A
Thesis Report

TO FIND THE OPTIMUM RESULTS FOR ENHANCING THE PROPERTIES OF CARBON NANOTUBES

Submitted in partial fulfillment of the requirement for the award of degree of

MASTER OF ENGINEERING

In

PRODUCTION AND INDUSTRIAL ENGINEERING

Submitted By

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CERTIFICATE

I hereby certify that the work which is being presented in this thesis entitled **"TO FIND THE OPTIMUM RESULTS FOR ENHANCING THE PROPERTIES OF CARBON NANOTUBES"** in partial fulfillment of requirement for the award of **Master's Degree in Production & Industrial Engineering** submitted in Mechanical Engineering Department, Thapar University, Patiala is an authentic record of the initial work carried out by me under the guidance of **Mr. Devender Kumar, Assistant Professor, Mechanical Engineering Department, Thapar University, Patiala.**

The matter embodied in this report has not been submitted in part or full to any other university or institute for the award of any degree.

Damanpreet Singh

Dated: 15/7/2012 **(Damanpreet Singh)**

This is to certify that above declaration made by the student concern is correct to the best of our knowledge & belief.

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ABSTRACT

This research is based on the link between molecular mechanics theory and solid mechanics theory through an analytical approach, investigating for the young's modulus of single-walled carbon nanotubes (SWCNT). The influence of diameter and chirality on the Young's modulus of SWCNT is also investigated. A SWCNT is considering as a continuum-shell model which is composed of the discrete molecular structures linked by the carbon-to-carbon bonds. The young's modulus is investigated for the SWCNT (both zig-zag and armchair) considering various parameters affecting it, in terms of the chiral indices (n, m). Based on the presented theory, it has been predicted that the optimum values of young's modulus for zig-zag lies in the range of (0.6346–1.0460 TPa) and for armchair, it lies in the range of (.5247–.9352 TPa). Also by varying the thickness of the SWCNT as 0.66 Å, the obtained values for the young's modulus lies in the range of (2.6734–.4027 TPa) for zig-zag. And for armchair, it lies in the range of (1.7504–.2366 TPa) respectively. Also, the effect of increasing temperature is investigated on the extreme points of nanotube's bond length. The theoretical prediction on elastic properties agreed reasonably with other existing experiment and theoretical results. The present formulas are able to serve as a good approximation of the young's modulus for SWCNTs.

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NOMENCLATURE

SYMBOLS	DESCRIPTIONS
CNTs	carbon nanotubes
SWNTs	single walled carbon nanotubes
DWNTs	double walled carbon nanotubes
MWNTs	multi walled carbon nanotubes
a_1,a_2	unit vectors of graphene
D_1	diameter of single walled carbon nanotubes
D_2	effective diameter of single walled carbon nanotubes
(b)	bond length
(t)	thickness
(n,m)	chiral indices
k_1	spring constant for axial deformation of carbon to carbon bonds
k_2	bending constant for angular distortion of bond angle
F_1, F_2	axial forces
M	bending moment
δ_{AB}^1	deformation of truss AB
δ_{AC}^1	deformation of truss AC
δ	deformation
$\Delta\theta$	angle variation
X_1, X_2	directions of axial force
σ_1, σ_2	tensile stresses
ϵ_1	strain in direction X1
E	young's modulus
T(k)	temperature in kelvin

CHAPTER 1

INTRODUCTION

1.1 Carbon Nanotubes:-

Carbon nanotubes(CNTs) are allotropes of carbon with a cylindrical nanostructure. Nanotubes have been constructed with length-to-diameter ratio of up to 132,000,000:1. These cylindrical carbon molecules have unusual properties, which are valuable for nanotechnology, electronics, optics and other fields of materials science and technology. In particular, owing to their extraordinary thermal conductivity and mechanical and electrical properties, carbon nanotubes find applications as additives to various structural materials. Nanotubes are members of the fullerene structural family, their name is derived from their long, hollow structure with the walls formed by one-atom-thick sheets of carbon known as graphene. These sheets are rolled at specific and discrete (chiral) angles, and the combination of the rolling angle and radius decides the nanotube properties. Nanotubes are categorized as single-walled nanotubes (SWNTs) and multi-walled nanotubes (MWNTs). Individual nanotubes naturally align themselves into "ropes" held together by vander Waal forces. Applied quantum chemistry, specifically, orbital hybridization best describes chemical bonding in nanotubes. These bonds, which are stronger than the sp3 bonds found in alkanes, provide nanotubes with their unique strength. One of the physical properties of carbon nanotubes is that it’s possible to make them only a single atomic layer thick. This means that they can be about 1/50,000th the thickness of a human hair. One of the interesting physical properties about carbon nanotubes is that when you have two of them which have slightly different physical structures and they are joined together, the junction (gap or small space) between them can function as an electronic device. Currently scientists are trying to make carbon nanotubes in large amounts (high yield) with a high degree of purity (little or no material defects), so that the physical structures are all the same. If they have similar physical and chemical properties then it becomes easier to predict their behavior. Since carbon nanotube science is relatively new, scientists from the fields of chemistry, physics and the material sciences are just beginning to unlock its mysteries and hypothesize about its potential applications.

