Single walled Carbon nanotubes and effect of defects & impurities

A thesis submitted in partial fulfilment of the requirements for the award of the degree of

Master of Science

In

Physics

By

Vaibhav Gupta

(2K20/MSCPHY/31)

Megha

(2K20MSCPHY/13)

Under the guidance of

Prof. Suresh C. Sharma

Professor

DTU, New Delhi

Department of Applied Physics

Delhi Technological University

New Delhi-110042

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DEPARTMENT OF APPLIED PHYSICS

DELHI TECHNOLOGICAL UNIVERSITY

(Formerly Delhi College of Engineering)

Bawana Road, Delhi-110042

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DEPARTMENT OF APPLIED PHYSICS

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(Formerly Delhi College of Engineering)

Bawana Road, New Delhi-110042

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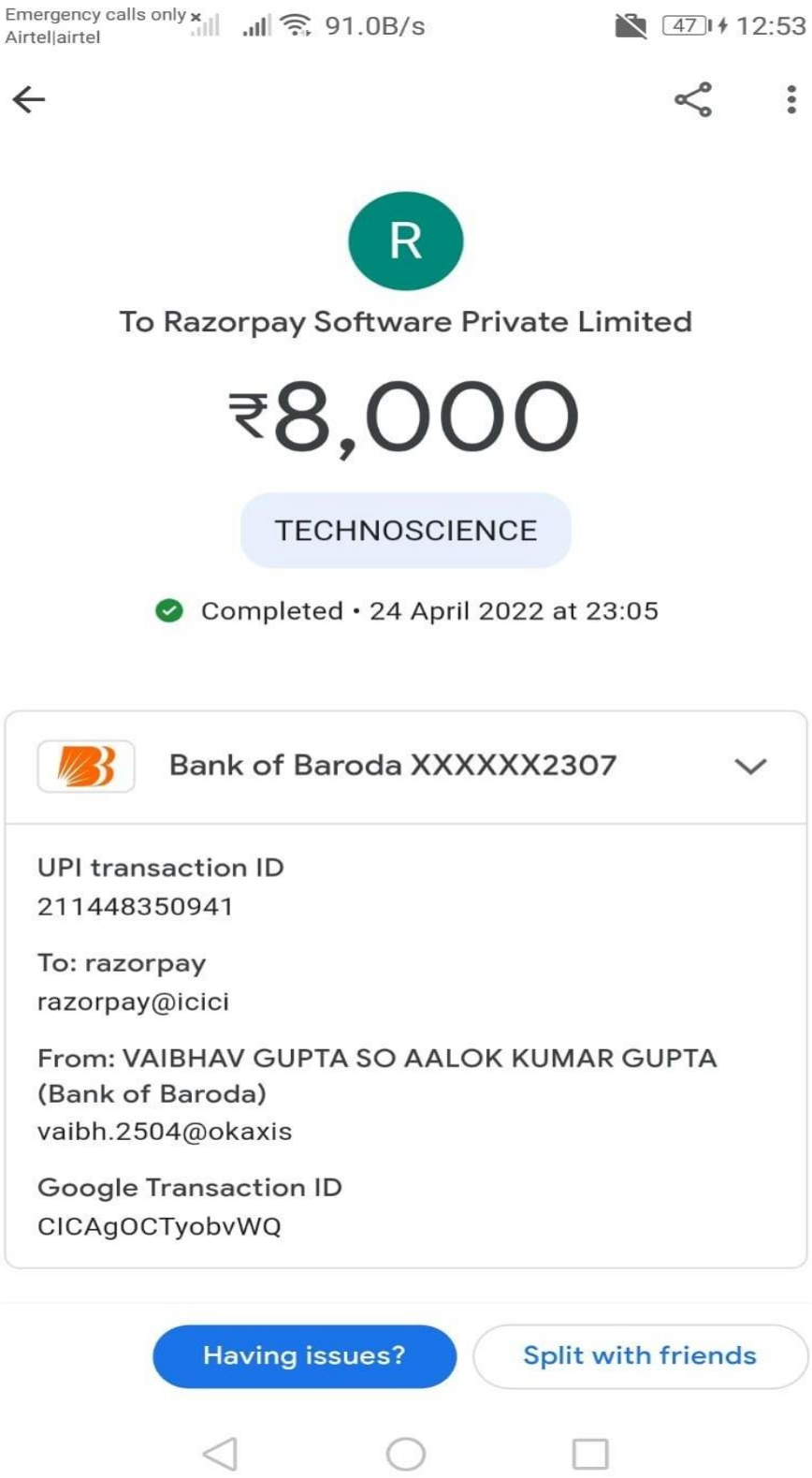

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ABSTRACT

In recent years, nanotechnology has been gaining a lot of attention due to the vast range of applications. CNTs are widely used because of extraordinary properties which make perfect use in different industries.In this study we are trying to find out energy changes in Singled Walled Carbon Nanotube (SWCNTs) while having some defects and impurity elements which will be helpful in determining different other physical properties of SWCNT. Molecular dynamics (MD) simulations, Avogadro and Origin have been used, for the analysis of SWCNTs, which is considered to be ideal Molecular structure (Mol-structure). The presence of vacancy defects and impurities in SWCNTs could lead to deviation from their ideal behaviour and thus affecting the original properties. SWCNTs with 1, 2, 3 & 4 carbon missing shows a trend by decreasing the energy as vacancy increases. Metal impurities (FE, Ni, Co) are taken in percentage of 0.5, 1, 1.5, 2 and optimisation energies is fond to be decreasing with increasing percentages of impurity.

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I. LIST OF FIGURES

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III. LIST OF ABBREVIATIONS

CNMS : Carbon nanomaterials

CNTs : Carbon nanotubes

CNFs : Carbon nanofibres

Nts : Nanotubes

Fig : figure

C_{60} : Buckminster fullerene Carbon

SWCNT : Single Walled Carbon Nanotube

MWCNT : Multi Walled Carbon Nanotube

YM : Young's modulus

CHAPTER 1

INTRODUCTION

Industries like Aeronautics, marines, automobiles, electronics and many more are primarily using Carbon nanomaterials. CNMs also found their potential use in construction industry. CNMs particularly known as carbon nanotubes or carbon nanofibres has some extraordinary mechanical properties like high tenile strength, elastic modulus and hardness. They also exihibit some astonishing electrical properties and thermo-physical properties[1]. Non-reactive property of CNTs make them a perfect cargo for drug delivery inside body[2]–[4].

1.1 History and Background

When the studies on C_{60} and C_{70} were on going, it suddenly came to the knowledge that a large variety of closed structures of graphine could be formed and each with unique properties. According to Euler's theorem, to form a closed hexagonal structure, 12 pentagons are needed in close[5]. C_{70} already shows a little elongated as compared to C_{60}[6].

A theoretical paper by the assembly of Naval Research Laboratory in 1991 on the electronic structure of small tubes[7], the results were believed too rough for publication as the production of CNTs seemed unlikely in not so far future.

But at the same time, a Japanese named Sumio Iijima used electron microscopy to analyze the carbon dust sample received from Meijo University. Carbon soot sample sent

was retrieved in carbon arc machine which is normally used to generate C_{60} [8]. Iijima noticed that the sample contains tubular like structure. The NTs generated were perfectly graphitized and had a pentagon capping at their end, just like the molecules of fullerene.

To study the properties of CNTs, there came a rush of researchers but the problem was the low amount of CNTs generation. By the spring of 1992, NEC Fundamental Research Laboratory, Tsukuba, Japan were trying to generation modified C_{60} by carbon arc method with boron. By accident, they found that under different conditions there is high yield of NTs and also the tubular structures were noticed[6] (fig 1).

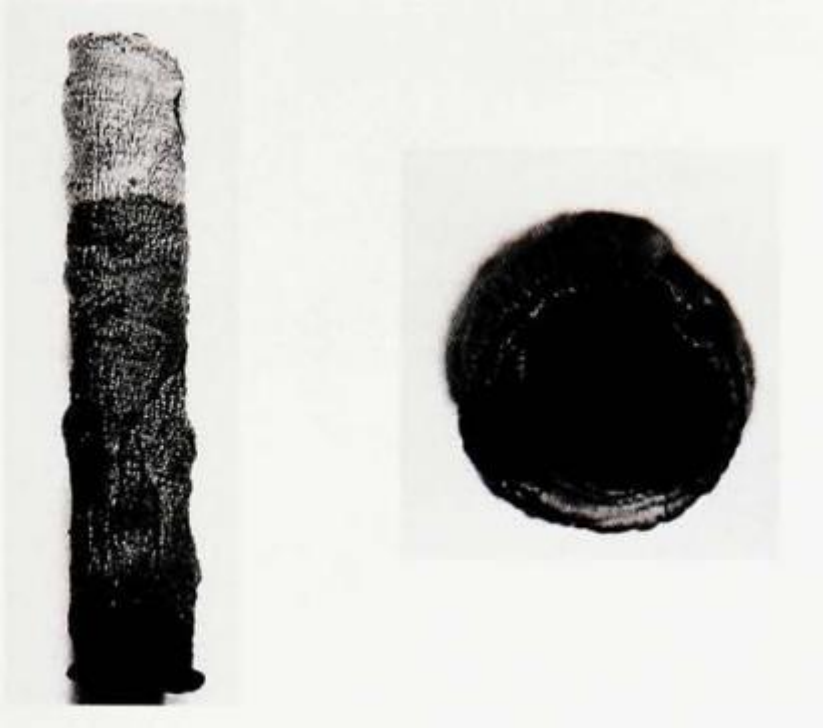

Fig 1. Tubular structure of diameter about 6mm[9].

1.2 Structure & Types

CNTs are first reported in 1991 by Sumio Iijima[8]. Soon after their discovery, they got quite lot of attraction because of their extraordinary mechanical and electronic

properties. A carbon nanotube (CNT) is a hexagonal array of Carbon-Carbon(C-C) bonded sp2 hybridised atoms shaped into a thin, long, hollow cylinder. CNTs can be think of rolled up layers of single Graphene (layer of carbon) or multiple. Later one is called as Multi walled (MWCNTs) nanotubes (fig 2(a)) and former one is known as Single walled (SWCNT) (fig 2(b))[10].

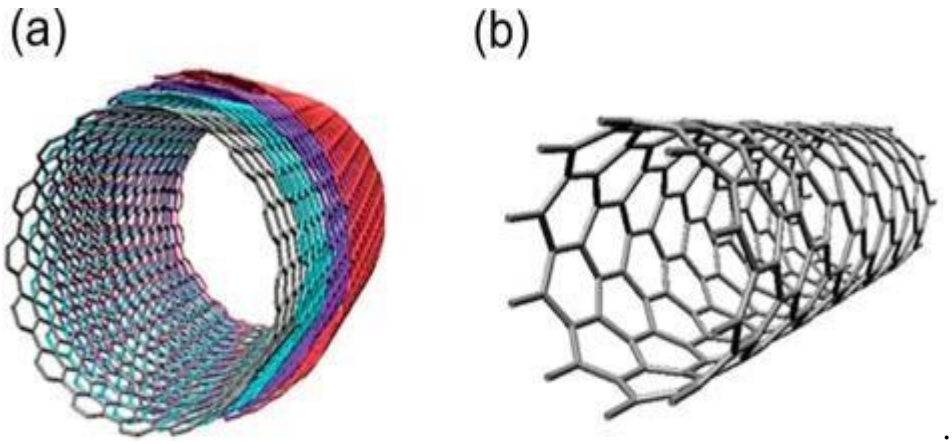

Fig 2. Schematic illustration of (a) Multi walled CNT (b) Single walled CNT[11].

