneling Microscopy (STM):-The scanneling tunneling microscopy of a single walled carbon nanotubes (SWCNT) is demonstrated in fig. 7. For tube no. 10(n=10), chiral angle be $7^0(\emptyset = 7^0)$, diameter be 1. 3nm (d=1. 3nm) correspond to vector (11, 7). Again taking the two dimensional graphene sheet as a starting point, then critical dependence of electronic spectra of nanotubes indices (n, m) can be understand. We apply the periodic boundary condition that is $c.k=2\pi q$, where, k=wave vector, q=integer, along c direction (circumferential direction). This follows a set of allowed values for k that can be substituted into the energy dispersion relation for a graphene sheet. Calculations show that armchair (n=m) tubes have bends crossing the Fermi level and therefore metallic[11]. There are existing two possibilities. First if n-m=3, where l=an integer, then tube is called metallic. Second, if $n-m\neq 3l$, then tube is semiconducting whose energy gap be in order of ~0. 5eV. This gap, should depend on the diameter, that is $E_{gap}=2\gamma_0 a_{c-c}/d$, where γ_0=c-c tight binding overlap energy, a_{c-c}=nearest neighbour, c-c=distance (0. 142nm) d=diameter

Atomic resolution is achieved on more than 25 tubes, corresponding to ~85%of the tubes investigated. In mostly cases only a few rows of atoms on the top of the tubes can be imaged. Very few armchair tubes were observed, which is in apparent contrast with earlier investigation on the same type of material. However unlike these earlier experiments, we have concentrated on individual tubes, and have neglected the ropes of tubes[12].

Fig. 7 shows atomically resolved STM images on five different nanotubes. The “m” maximum important feature is triangular lattice of dark dots with lattice spacing in the order of 0. 25nm, as expected by graphene lattice. We find the dark dots on the centre of hexagons. The atomic resolution images help us to determine the chiral angle. This also enables to distinguish chiral tubes from zig zag. Chiral tubes are shown in 1, 10 and 11 zig-zag in 7 and armchair in 8 as demonstrated in fig. 8. A wider variety of chiral angle is observed in contrast

to earlier electron diffraction studies on ropes of single walled carbon nanotubes. The vacuum barrier between the STM tip and sample provides a junction for scanning tunnelling spectroscopy(STS). It allows tunnel current at large bias voltage. In STS current- I is recorded as a function of applied bias voltage applied to the sample, where scanning and feed back are switched off. When tube is examined the differential conductance(dI/dV) can be considered to be proportional to the density of states(DOS). Reference measurements we performed on the gold substrate after and before taking STS measurements. Only when the curves on the gold were approximately linear and did not show kinks or steps, where data on a tube is recorded. I.V. Traces are taken only far from the tube where tubes are isolated with each other. Here all the tubes are reported. STS curves are taken at different positions that is in order of 40nm[13].

Geometry of figure-7:-This figure bears the atomically resolved STM images of individual single walled carbon nanotubes(SWCNT). The lattice on the surface of cylinders give the clear identification of the tube chirality. Dashed arrow represent the tube axis vector-T, and solid arrows indicate the solid vector –H(direction of nearest neighbours hexagon rows). Tubes no 10, 11 and 1 are chiral where as tube no 7 and 8 have a zig-zag and armchair structures respectively. Tube no 10 has a chiral angle $\emptyset=7^0$ and a diameter 1. 3nm, which corr espond to the(11, 7) type of panel as clear from fig. 7. Studies have shown that the material consists of mainly ~1. 4nm single walled nanotubes. These are deposited from a dispersion 1.2 dichloromethane on single Au(111) faces. Topogram images are obtained by recording the tip height at constant tunnelling current(I) in a home built STM operated at 4k.