1.2 Nanotube geometry:-

1.2.1 Armchair arrangement of carbon atoms:-

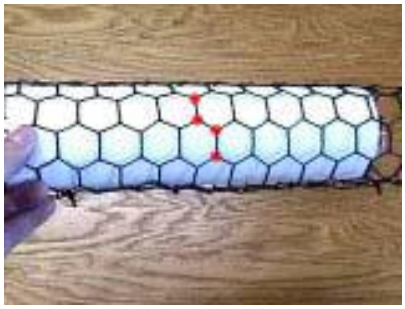

Fig.1(Armchair geometry)[19]

1.2.2 Zig-zag arrangement of carbon atoms:-

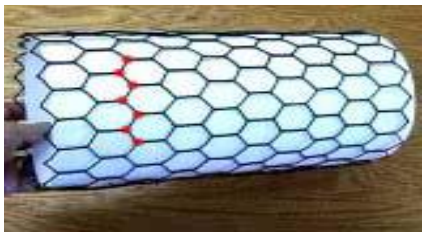

Fig.2(Zig– zag geometry)[19]

1.2.3 Chiral arrangement of carbon atoms:-

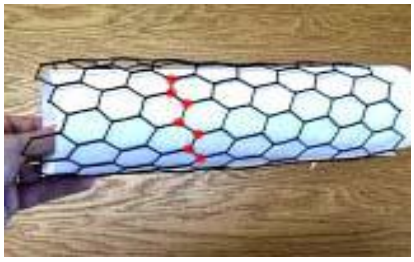

Fig.3(Chiral geometry)[19]