MWCNTs have multiple walls and again can be classified into two types depending on their structures. One is Parchment structure and other is Russian doll structure. In Parchment type structure, a single sheet of graphene is rolled up in the form of parchment to form a multi walled nanotube (fig 3(A)). While in Russian doll structure, several concentric layers of graphene are present to form multi walled nanotube (fig 3(B))[12]. The inter layer separation between two layers in Russian doll is approximately 3.4 Angstrom which is same in interlayer separation in graphite[9].

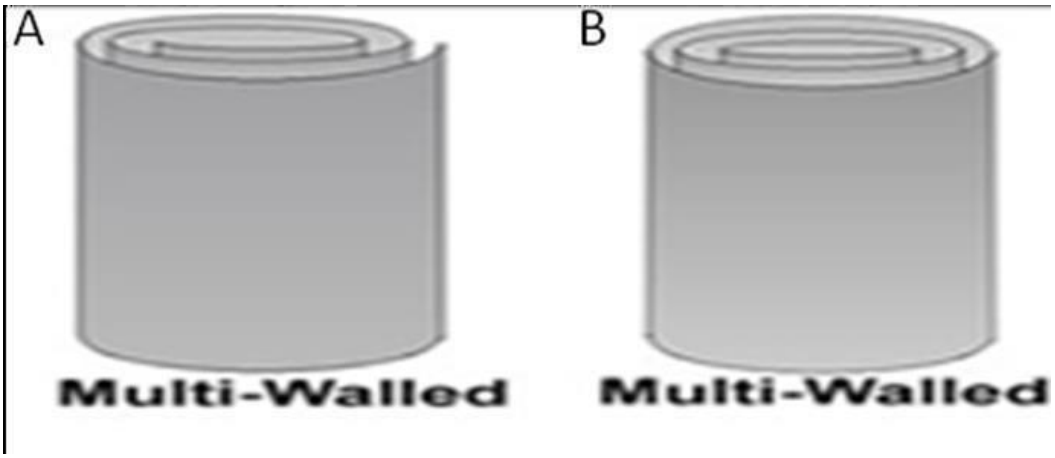

Fig 3. MWCNT (A) Parchment structure (B) Russian doll structure[12]

1.3 Morphology

Apart from two different types of CNT, there 3 other different basic structure of CNT. These three types of CNTs are Chiral, zigzag and armchair NTs (fig 4(b)). Difference in them arises when they are getting rolled up during their production.

Representation of chiral vectors is done selecting a pair of indices, termed here as n and m, where these two integer designates two unit vectors in different directions in graphene's honeycomb lattice structure. When unit vectors are equal to each other i.e. n=m, then it is called armchair. When m=0, NT is called zigzag. And the left ones are called Chiral[14][16] (fig 4(a)).

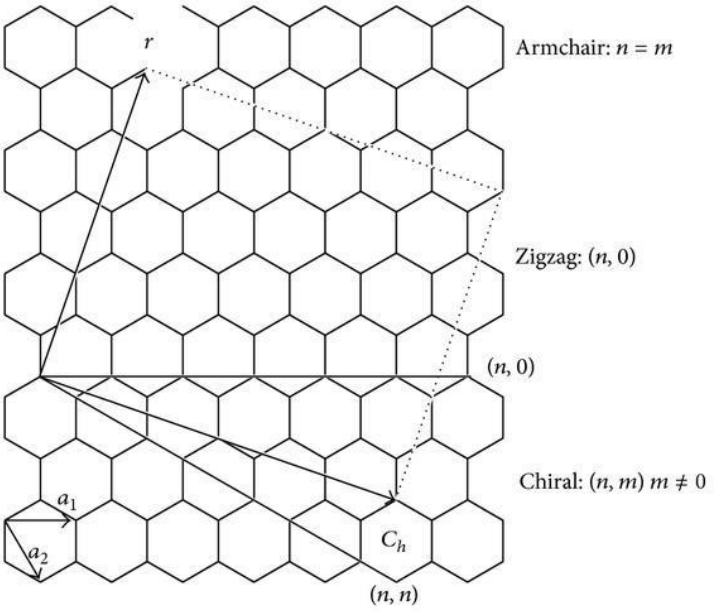

Fig 4. (a) Construction of chiral CNT from graphene sheet[17]

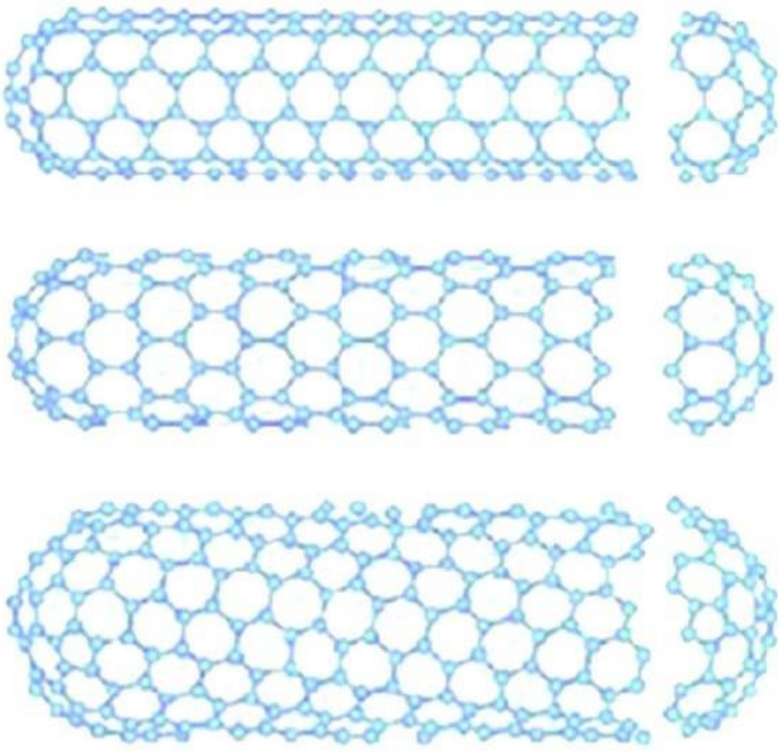

Fig 4(b) armchair, zigzag and chiral types of NTs[17]

Classification also depends on the chiral angle. If chiral angle, Θ, is zero, SWCNT is Zigzag. If Θ=30 degrees the armchair. If 0<Θ<30, then chiral[10].

1.4 Properties

Since the breakthrough of CNTs in 1991[8], CNTs have made their strong place in some the leading industries like aeronautics, marine, sports, automobiles, electronics ,and many more. They are considered as one of the most favourable class of material for advancement in nanotechnology. CNTs possess some very unusual properties that make valuable for optics, electronics, nanotech and various other fields. Let see some of their properties in brief.

1.4.1 Mechanical Properties

As the bonding found in CNTs is sp2, they are assumed to have axial strength and high stiffness[18]. We need to study the properties like fracture, yield strength, inelastic and buckling behaviour and elastic response in order to utilize the CNTs in mechanical industries. Right now, the stiffest fibre is CNT with YM of 1.4 TPa[19]. For comparison, tensile strength of steel is 1-2 GPa and YM is approx 200 GPa. Elongation to failure n CNTs is about 20-30%, together with stiffness, which concludes to tensile strength more than 100 GPa, highest yet known.

1.4.2 Electronic Properties

One dimensional character of CNTs are the one the major contributing reason for their electrical potential[20]. Low resistance is one of the very unusual properties exhibit by CNTs. Current density CNTs have yet highest known[21] of about $10^9 \frac{A}{cm^2}$ [22]. Superconducting effect has also been shown by CNTs.

1.4.3 Thermal properties

Before CNTs, diamonds have highest thermal conductivity. CNTs have twice the thermal conductivity of diamond[23]. Thermal conductivities and specific heat of CNTs is calculated by using phonos[24].

CHAPTER 2

VACANCY DEFECTS AND IMPURITIES

Like with any other material, the problem of defects always arises which can't be ignored. Because of presence of defects in CNTs, consistent results have not been carried out. Properties of CNT alter in presence of defects. Defects have been classified into 3 categories- (i) topological (ii) rehybridization (iii) incomplete bonding defects. But in this thesis, we will only discuss incomplete bonding or vacancy defect. And later presence of impurities during their synthesis.

2.1 Vacancy defects

Vacancy defects arise when one or more than one carbon atoms are missing from their original site (fig 5). Electronic property gets affected by these defects. Resistance in CNTs increases due to increase in vacancy defects. When electrons collide with defects, the resistance increases[25].

The mechanical properties and the YM are affected due to the defects in CNTs. In fuel cells, CNTs with vacancy defects are perfect to be used as platinum carrier electrodes. Because of the vacant positions the adsorption at sites increases, hence binding energy increases. SWCNTs with deficiency always have larger binding energy than ideal SWCNTs, and the binding energy at carbon deficit positions are found to be approximately double of any other configuration. If the no. of carbon atoms were missing or the position of missing carbon atom, mechanical properties also show variations[26].

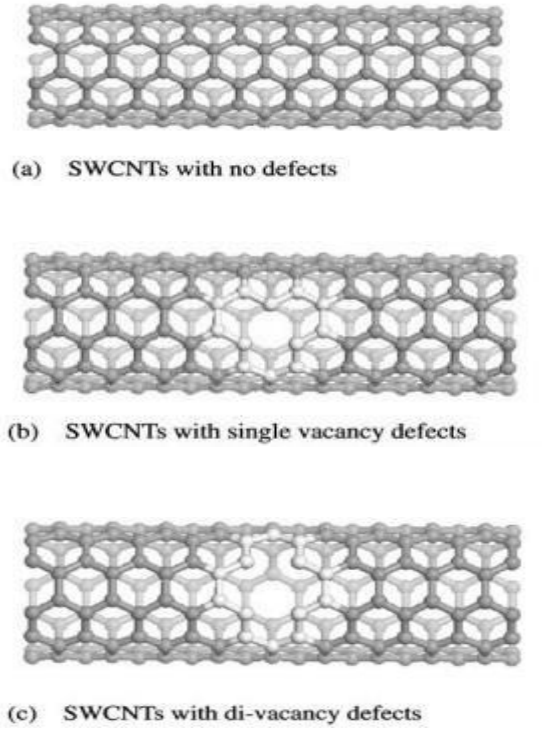

Fig 5. Vacancy defects in SWCNTs (5,5)[27].