I-V Curves of Structure by STS:-I-V curves obtained by STS are shown in fig. 8. This figure contains part a, b and c. In this figure most of curves show that a low conductance at low bias, followed by several kinks at large bais voltages. We have investigated that for all chiral tubes are distinguished into two categories: One has a well defined value of gap from 0. 5-0.6eV. where as other having larger gap values from 1.7-2. 0eV. This is demonstrated in fig. 2(b). The gap value of first category coincides with the expected gap values of semiconducting tubes. Now fig. 2(c) that displays gap versus tube diameter the measurement degree will be theoretical gap values, obtained for an overlap energy $\gamma_0=2.7\pm0.$ 1eV. Which is a close to the value of$\gamma_0=2.5$eV, suggested for a single graphene sheet[14]. The very large gap that we observe for second category of tubes, 1.7-2. 0eV, are in good agreement with the values 1.6-1. 9eV, that we obtained from one dimensional relations for a number of metallic -tubes. For metallic tubes, m-n=3l and its diameter be 1. 4nm. Metallic nanotubes having small but finite DOS near the Fermi energy[E_f] and apparent gap is associated with DOS peaks at the band edges of one dimensional modes. The gaps seen in fig. 8 are not symmetrical around the zero bias voltage. This shows that the tubes adopted by charge transfer from the Au(111) substrate. The work function of the order of 5. 3eV, that is much higher than that of nanotube but similar to 4. 5eV, which is equal to the graphite. This shifts the Fermi energy towards the valance bond of tube. In the semiconducting tubes, the Fermi energy seems to have shifted from the centre of gap to the valance band edge. In the metallic tubes it is shifted by 0. 3eV, which is much lower than half of the gap. This provides experimental proof that these tubes have a finite DOS within the gap. The chiral to tubes seem to be either semiconducting or metallic with gap values are predicted[15]. The data provide a ballistic proofs band gap structure calculation of nanotube electronic properties. The electronic spectra for armchair and zig zag tubes are also consistent with the calculations but small number of such tubes in our experiments prevent a more general statement. We suggest for chiral metallic tubes, that a small gap of value approximately 0. 01eV will open up owing to the tube curvature. But we cannot find or observe such a small gap at the centre of large gap in chiral metallic tubes. This condition provides the hybridisation between wave function of tube and the gold substrate[16].

Geometry of Figure-8. This fig. 8 provides the electronic properties of single walled carbon nanotubes(SWCNT) in the form I-V characteristics. Fig. 8(a). -Tube no 1-6 are chiral, no. 7 is zig-zag and no. 8 is armchair. The bias voltage is applied to the sample. It means the sign of bias voltage, corresponding to the relative energy of Fermi level. Curves no 1 to 7 are menat for low conductance at low bias followed by several kink at large bias voltages. Fig. 8(b):-The derivative dI/dv clearly curves are offset vertically. Gaps are represented by rows. Here two categories can be separated, one with gap values 0. 5 to 0. 6eV the other with significantly larger gap values. The first category of tube is identified as a semiconducting types where as second type be metallic tubes. In nanotubes about 12 out of 18 tubes were semiconducting [17]. These tubes besides the primary gap and also show peaks associated with secondary and higher order gaps. For the secondary gaps we find: 1.4Ev(n=1), 1.1eV(n=2), 1. 2eV(n=3), 1.4Ev(n=4) and so on. All the gaps have shifted to right, which indicates doping of the tube by substrate. We hold back from finding a zero or finite DOS from the values of dI/dv in the gap. The doping behaviour however indicates a finite DOS for metallic tubes and a zero DOS for semiconducting tubes. At zero bias the small dops in dI/dv represents some of the curves are not yet understand. The displayed dI/dv data are the result of averaging over approx 50 individual I-V curves for improved signal to noise ratio. The all individual curves contains same physical nature[18].

Fig. 8(c):-The data give the clear account for the theoretical prediction. The solid line indicates a fit of $E_{gap}=2\gamma_0 a_{c\text{-}c}/b$, with $\gamma_0=2.$ 7eV. Here tunnel current I as a function the bias voltage V applied to the sample. This is recorded as STM, where scanning and feed back were switched off[19].

Confirmation of one Dimensional Nature of Conduction within Nanotube:-Explanation of this conduction within nanotube is demonstrated in fig. 9. We study and find that (dI/dV)/(I/V) be on the ordinate. Sharp peaks are observed with a shape that indicates that prediction for Van Hove singularities. Since this singularities acts just like as an indicator that responsible for the conformation of strongly one dimensional nature of conduction within nanotube[20], with increasing V, (dI/dV)/(I/V) rises steeply, followed by a slow decrease. We find that the experimental peaks have finite height and are produced, that indicates properties of hybridisation of wave functions[21].