1.2.4 The armchair model:-

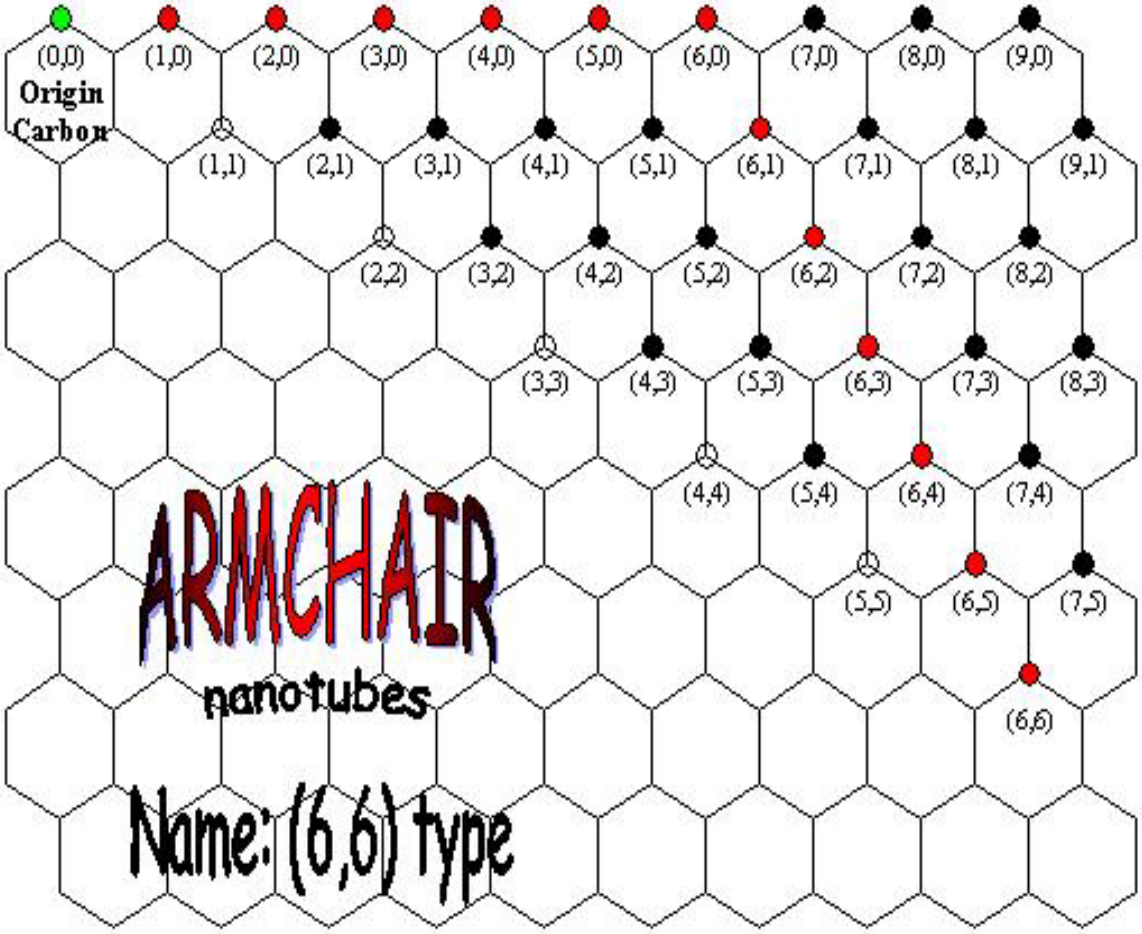

Fig.4 (zoom in for armchair)[19]