2.2 Impurities

Impurities in CNT is one of the leading problems researchers dealing with. Metal impurities in CNT get added during their synthesis[28]. Transition metals like Iron, Nickel, Cobalt are used as catalyst residues[29]. Nanoparticles of metal formed from decpmposition of metal precursor. CNTs when manufactured consists of some impurity. These impurities can be washed off by several methods but they can't be washed off perfectly. Some hints of impurities will remain intact. Presence of these impurities effects the mechanical properties (like YM) of CNTs. Presence of contaminants in CNTs develop the toxic effects, the amount of residual oxygen reactive metal present in CNT decides the toxicity factor.

Impurities mainly consists of metals- Fe, Co, Mo and Ni all of which have reported the toxic effects[31], [32].

CHAPTER 3

SYSTEM ARCHITECHURE & SIMULATION

Configurations of device are of great importance when it comes to simulation. Configuration on which the simulations has been carried out are-

Processor	AMD A6-7310 APU with AMD Radeon R4 Graphics 2.00 GHz
Installed RAM	4.00 GB
System type	64-bit operating system, ×64-based processor

3.1 Simulator

Avogadro is a molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It is extensible via a plugin architecture. Avagadro is an open source software.

3.1.1 Molecular dynamics

Molecular dynamics (MD) modelling gives in summary the idea of dynamic individual motion of particle(or in our study, atoms) and structural developments as a function of time. MD has been the predominant computational outlook for estimating the mechanical properties and contaminated behaviour of CNTs. In this study, several

SWCNT models with different vacancy defects and different concentration of impurity are added and their energy dependence, the effects of contamination on energy of the SWCNTs were investigated based on MDs method.

3.1.2 Universal force field

Non-stochastic MD re-enactment strategies inevitably based on Newton's second law, F=ma, where F is the force applied on atoms, m is the mass, a is speeding up. As from the force on every atom, acceleration on each atom can be found. Parameters like acceleration, velocity and position can be determined by the trajectories which are depicted by the eq^{ns} of motions. Average value of these parameters can be evaluated by the trajectories formed. Summation of bonding and non-bonding energies is the total PE, $U=U_{bonding} + U_{non\text{-}bonding}$. For CNTs, van-der-Waal forces are the non-bonding energies, which ordinarily have a frail effect on the mechanical properties among the other interrelations present in C-C interactions. Lennard-Jones PE functions are most often used in order to know about the Vann-der-waal forces[33].

$$U_{van\text{-}der\text{-}waal} = \sum\left(\frac{Aij}{rij} - \frac{Cij}{rij}\right). \quad (1)$$

In above equations, A and C represent atom type subordinate constants. $r_{ij}=|r_{ij}|=|r_i r_j|$ gives the separation between two atoms, i and j, and r_i and r_j are the position vectors of i^{th} and j^{th} atom.

The prevailing portion of whole potential vitality, bonding vitality, may be an entirety of three diverse connections among atoms: bond extending, bond twisting, and bond torsion.

$$U_{bonded} = U_{bonded\text{-}stretch} + U_{angle\text{-}bend} + U_{torsion.} \quad (2)$$

Most frequently used PE functions are written as,

$$U_{bonded} = \sum K_s (rij - r)^2 \quad (3)$$

$$U_{angle\text{-}bend} = \sum K\theta(\theta - \theta o)^2 \quad (4)$$

$$U_{torsion} = \sum K\varphi(1 - \cos(t\varphi + \varphi o)) \quad (5)$$

Each term in above equation represents different parameters. r is equilibrium separation of the bond, K_s represents spring constant of stretching of bond, $K\theta$ represents force constant of bending, θo is rest angle for this bond, $K\varphi$ is force constant of torsion, φo represents the ideal bond phase and t is the periodicity of bond. By underlying the interaction of different carbon atoms with the quantum interaction of electron wave functions helped in finding the above written coefficients. In order to determine mutual interaction forces, program of gradient of potential energy will be our way out i.e. F= -∇U.

3.3 Procedure

This concentrate primarily centers around working out energy in presence of pollutions and in opening imperfections. Reads up done on MD for foreseeing the Young's modulus has utilized a few strategies. Strategies like observational power field technique, atomic primary mechanics strategy and so forth. Here we have utilized Universal power field (UFF) strategy (up to 4 folds) for registering the advancement energy. Subsequent to opening Avogadro programming, go to the form tab. A drop down menu will show Nanotube developer. On clicking this menu a window shows up. In this menu, we need to

put the necessary boundaries we need for our SWCNT. Various instruments are accessible for length, chirality, twofold bonds and so on. Opening can be made by tapping on draw instrument and select the molecule and press erase the carbon we need to eliminate. CNTs when produced in labs have debasements. For their actual use we add contamination. Pollution can be added by first eliminating the carbon and adding one more iota instead of it. This is accomplished by tapping on the draw instrument and choosing the ideal component from component list.

The improved energy will be utilized to concentrate on various mechanical properties like security strength under rigidity and so on. Different CNTs were ready and their relating energies were improved. Further, iron, nickel and cobalt were added as contaminations at various arrangements, for example, 0.5%, 1.0%, 1.5%, 2.0% and afterward again the examples were upgraded. For deserts, CNTs were noticed utilizing various sytheses of carbon, for example, one, two, three and four carbon molecules were absent from each CNT separately.

3.3.1 Molecular modelling

Carbon nanotubes are large molecules of the similar size structured in chemical bonding of nanotubes which are bound together by force of vander waals ,CNTs represents one of the most unique inventions, in field of nanotechnology. The diameter and length of a nanotube is taken in the order of a few nanometers. CNTs are categorized as single-walled nanotubes (SWNTs) as shows the Fig 6, SWCNTs of length 10 nm and diameter 4 nm with chirality (6, 6) has been created on Avogadro software.

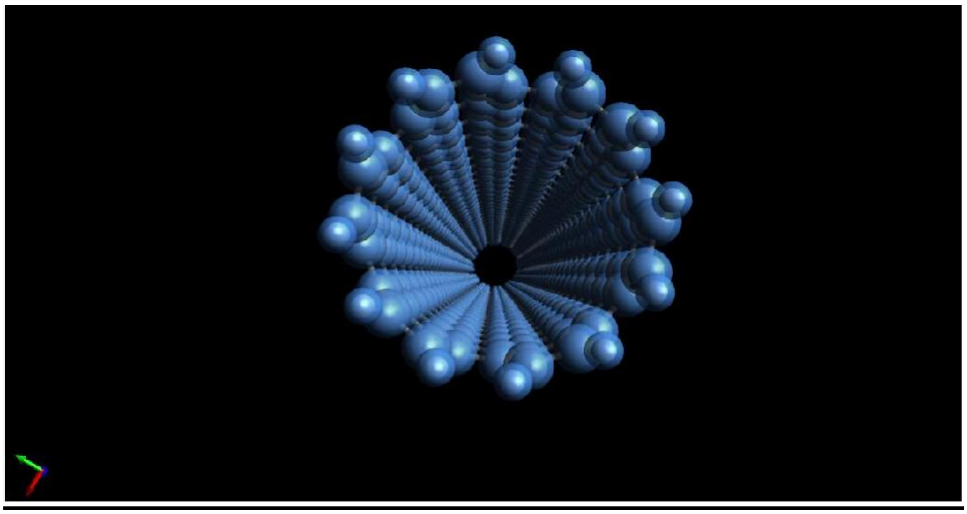

Fig 6. Molecular simulation of a Single walled carbon nanotube (SWCNT) using Avogadro software

3.3.2 CNTs created

For carrying out the calculations, CNTs made on Avogadro as shown in figures.

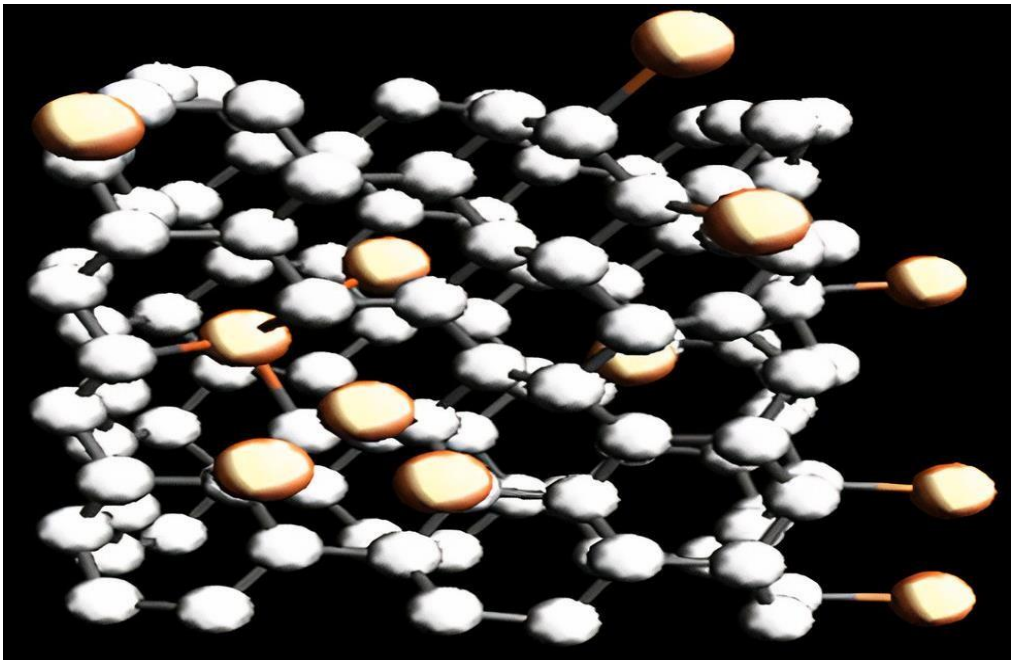

Fig 7. SWCNT with 1% iron doped impurity.

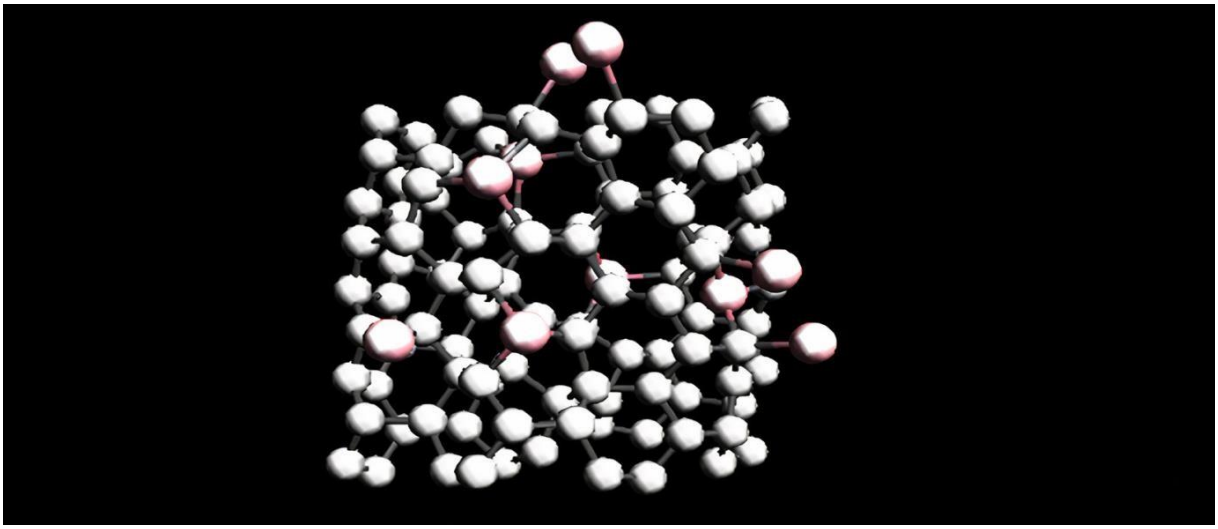

Fig 8. SWCNT with 1% Cobalt doped impurity.