Geometry of fig. 9:-In this figure (dI/dV)/(I/V) is a measure of density of states versus V for a single walled nanotube-9. Here the symmetric peaks correspond to Van Hove singularities at the onsets of one dimensional energy bonds of the nanotube. The experimental peaks have a finite height and are broadened, which we conclude to hybridisation between the wave function of the tube and gold bsubstrate. The all shapes of experimental peaks however be still resembles that detected by theory. Sharp Van Hove Singularities in the DOS are predicted at the onsets of subsequent energy bands, reflecting the one dimensional character of carbon nanotubes[22].

Review of the experimental STM and STS results:-In our re search paper we have consider n is a number of nanotubes, ∅ is chiral angle, d is diameter of nanotubes in nm. E_{gap} is the apparent band gap in eV in STS, I-V, spectra and δE is the shift of Fermi energy due to doping of the tube by the substrate[23]. Chiral agle of 0^0 denotes an armchair nanotubes and angle of 30^0 a zig zag tubes. The flat surface Au allowed the diameter d of nanotube to determine an accuracy of o. 1nm by measuring the tube height relative to the surface. A possible systematic uncertainty in determining the diameter is due to difference in barrier heights for gold substrate and the tubes. The bending angle ∅ can be determined with an accuracy of~$1^{0.}$ Accuracy ∅ in is limited by the curvature of the tubes[24]. A combination of high accuracy in both ∅(~1^0) and d(0, 05nm) is required for a sharp identification of the n, m indices. Accuracy in E_{gap} and δE is 0.05-0.1eV. For this sample we observe that shift in the Fermi energy towards the conduction band instead of a shift towards the valence band as observed in the other samples. We speculate that the gold substrate for the sample may have had an anomalously low work function. These descriptions are summarized in table-1(a,b,c)[25].

3. CONCLUSION

In most cases only a few rows of atoms on top of the tube could be imaged. Very few armchair tubes were observed. All the gaps seem to have shifted to right which indicates doping of the tubes by the substance. We refrain from come concluding a zero or finite DOS from the value of dI/dV data in the gap. The central theoretical prediction, that chiral tubes are either semiconducting or metallic depending on minor variations of bending angle or diameters has been verified.

Use of this work:-We find that bending angle of tube is the function of its electronic properties and diameter. Hence by increasing of its bending angle we can understand of its electronic properties and measure its diameter.

FIGURES AND TABLES:-

Tables:-1-Overview of experimental STM and STS results are demonstrated in this table

Tube No(n)	1	2	3	4	5	6	7	8	9	10
Chiral angle(∅)	15	3	7	14	8	14	30	0	2	7
Diameter (d)	1. 4	1. 4	1. 2	1. 7	1. 3	1. 1	1. 3	1. 3	1. 3	2. 0
E_{gap}(eV)	0. 55	0. 60	0. 50	0. 65	1. 7	1. 8	1. 8	1. 9	0. 65	0. 2
δE(eV)	0. 25	0. 30	0. 25	0. 3	0. 3	0. 2	0. 2	0. 1	0. 2	0. 2

(a)

Tube No(n)	11	12	13	14	15	16	17	18	19	20
Chiral angle(∅)	14	12	7	15		4	9	16	6	29
Diameter (d)	1. 3	1. 5	1. 5	1. 4	1. 2	1. 2	1. 4	1. 2	1. 3	1. 3
E_{gap}(eV)			3. 0	1. 8	0. 50	0. 65	0. 61	0. 61	0. 5	0. 52
δE(eV)	0. 2	0. 4	0. 3	0. 2	0. 3	0. 3	0. 2	0. 3	-	-

(b)

Tube No(n)	21	22	23	24	25	26	27	28	29	30
Chiral angle(∅)	15	16	18	09	07	28	27	5	5	4
Diameter (d)	1. 8	1. 0	1. 4	1. 5	1. 7	1. 4	1. 4	1. 3	1. 5	1. 4
E_{gap}(eV)	0. 3	-	-	-	-	-	-	-	-	-
δE(eV)	-0. 3	-	-	-	-	-	-	-	-	-