1.2.5 The zig-zag model:-

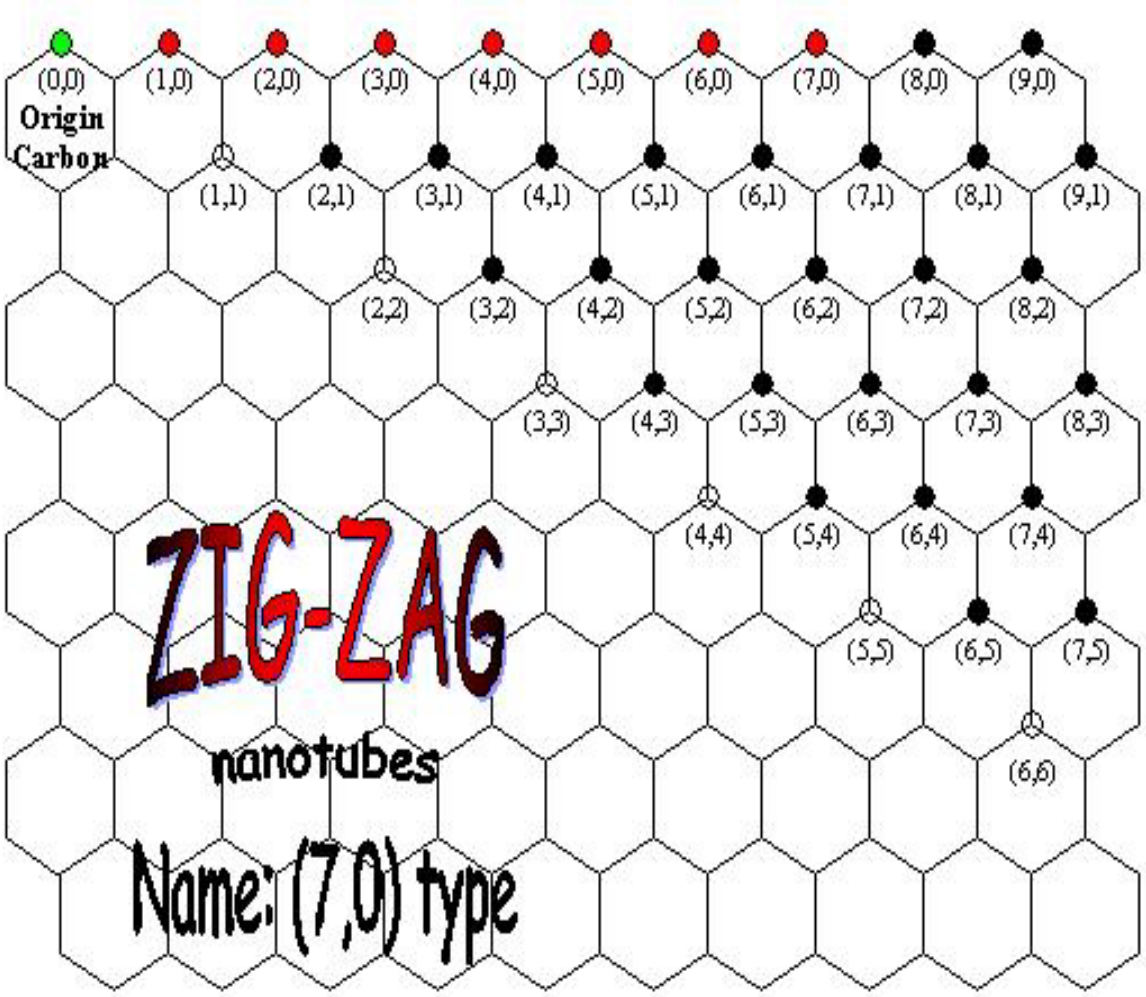

Fig.5 (zoom in for zig-zag)[19]

1.2.6 The chiral model:-

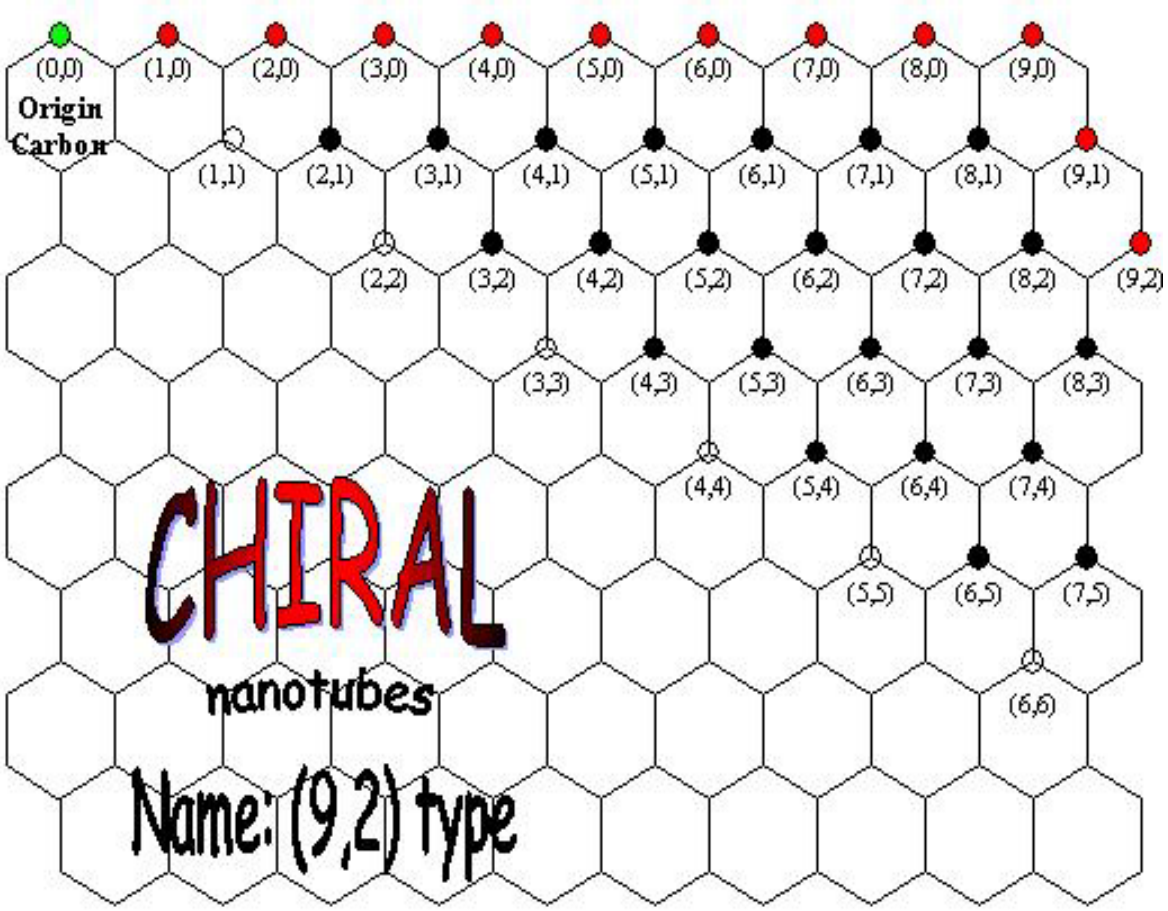

Fig.6 (zoom in for chiral)[19]