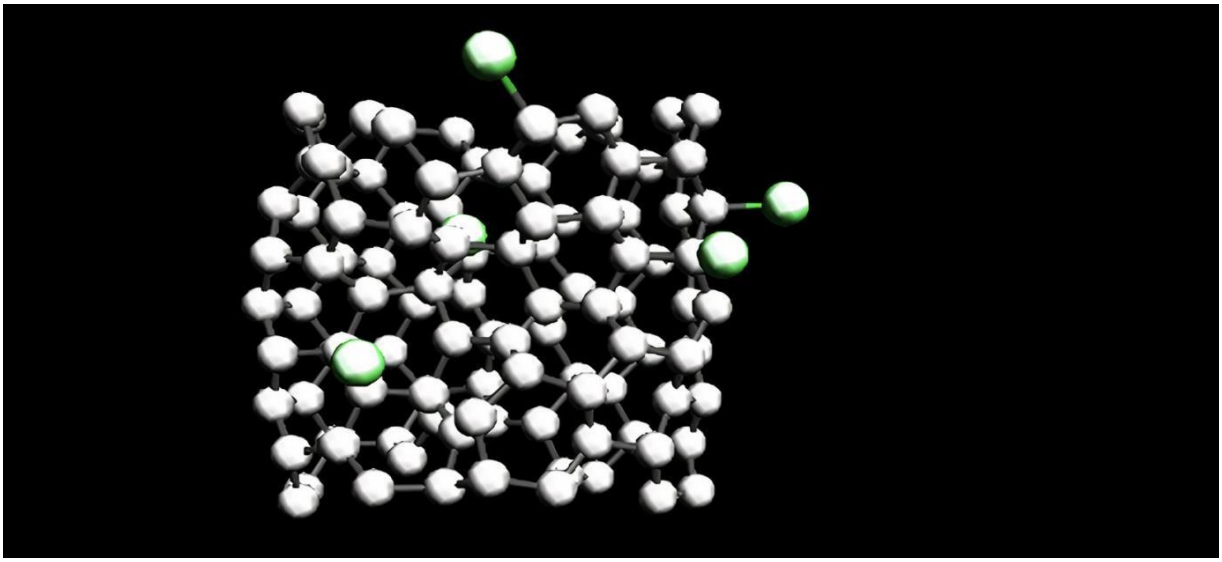

Fig 9. SWCNT with 1% Nickel doped impurity.

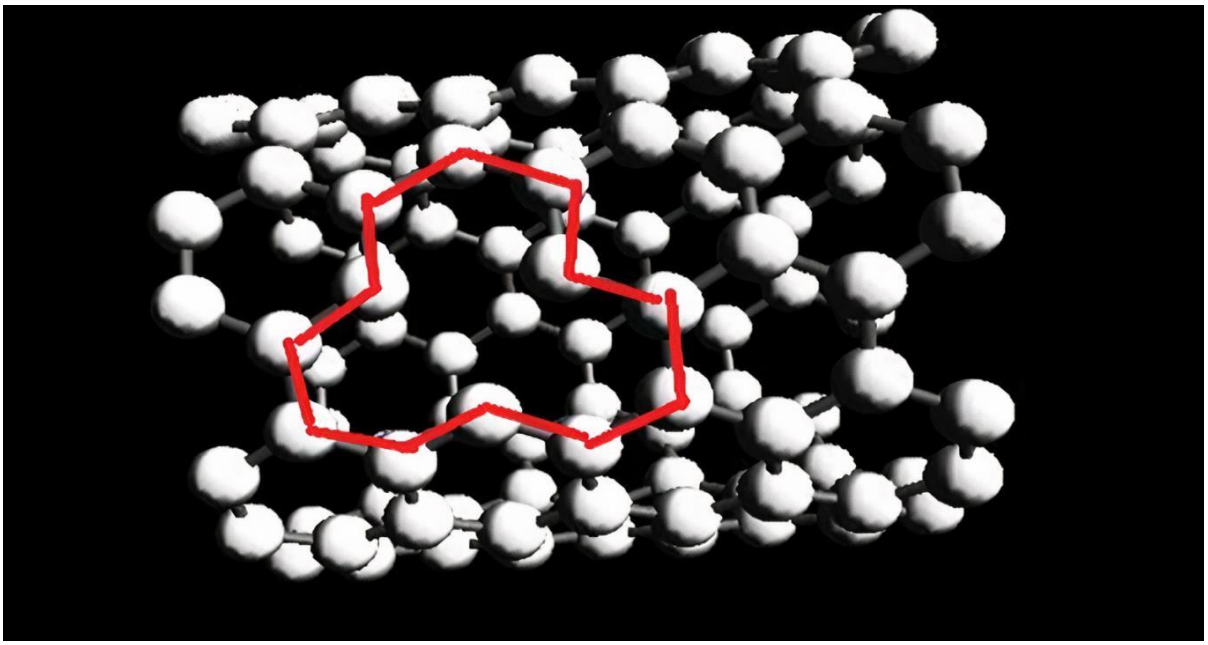

Fig 10. SWCNT with 1 carbon missing defect.

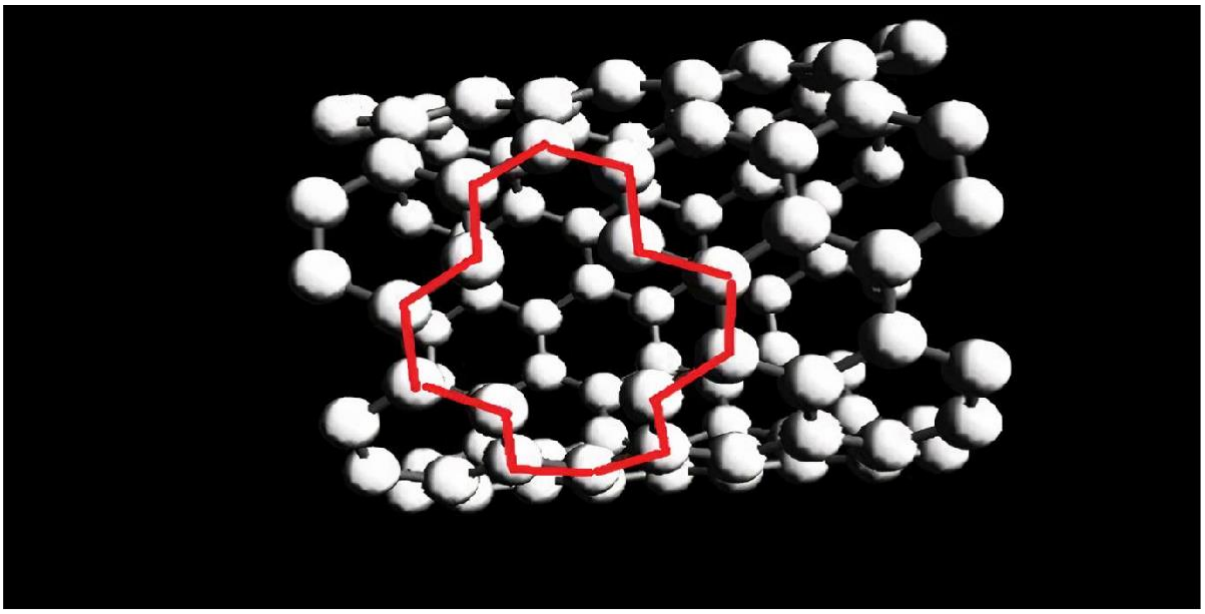

Fig 11. SWCNT with 2 carbons missing defect.

CHAPTER 4

LITERATURE REVIEW

4.1 Effect of impurities

Cuicui Ge, 2012, reviewed that because of the presence of extensive amounts of metallic and carbonaceous pollutions, the vital variable and component for the announced harmfulness of carbon nanotubes (CNTs) are indistinct. Here, we initially measure the commitment of metal deposits and fiber design to the poisonousness of CNTs. Huge amounts of metal particles could be activated from CNTs into encompassing liquids, contingent upon the properties and constituents of the natural microenvironment, as well as the properties of metal particles. Moreover, electron turn reverberation estimations affirm that hydroxyl revolutionaries can be created by both CNTs containing metal pollutions and corrosive leachable metals from CNTs. A few biomolecules work with the age of free revolutionaries, which may be because of the support of these biomolecules in redox cycling impacted by pH. Among a few significant metal buildups, Fe plays a basic part in creating hydroxyl revolutionaries, lessening cell reasonability and advancing intracellular responsive oxidative species. Cell suitability is profoundly subject to how much metal buildups and iron specifically, however not tube structure, while the adverse consequence of CNTs themselves on cell feasibility is extremely restricted in a specific fixation range under

80 μg ml−1. It is vital to deliberately comprehend how these exogenous and endogenous elements impact the harmfulness of CNTs to stay away from their unfortunate poisonousnes

4.2 Effect of vacancy defects

Keiichi Shirasu, 2021, reviewed that to apply carbon nanotubes (CNTs) as building up specialists in cutting edge composites, further developing their ostensible strength is fundamental. In any case, since it is hard to totally eliminate the imperfections, the combination rule for further developing ostensible strength is as yet hazy, i.e., the viable strength and the quantity of nanotube layers expected to further develop the ostensible strength has been sabotaged.

. In this review, sub-atomic elements reenactments were utilized to explain the impacts of opening on the mechanical properties of CNTs. Furthermore, the connections between the number of layers and compelling and ostensible qualities of CNTs were examined hypothetically. The presence of broad opening gives a potential clarification to the low ostensible qualities acquired in past exploratory estimations of CNTs. This study demonstrates that the ostensible strength can be expanded from the tentatively gotten upsides of 10 GPa to around 20 GPa by utilizing six to nine nanotube layers, regardless of whether the expansion in compelling strength of each layer is little. This enjoys upper hands over twofold walled CNTs, in light of the fact that the powerful strength of such CNTs should be around 60 GPa to accomplish an ostensible strength of 20 GPa.