(c)

(b)Figures:-

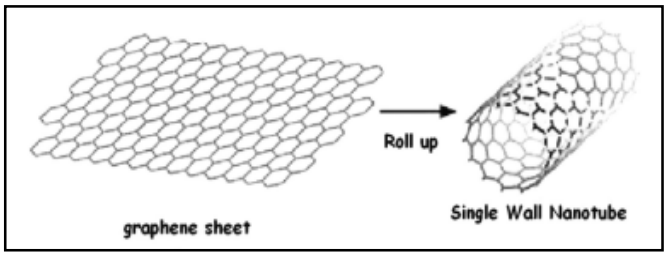

Fig. 1: Preparation of Nonotubes

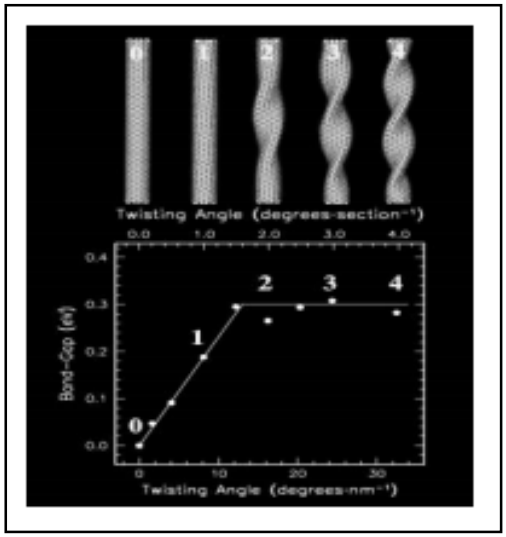

Figure 2: Brand gap varies with twisting angle

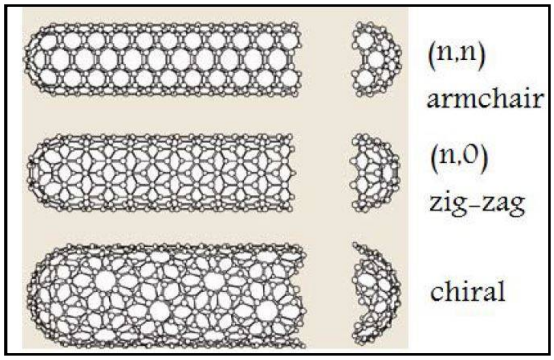

Figure 3: Carbonnonotubes based on Chirality

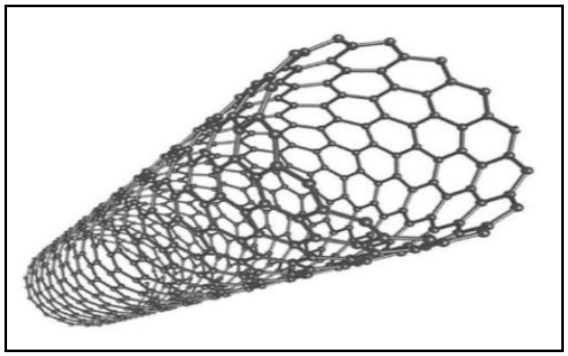

Figure 4: Single walled Carbonnonotube

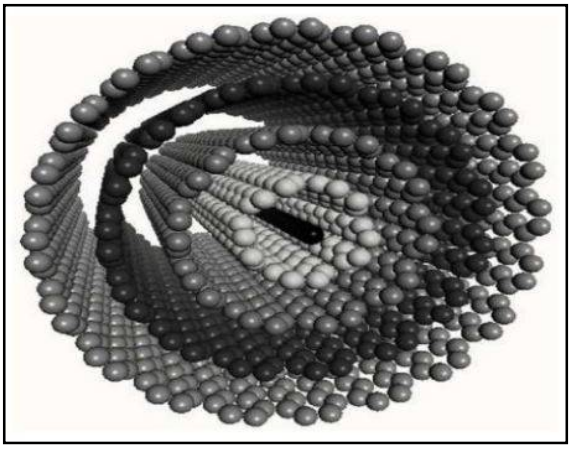

Figure 5: Multiwalled carbon nonotube