1.3 Types of carbon nanotubes and related structures:-

There is no consensus on some terms describing carbon nanotubes in scientific literature: both "-wall" and "-walled" are being used in combination with "single", "double", "triple" or "multi", for example, multi-walled carbon nanotube (MWNT).

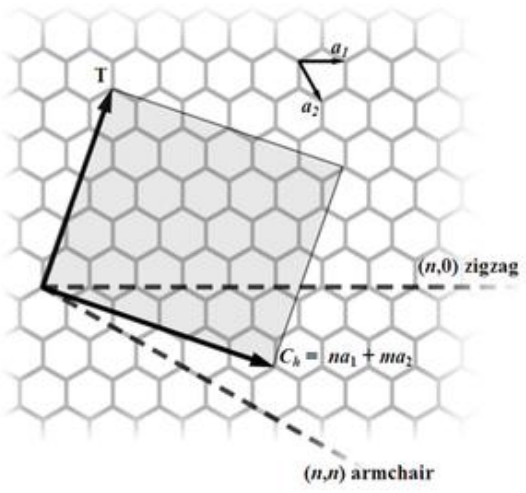

Fig.7 (3-D geometry of nanotubes)[18]

The (n,m) nanotube naming scheme can be thought of as a vector in an infinite graphene sheet that describes how to "roll up" the graphene sheet to make the nanotube. “T” denotes the tube axis, and a_1 and a_2 are the unit vectors of graphene in real space.

1.3.1 Single-walled nanotubes:

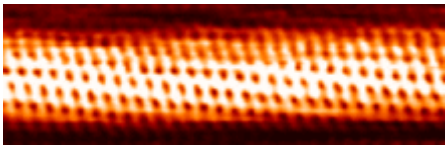

Fig.8 (Scanning tunneling microscopy image of single-walled carbon nanotube)[18]

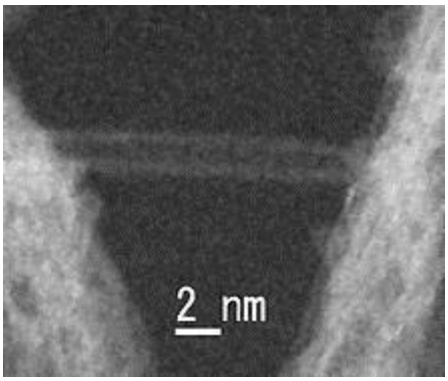

Fig.9 (Transmission electron microscopy image of a single-walled carbon nanotube)[18]

Most single-walled nanotubes (SWNT) have a diameter of close to 1 nanometer, with a tube length that can be many millions of times longer. The structure of a SWNT can be conceptualized by wrapping a one-atom-thick layer of graphite called graphene into a seamless cylinder. The way the graphene sheet is wrapped is represented by a pair of indices (n,m) . The integers n and m denote the number of unit vectors along two directions in the honeycomb crystal lattice of grapheme .If m = 0, the nanotubes are called zigzag nanotubes, and if n = m, the nanotubes are called armchair nanotubes. Otherwise, they are called chiral. The diameter of an ideal nanotube can be calculated from its (n,m) indices as follows:-

$$D_1 = \frac{\sqrt{3}b}{\pi}\sqrt{(n^2 + m^2 + mn)}$$

where (b) = 1.42 Å

1.3.2 Multi-walled:-

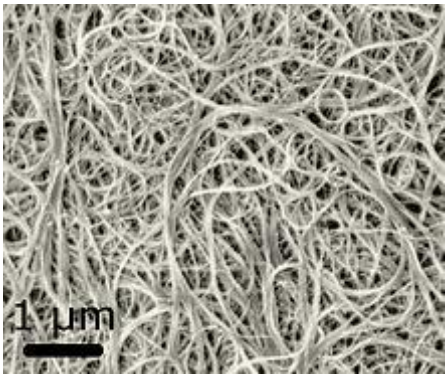

Fig.10 (Scanning electron microscopy image of carbon nanotubes bundles)[12]