Elvis G. Fefey, 2011, reviewed that most atomic elements (MD) recreations for single divider carbon nanotubes (SWCNT) depend on an amazing sub-atomic material design. The presence of opportunity absconds in SWCNTs could prompt deviations

from this ideal construction accordingly influencing the anticipated properties. The current paper researches the impact of carbon opening imperfections in the sub- atomic construction of SWCNT on the Young's modulus of the SWCNT utilizing MD reenactments performed by means of Accelrys and Materials Studio. The impact of the position of the imperfections in the nanotube ring and the impact of the quantity of deformities on the Young's modulus are considered. The examinations show that for an encased deformity with a similar shape in a SWCNT structure, its position caused no adjustment of the Young's modulus. Notwithstanding, as the quantity of imperfections expanded, the anticipated Young's modulus was found to diminish. For a 10 ring (6, 6) SWCNT, six opportunity surrenders (comparing to an imperfection level of 2.5%) decreased the Young's modulus by 13.7%

CHAPTER 5

RESULTS & DISCUSSION

Energy streamlining is done to figure the impacts of deformities and pollution, Optimization of energy under UFF technique for SWCNTs with opportunity deserts has been gotten.

Figure 12 shows that Optimization energy pursues a direction, for example its diminishing with expansion in no. of missing carbon iotas. Aside from CNT4, this shows position of deformities significantly affect enhancement energy. On expanding the deformities, the energy diminishes.

Figure 13 shows the variety of streamlining energy with expansion in level of contamination of various components the pollution added are copper, nickel and iron. Advancement energy is viewed as expanding with expanding doping. And furthermore the energy increments pointedly when CNTs have Co debasement. Energy increments gradually when CNTs have Fe debasement.

Table 1. Variation of Optimised energy with the number of missing carbon atoms.

Missing Carbon atoms from SWCNT	Optimised energy (KJ/mol)
1	3754.92
2	3554.25
3	3100.00
4	4781.73

Table 2. Variation of Optimised energy with percentage of impurity of different metals.

Metal impurity	Percentage of impurity	Optimised energy(KJ/mol)
Fe	0.5	3416.91
	1.0	4121.26
	1.5	4424.38
	2.0	4678.45
Co	0.5	2112.16
	1.0	3711.82
	1.5	5729.99
	2.0	11075.4
Ni	0.5	2735.67
	1.0	5927.74
	1.5	7281.34
	2.0	7325.38

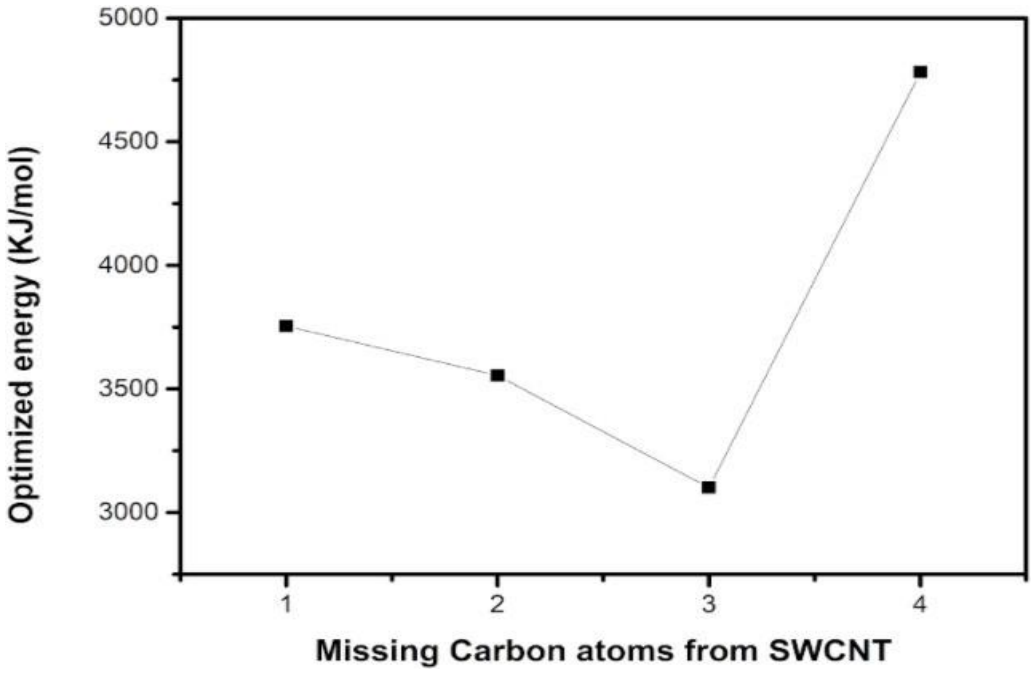

Fig 12. Graph showing variation of optimization energy w.r.t missing carbon atoms (defects)

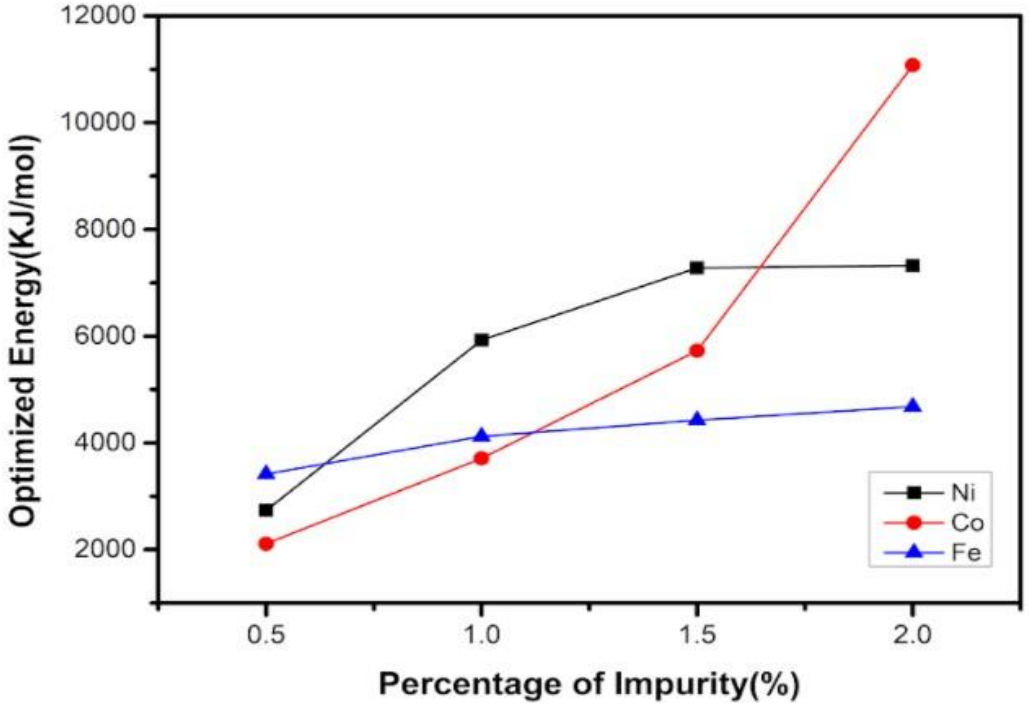

Fig 13. Graph showing variation of optimization energy w.r.t percentage of impurity

CHAPTER 6

CONCLUSION

Different CNTs were ready and streamlined with their particular contamination and deformities parts independently. Their comparing improvement energies were plotted against the level of separate debasements and imperfections. For every one of the metal debasements, the comparing enhancement energies are diminishing with expanding rates of pollution and it's diminishing with expansion in no. of missing carbon particles. The graphical portrayal of such a variety is displayed in Figureure 9 and Figureure 10, individually.

This streamlining energy can be useful in computing mechanical boundaries like YM, Stress and Strain, twisting capacity and so forth and utilizing boundaries, poisonousness of the CNTs can be determined which thus would be useful in tracking down the utilizations of these CNTs.

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RESEARCH PAPER

SINGLE-WALLED CARBON NANOTUBE AND EFFECT OF DEFECTS AND IMPURITIES

Vaibhav Gupta[A], Megha Prajapati[B] and Suresh C. Sharma*

[A,B] Department of Applied Physics, Delhi Technological University, Bawana Road, Delhi 110042, India.

ABSTRACT

The conventional approaches to assess the potential cytotoxic effects of nanomaterial's (NMs) rely mainly either on in-vitro or on in-vivo studies. Here, in this study we are trying to find out energy changes in Singled Walled Carbon Nanotube (SWCNTs) while having some defects and impurity elements which will be helpful in determining different other physical properties of SWCNT. Molecular dynamics (MD) simulations, Avogadro and Origin have been used, for the analysis of SWCNTs, which is considered to be ideal Molecular structure (Mol-structure). The presence of vacancy defects and impurities in SWCNTs could lead to deviation from their ideal behaviour and thus affecting the original properties.

Keywords: carbon nanotubes (CNT), Defects, Molecular dynamics (MD), Potential energy.

1. INTRODUCTION

A carbon nanotube (CNT) is a hexagonal array of Carbon-Carbon(C-C) bonded atoms shaped into a thin, long, hollow cylinder. Two type of CNTs that exist: Single Walled (SWCNTs) (Figure. 1(a)) and Multi walled (MWCNTs) nanotubes (Figure 1(b)). After the discovery of CNT in 1991 by Iijima[1] , CNTs found their potential applications in several industries like Aerospace engineering, electrical and electronic applications, air craft stress reduction, in-air purification and many more. A few of the rising technologies aim to utilize nanomaterials (NMs) as a new way to deliver molecular medicines and drugs into the cell which directly affect the affected parts (including cells) inside the body. CNTs are promising for clinical and biomedical sciences, especially in bio imaging, diagnosis and biosensors, although they also have reasonable harms. In cancer treatment, CNT have vast applications, hence can also be taken into work as an intracellular delivery unit for medical active freight .

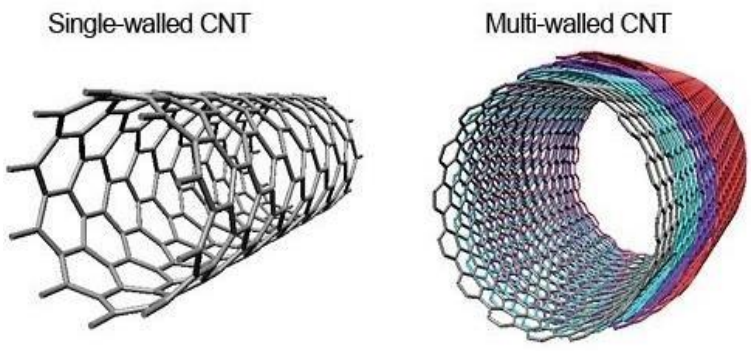

Figure 1. Different types of CNTs[4]

Despite of all valuable characteristics of CNTs, there are several issues linked to the toxicity of CNTs for there application in the treatment of disease and drug therapy [3]. Due to the large scale concentration of nano-sized tubes(NSTs) per given mass have toxological consequence when NSTs interrelate with cells and subcellular vital organs. Functional group, chirality and and surface structure are also major parameters of toxicity. Bunch

of properties of nanosized particles are because of respective vast surface area and tiny size. On increasing the surface to the atom are exponentially. On comparison to the larger particles, surface reactivity of nanosized particles rises causing higher biologic activity per given mass. There is potential to cause the toxicity in a nanosized particles[4]. Change in molecular arrangements, presence of vacancy defects in CNTs are known to be causes that changes the original behaviour and properties [5][6]. Failure stresses of CNTs is reduced approximately 26% with noticeably reduced failure strains even for one and two atom vacancy defects. It is observed experimentally that strength of the carbon nanotubes greatly reduced due to large holes, like those which are introduced by oxidative purification processes[7], [8]. Young's modulus(YM) of CNTs is a matter of substantial interest [9][10][11]. The computation of mechanical properties of CNTs may be classified into two categories. First is MD simulation using a potential energy(PE) function got by empirical, tight-binding [18] – [22]. The second method counts on the advancement of models based on molecular and continuum mechanics (cont. Mechanics). The behaviour of Nano scale fillers and their influence on mechanical characteristics are not fully described by continuum models. Predicting the properties of Nano composites can also be done using a method that combines MD and continuum mechanics. The physics of molecules at the Nano scale can be combined with the precision and pace of computation on larger length scales using a combination of molecular dynamics and continuum mechanics. As a result, it is widely used method for simulating CNT reinforced composites.