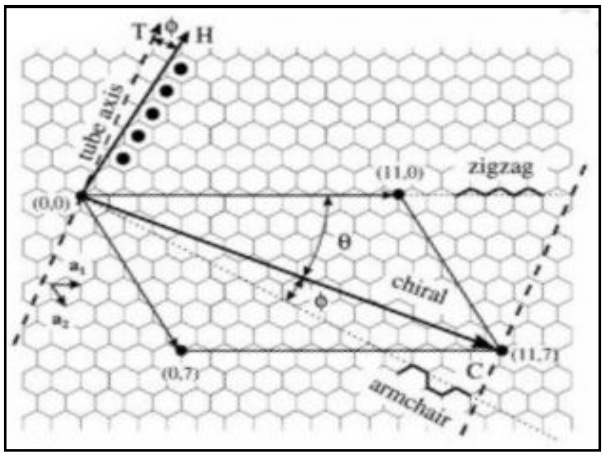

Figure 6: Sites of Hexagonal Lattice

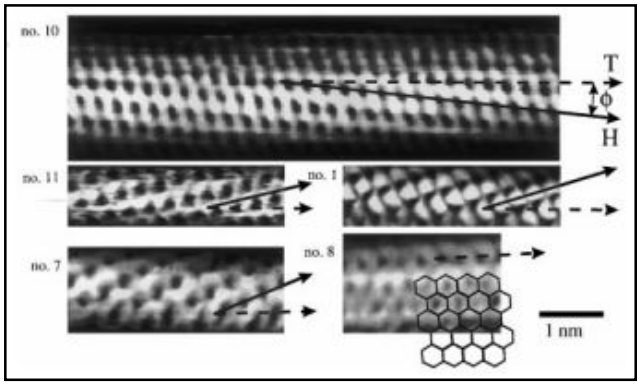

Figure 7: STM images of single walled carbon nonotubes

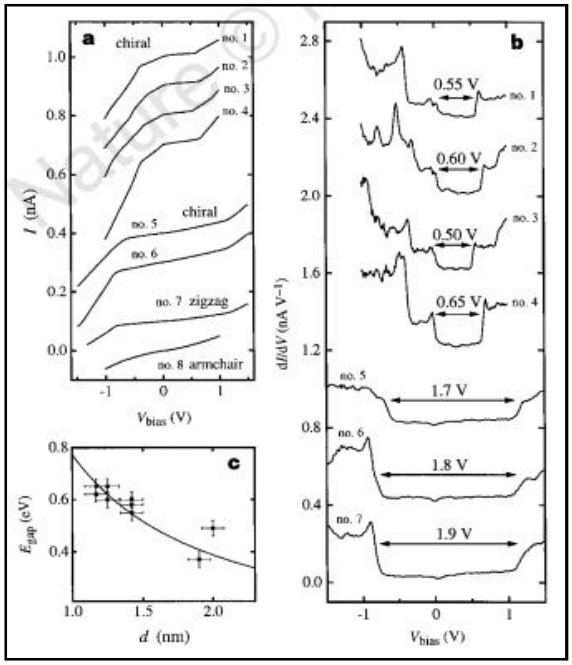

Figure 8: Electronic properties of single walled carbon nanotubes

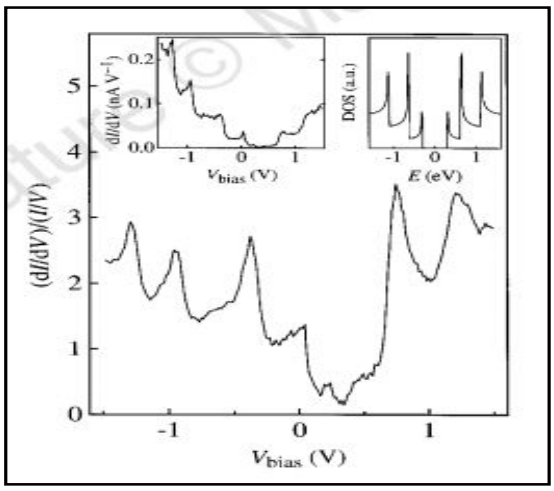

Figure 9: Van have singularities of single walled carbon nonotubes

4. ACKNOWLEDGEMENT

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