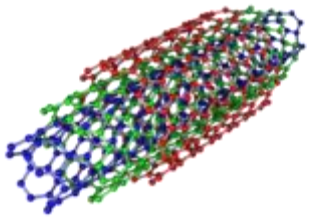

Fig.11 (Triple-walled armchair carbon nanotube)[12]

Multi-walled nanotubes (MWNT) consist of multiple rolled layers (concentric tubes) of graphite. There are two models that can be used to describe the structures of multi-walled nanotubes. In the Parchment model, a single sheet of graphite is rolled in around itself, resembling a scroll of parchment or a rolled newspaper. The interlayer distance in multi-walled nanotubes is close to the distance between graphene layers in graphite, approximately 3.4 Å. The Russian Doll structure is observed more commonly. Its individual shells can be described as SWNTs, which can be metallic or semiconducting. Because of statistical probability and restrictions on the relative diameters of the individual tubes, one of the shells, and thus the whole MWNT, is usually a zero-gap metal. Double-walled carbon nanotubes (DWNT) form a special class of nanotubes because their morphology and properties are similar to those of SWNT but their resistance to chemicals is significantly improved. This is especially important when functionalization is required (this means grafting of chemical functions at the surface of the nanotubes) to add new properties to the CNT.

1.3.3 Extreme carbon nanotubes:-

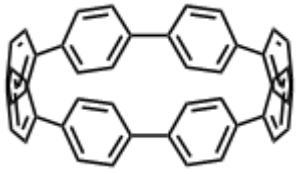
[3][4][5]

Fig.12 (Cycloparaphenylene)

The observation of the longest carbon nanotubes (18.5 cm long) was reported. These nanotubes were grown on Si substrates using an improved chemical vapor deposition method and represent electrically uniform arrays of single-walled carbon nanotubes[1]. The shortest

carbon nanotube is the organic compound cycloparaphenylene, which was synthesized in early 2009[3][4][5] The thinnest carbon nanotube is armchair (2,2) CNT with a diameter of 3 Å. This nanotube was grown inside a multi-walled carbon nanotube. Assigning of carbon nanotube type was done by combination of high-resolution transmission electron microscopy, Raman spectroscopy and density functional theory.[6]

1.4 Properties :

1.4.1 Strength: Carbon nanotubes are the strongest and stiffest materials yet discovered in terms of tensile strength and elastic modulus respectively. This strength results from the covalent sp2 bonds formed between the individual carbon atoms. In 2000, a multi-walled carbon nanotube was tested to have a tensile strength of 63 gigapascals (GPa).[7] Further studies, conducted in 2008, revealed that individual CNT shells have strengths of up to ~100 GPa, which is in good agreement with quantum/atomistic models[8]. Since carbon nanotubes have a low density for a solid of 1.3 to 1.4 g/cm3[9], its specific strength of up to 48,000 kN·m·kg−1 is the best of known materials, compared to high-carbon steel's 154 kN·m·kg−1. Under excessive tensile strain, the tubes will undergo plastic deformation, which means the deformation is permanent. This deformation begins at strains of approximately 5% and can increase the maximum strain the tubes undergo before fracture by releasing strain energy. Although the strength of individual CNT shells is extremely high, weak shear interactions between adjacent shells and tubes leads to significant reductions in the effective strength of multi-walled carbon nanotubes and carbon nanotube bundles down to only a few GPa's.[10] This limitation has been recently addressed by applying high-energy electron irradiation, which crosslinks inner shells and tubes, and effectively increases the strength of these materials to ~60 GPa for multi-walled carbon nanotubes[8] and ~17 GPa for double-walled carbon nanotube bundles.[10] CNTs are not nearly as strong under compression. Because of their hollow structure and high aspect ratio, they tend to undergo buckling when placed under compressive, torsional, or bending stress.[11]

1.4.2 Hardness: Standard single-walled carbon nanotubes can withstand a pressure up to 24GPa without deformation. They then undergo a transformation to super hard phase nanotubes. Maximum pressures measured using current experimental techniques are around 55GPa. However, these new super hard phase nanotubes collapse at an even higher pressure.The bulk modulus of super hard phase nanotubes is 462 to 546 GPa, even higher than that of diamond(420 GPa for single diamond crystal).