2. Molecular dynamics

Molecular dynamics (MD) modelling gives in summary the idea of dynamic individual motion of particle(or in our study, atoms) and structural developments as a function of time. MD has been the predominant computational outlook for estimating the mechanical properties and contaminated behaviour of CNTs. In this study, several SWCNT models with different vacancy defects and different concentration of impurity are added and their energy dependence, the effects of contamination on energy of the SWCNTs were investigated based on MDs method.

2.1 Universal Force – Fields (UFF) and Potential Energy(PE)

Non-stochastic MD re-enactment strategies inevitably based on Newton's second law, F=ma, where F is the force applied on atoms, m is the mass, a is speeding up. As from the force on every atom, acceleration on each atom can be found. Parameters like acceleration, velocity and position can be determined by the trajectories which are depicted by the eq^{ns} of motions. Average value of these parameters can be evaluated by the trajectories formed. Summation of bonding and non-bonding energies is the total PE, $U=U_{bonding} + U_{non\text{-}bonding}$. For CNTs, van-der-Waal forces are the non-bonding energies, which ordinarily have a frail effect on the mechanical properties among the other interrelations present in C-C interactions. Lennard-Jones PE functions are most often used in order to know about the Vann-der-waal forces[24].

$$U_{van\text{-}der\text{-}waal} = \sum\left(\frac{Aij}{rij} - \frac{Cij}{rij}\right) . \quad (1)$$

In above equations, A and C represent atom type subordinate constants. $r_{ij}=|r_{ij}|=|r_i r_j|$ gives the separation between two atoms, i and j, and r_i and r_j are the position vectors of i^{th} and j^{th} atom.

The prevailing portion of whole potential vitality, bonding vitality, may be an entirety of three diverse connections among atoms: bond extending, bond twisting, and bond torsion.

$$U_{bonded} = U_{bonded\text{-}stretch} + U_{angle\text{-}bend} + U_{torsion.} \quad (2)$$

Most frequently used PE functions are written as,

$$U_{bonded} = \sum K_s (rij - r)^2 \quad (3)$$

$$U_{angle\text{-}bend} = \sum K\theta(\theta - \theta o)^2 \quad (4)$$

$$U_{torsion} = \sum K\varphi(1 - \cos(t\varphi + \varphi o)) \quad (5)$$

Each term in above equation represents different parameters. r is equilibrium separation of the bond, K_s represents spring constant of stretching of bond, $K\theta$ represents force constant of bending, θo is rest angle for this bond, $K\varphi$ is force constant of torsion, φo represents the ideal bond phase and t is the periodicity of bond. By underlying the interaction of different carbon atoms with the quantum interaction of electron wave functions helped in finding the above written coefficients. In order to determine mutual interaction forces, program of gradient of potential energy will be our way out i.e. $F = -\nabla U$.

3. Morphology of SWCNTs

Periodic arrangements of C-C atoms having a lattice like structure with end caps like fullerene. For the honeycomb crystal lattice of Graphene, the number of unit vectors across two ways is decided by the integer's n and m. Chiral-vector in Figure. 2 identifies as (n,0) as zigzag and (n,n) as Armchair nanotubes indicates the sort of nanotube. Chiral vectors defines the structure of CNTs.

Atomistic construction of CNTs can be explained via Chiral Index. Chiral-vectors shown in Figure 2 state the different categories of nanotubes.

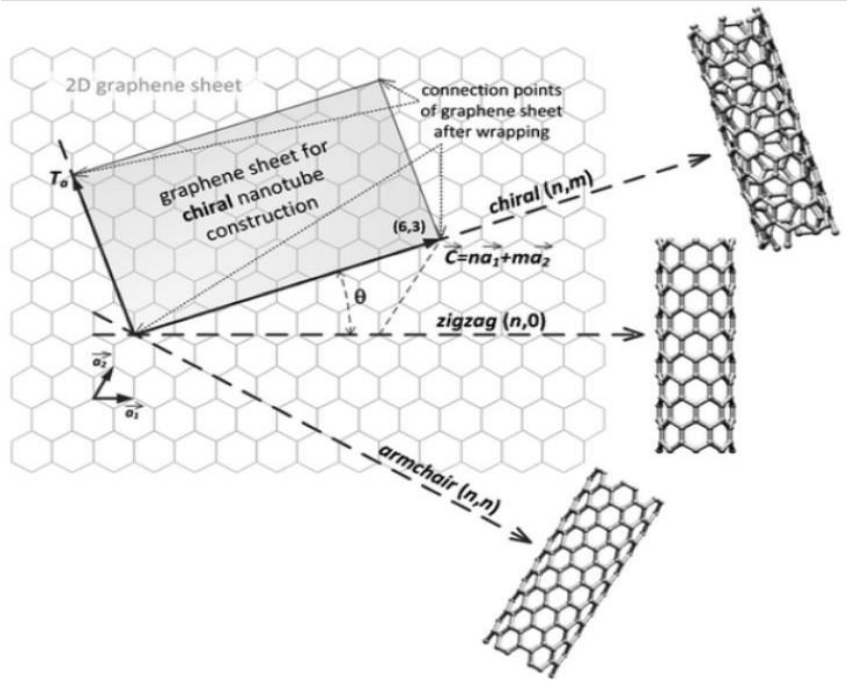

Figure 2. Construction of chiral CNT from graphene sheet[10]

As a general opinion, when n = 0, the CNTs are termed as Zigzag (Figure. 3(a)), and when n = m, the CNTs are termed as Armchair CNTs (Figure. 3(b)) and other state are called chiral (Figure. 3(c)) [25].

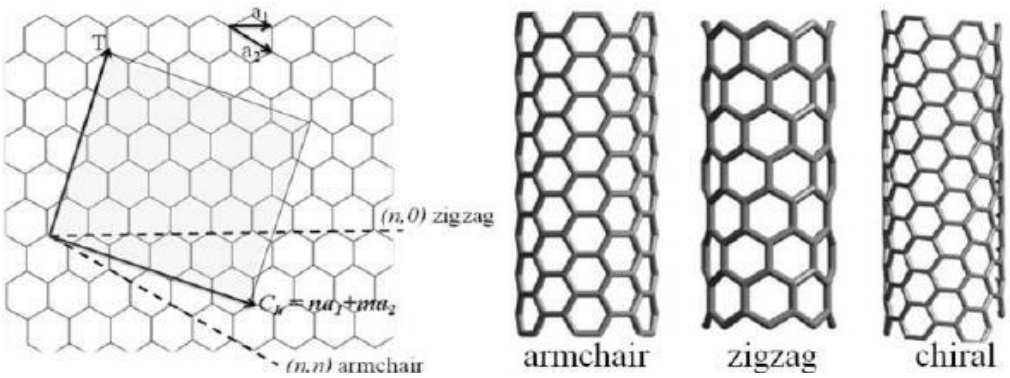

Figure 3. Armchair, zigzag and chiral types of nanotubes[6]

Each single divider nanotube is recorded by pair of integer(n,m) , comparing to a grid vector L = n*a_1 + m*a_2, where a_1, a_2 are the unit cell vectors of the graphite sheet. The nanotube radius is given by

$$r = a\sqrt{[3(n^2 + m^2 + nm)]}/2\pi \ , \qquad (6)$$

where a=1.53 A^o which is C-C bond-length.

4. Literature Review

The dynamic discrete particle motions and constructions are well detailed by Molecular dynamics (MD) modelling as a function of time [5] and thus serves as a good tool to examine the properties of a material system. There are various computational studies based on MD simulations and experimental studies have been done on Young's modulus of CNTs [17]. Some results of previous studies are shown in table 1 and in table 2.

Table 1. Showing some experimental data of previous studies

Name	**Method**	**Young's modulus**
Liu et al.[18]	Increasing diameter from 8 - 40 nanometer by measure resonance frequency of SWCNTs.	1-0.1 Tetra pascal
Krishnan et al.[15]	TEM to observe vibrations	0.90-1.7 Tetra pascal
Tombler et al.[19]	AFM to bend an SWCNT	1.2 Tetra pascal
Yu et al.[20]	Nano scale tensile investigation of SWCNT.	0.32-1.47 Tetra pascal
Demczyk et al. [21]	TEM to bend an individual MWCN tubes.	0.8-0.9 Tetra pascal

Table 2. Showing theoretical results of previous studies done

Name	Methods	Young' Modulus
Lu et al. [22]	empirical force-constant model	1 tetra pascal
Li et al.[23]	molecular structural mechanics method	1000-1100 Gigapascal
GPa Jin et al.[24]	MD and force-constant approach	1230-1245 GPa
Zhou et al.[25]	Young's modulus of SWCNTs	0.76 Tetra pascal
Vodenitcharova et al.[26]	Cont. Mechanics modelling	4.88etra pascal

4.1 Effect of impurity: CNTs when manufactured consists of some impurity. These impurities can be washed off by several methods but they can't be washed off perfectly. Some hints of impurities will remain intact. Presence of these impurities effects the mechanical properties (like YM) of CNTs. Presence of contaminants in CNTs develop the toxic effects, the amount of residual oxygen reactive metal present in CNT decides the toxicity factor. Depending on the mode of synthesis of CNTs, toxic metals that can be considered as contaminants as they are not welcomed in application of CNTs get added and alter their properties [30]. Impurities mainly consists of metals- Fe, Co, Mo and Ni all of which have reported the toxic effects[31], [32].

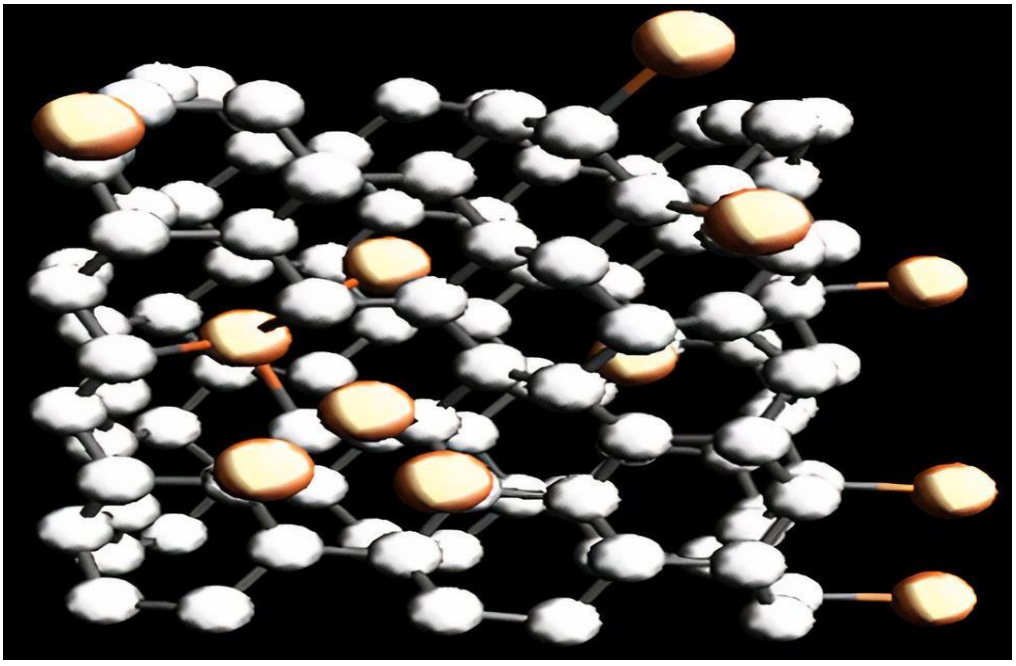

Figure 4. SWCNT with 1% iron doped impurity.

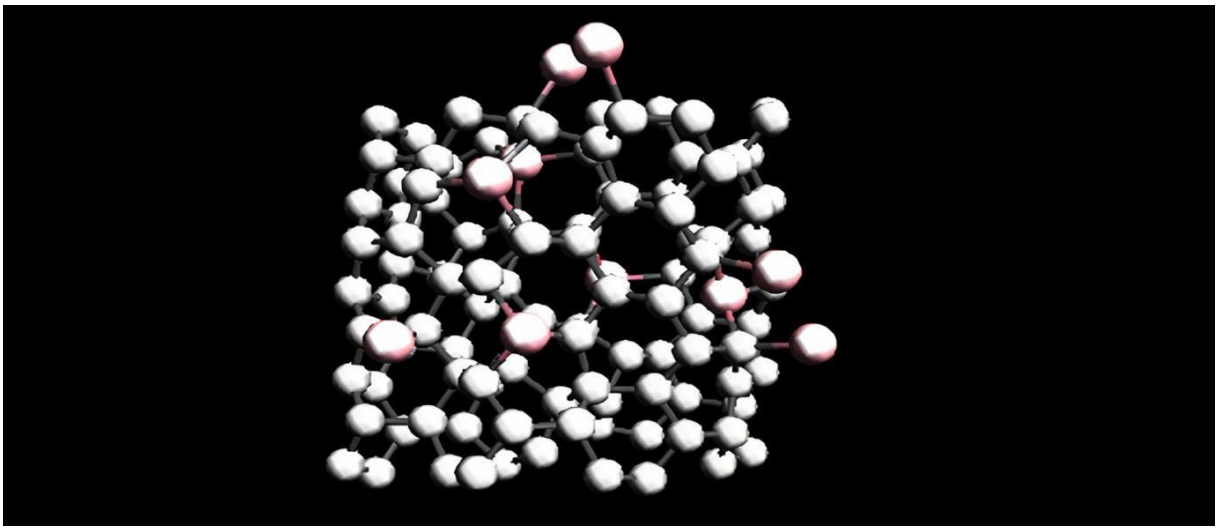

Figure 5. SWCNT with 1% Cobalt doped impurity.

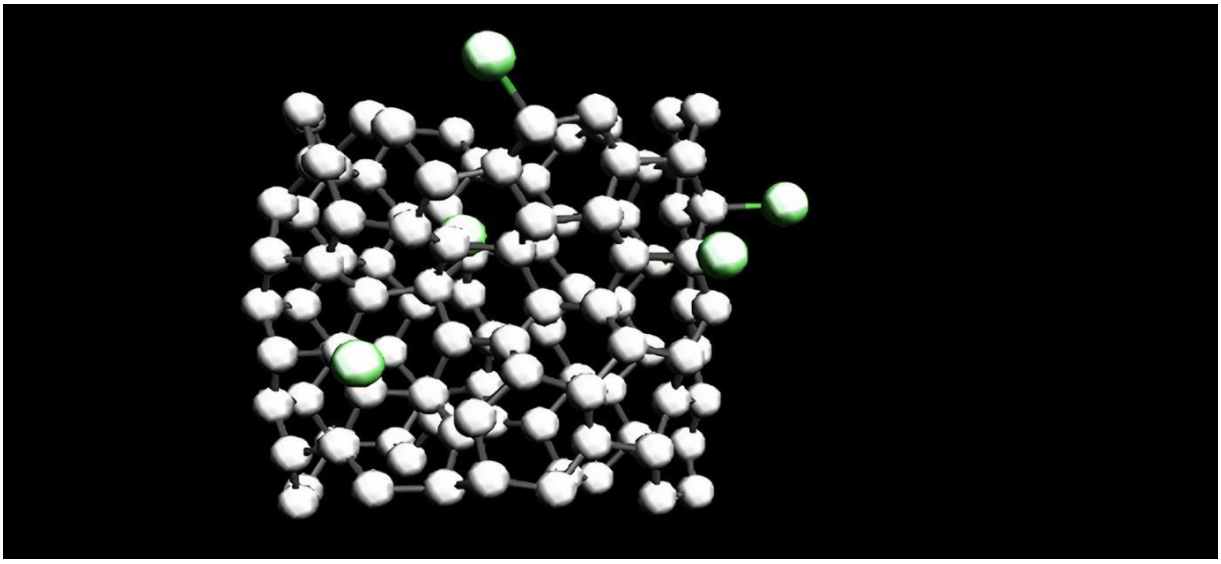

Figure 6. SWCNT with 1% Nickel doped impurity.

4.2 Effect of defects: The mechanical properties and the YM are affected due to the defects in CNTs. In fuel cells, CNTs with vacancy defects are perfect to be used as platinum carrier electrodes. Because of the vacant positions the adsorption at sites increases, hence binding energy increases. SWCNTs with deficiency always have larger binding energy than ideal SWCNTs, and the binding energy at carbon deficit positions are found to be approximately double of any other configuration. If the no. of carbon atoms were missing or the position of missing carbon atom, mechanical properties also show variations [29].

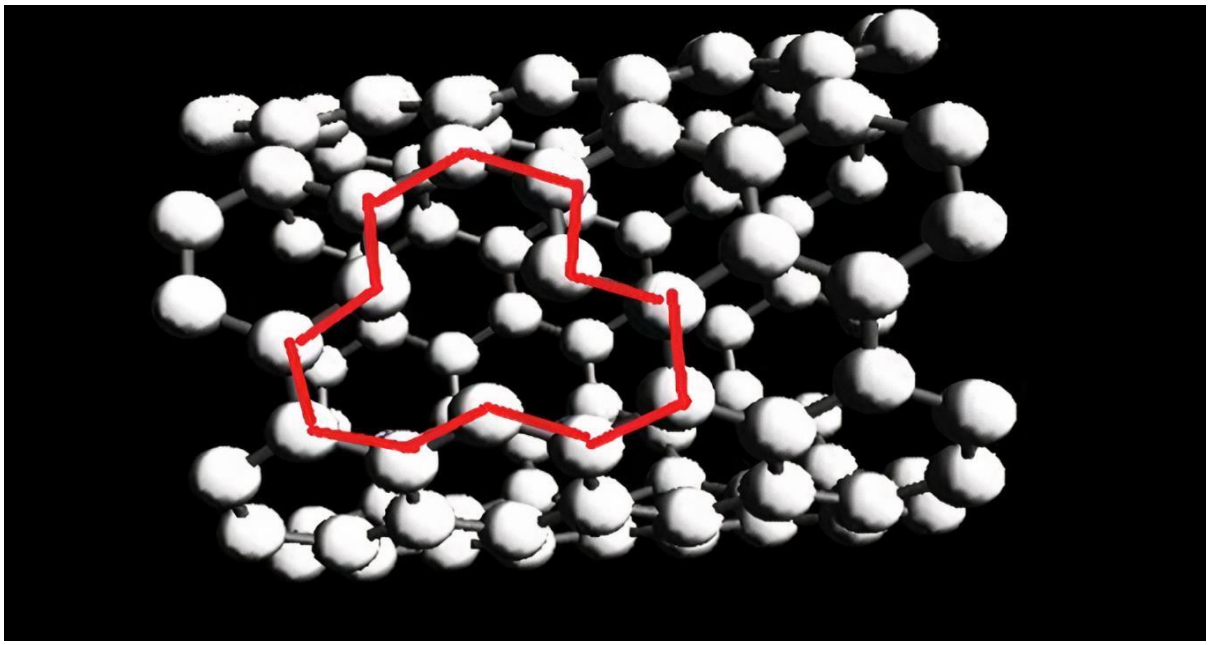

Figure 7. SWCNT with 1 carbon missing defect.

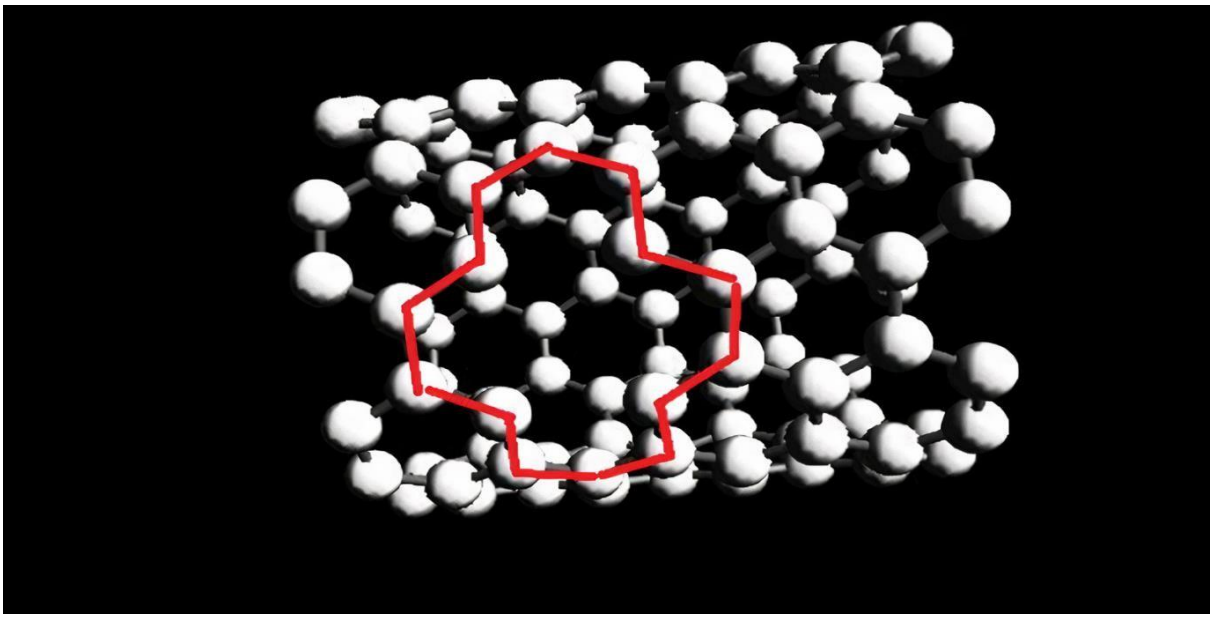

Figure 8. SWCNT with 2 carbons missing defect.

5. METHODOLOGY

This study mainly focuses on calculating energy in presence of impurities and in vacancy defects. Studies done on MD for predicting the Young's modulus has used several methods. Methods like empirical force- field

method, molecular structural mechanics method etc. Here we have used Universal force field (UFF) method (up to 4 folds) for computing the optimization energy. After opening Avogadro software, go to the build tab. A drop down menu will show Nanotube builder. On clicking this menu a window appears. In this menu, we have to put the required parameters we want for our SWCNT. Different tools are available for length, chirality, double bonds etc. Vacancy can be created by clicking on draw tool and select the atom and press delete the carbon we want to remove. CNTs when manufactured in labs have impurities. For their physical use we add impurity. Impurity can be added by first removing the carbon and adding another atom in place of it. This is achieved by clicking on the draw tool and selecting the desired element from element list.

The optimized energy will be used to study different mechanical properties like bond strength under tensile strength etc. Different CNTs were prepared and their corresponding energies were optimised. Further, iron, nickel and cobalt were added as impurities at different compositions such as 0.5%, 1.0%, 1.5%, 2.0% and then again the samples were optimised. For defects, CNTs were observed using different compositions of carbon such as one, two, three and four carbon atoms were missing from each CNT respectively.

5.1 Molecular modelling : Carbon nanotubes are large molecules of the similar size structured in chemical bonding of nanotubes which are bound together by force of vander waals ,CNTs represents one of the most unique inventions, in field of nanotechnology. The diameter and length of a nanotube is taken in the order of a few nanometers. CNTs are categorized as single-walled nanotubes (SWNTs) as shows the Figureure 9 ,SWCNTs of length 10 nm and diameter 4 nm with chirality (6, 6) has been created on Avogadro software.

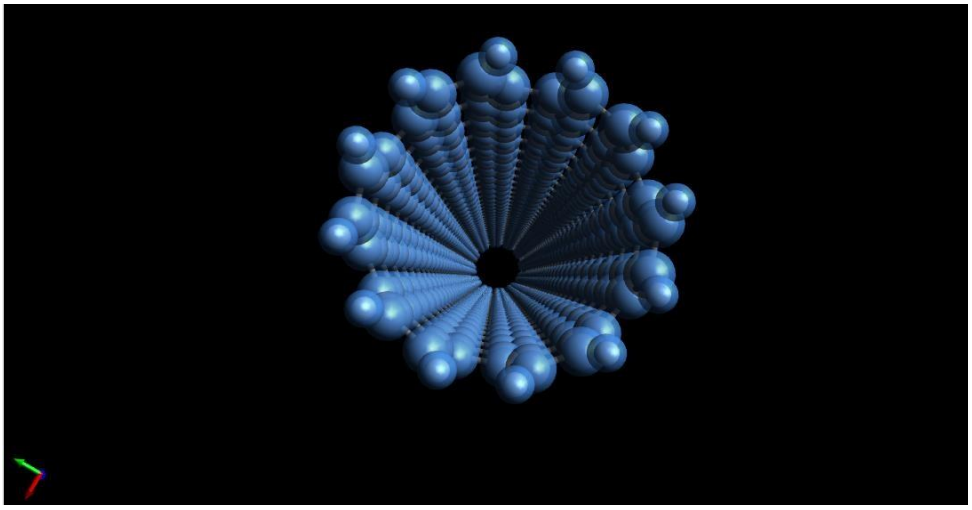

Figure 9. Molecular simulation of a Single walled carbon nanotube (SWCNT) using Avogadro software

6. RESULTS and DISCUSSION

Energy optimization is done to compute the effects of defects and impurity, Optimization of energy under UFF method for SWCNTs with vacancy defects has been obtained.

Figure. 10 shows that Optimization energy follows a trend, i.e. its decreasing with increase in no. of missing carbon atoms. Except for CNT4, this shows position of defects have effect on optimization energy. On increasing the defects, the energy decreases.

Figureure 11 shows the variation of optimization energy with increase in percentage of impurity of different elements the impurity added are copper, nickel and iron. Optimization energy is found to be increasing with increasing doping. And also the energy increases sharply when CNTs have Co impurity. Energy increases very slowly when CNTs have Fe impurity.

Table 3. Variation of Optimised energy with the number of missing carbon atoms.

Missing Carbon atoms from SWCNT	Optimised energy (KJ/mol)
1	3754.92
2	3554.25
3	3100.00
4	4781.73

Table 4. Variation of Optimised energy with percentage of impurity of different metals.

Metal impurity	Percentage of impurity	Optimised energy(KJ/mol)
Fe	0.5	3416.91
	1.0	4121.26
	1.5	4424.38
	2.0	4678.45
Co	0.5	2112.16
	1.0	3711.82
	1.5	5729.99
	2.0	11075.4
Ni	0.5	2735.67
	1.0	5927.74
	1.5	7281.34
	2.0	7325.38

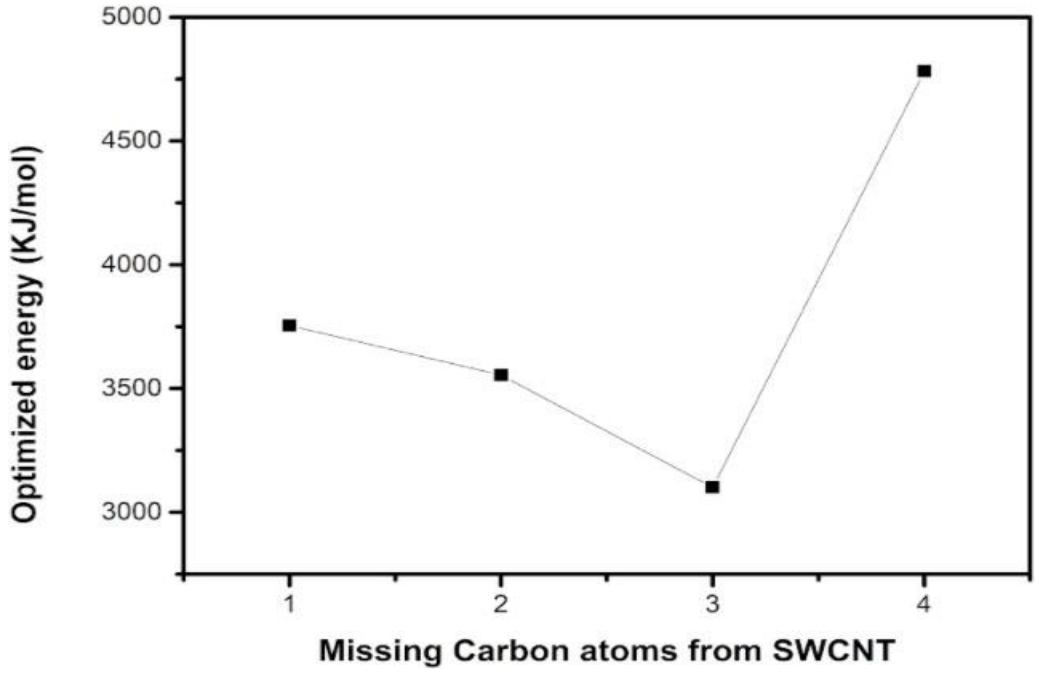

Figure 10. Graph showing variation of optimization energy w.r.t missing carbon atoms (defects)

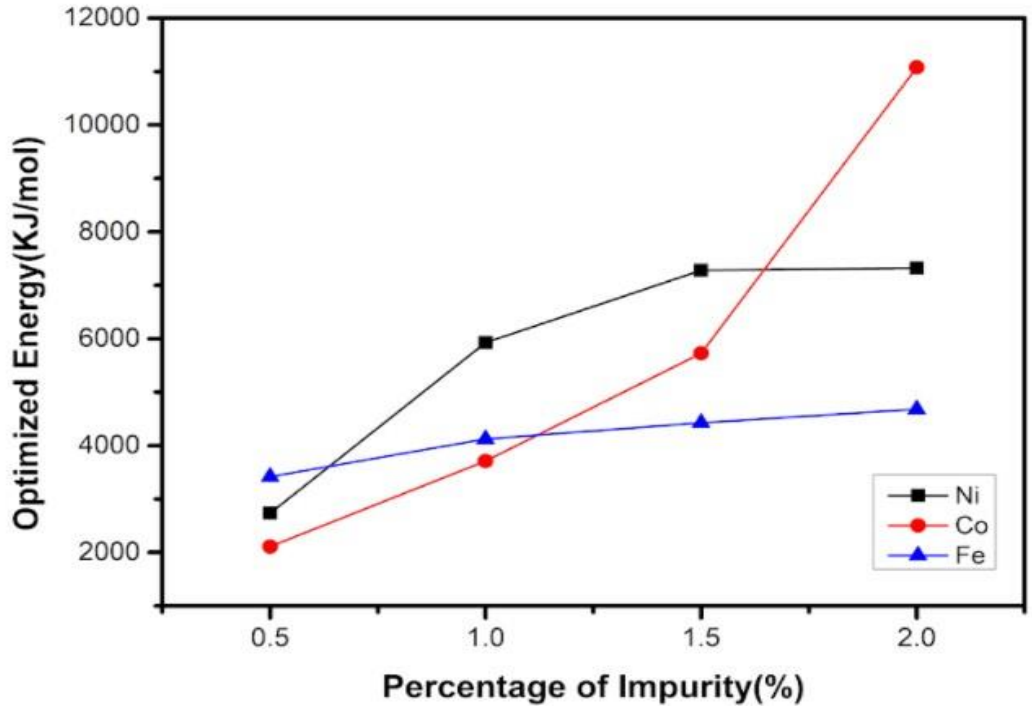

Figure 11. Graph showing variation of optimization energy w.r.t percentage of impurity

7. CONCLUSION

Different CNTs were prepared and optimised with their respective impurity and defects components separately. Their corresponding optimisation energies were plotted against the percentage of respective impurities and defects. For all the metal impurities, the corresponding optimisation energies are decreasing with increasing percentages of impurity and it's decreasing with increase in no. of missing carbon atoms. The graphical representation of such a variation is shown in Figureure 9 and Figureure 10, respectively.

This optimisation energy can be helpful in calculating mechanical parameters like YM, Stress and Strain, bending ability etc. and using parameters, toxicity of the CNTs can be calculated which in turn would be helpful in finding the applications of these CNTs.

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