1.4.3 Kinetic: Multi-walled nanotubes are multiple concentric nanotubes precisely nested within one another. These exhibit a striking telescoping property whereby an inner nanotube core may slide, almost without friction, within its outer nanotube shell, thus creating an atomically perfect linear or rotational bearing. This is one of the first true examples of molecular nanotechnology, the precise positioning of atoms to create useful machines. Already, this property has been utilized to create the world's smallest rotational motor.[13] Future applications such as a gigahertz mechanical oscillator are also envisaged.

1.4.4 Electrical: Band structures computed using tight binding approximation for (6,0) CNT (zigzag, metallic) (10,2) CNT (semiconducting) and (10,10) CNT (armchair, metallic). Because of the symmetry and unique electronic structure of graphene, the structure of a nanotube strongly affects its electrical properties. For a given (n,m) nanotube, if n = m, the nanotube is metallic; if (n – m) is a multiple of 3, then the nanotube is semiconducting with a very small band gap, otherwise the nanotube is a moderate semiconductor. Thus all armchair (n = m) nanotubes are metallic, and nanotubes (6,4), (9,1), etc. are semiconducting. Thus, a (5,0) SWCNT that should be semiconducting in fact is metallic according to the calculations. Likewise, vice versa zigzag and chiral SWCNTs with small diameters that should be metallic have finite gap (armchair nanotubes remain metallic)[15], where for copper interconnects current densities are limited by electromigration. Multiwalled carbon nanotubes with interconnected inner shells show superconductivity with a relatively high transition temperature.[16]

1.4.5 Thermal: All nanotubes are expected to be very good thermal conductors along the tube, exhibiting a property known as "ballistic conduction", but good insulators laterally to the

tube axis. Measurements show that a SWNT has a room-temperature thermal conductivity along its axis.

1.4.6 One-dimensional transport: Because of the nano scale dimensions, electrons propagate only along the tube's axis and electron transport involves many quantum effects. Because of this, carbon nanotubes are frequently referred to as “one-dimensional”.

1.5 Applications:

1.5.1 AFM probe tips. Single-walled carbon nanotubes have been attached to the tip of an AFM probe to make the tip "sharper". This allows much higher atomic resolution of the surface under investigation. Also, the flexibility of the nanotube prevents damage to the sample surface and the probe tip if the probe tip happens to "crash" into the surface. A company started by Max Legally that attaches carbon nanotubes to AFM probes for the purpose of increased resolution as well as decreased wear on sample and probe tip.

1.5.2 Flat panel display screens. When a nanotube is put into an electric field, it will emit electrons from the end of the nanotube like a small cannon. If those electrons are allowed to bombard a phosphor screen then an image can be created. Several companies are using this technology to replace the bulky electron guns of conventional television sets with these significantly smaller carbon nanotube electron guns. When scientists instead use millions of carbon nanotubes as tiny electron guns, the required dimensions change and the creation of a flat panel display (that can hang on your wall) becomes possible. In fact, some advertising billboards have already been made and are being used.

1.5.3 Hydrogen storage. When oxygen and hydrogen react in a fuel cell, electricity is produced and water is formed as a byproduct. If industry wants to make a hydrogen-oxygen fuel cell, scientists and engineers must find a safe way to store hydrogen gas needed for the fuel cell. Carbon nanotubes may be a viable option. Carbon nanotubes are able to store hydrogen and could provide the safe.

1.5.4 Actuators/Artificial muscles. An actuator is a device that can induce motion. In the case of a carbon nanotube actuator, electrical energy is converted to mechanical energy

causing the nanotubes to move. Two small pieces of "Bucky paper" paper made from carbon nanotubes, are put on either side of a piece of double-sided tape and attached to either a positive or a negative electrode. When current is applied and electrons are pumped into one piece of Bucky paper and the nanotubes on that side expand causing the tape to curl in one direction. This has been called an artificial muscle, and it can produce 50 to 100 times the force of a human muscle the same size. Applications include: robotics.

1.5.5 Nanoscale electronics/nanocomputing. Scientists have exploited the mechanical and electrical properties of carbon nanotubes to produce molecular electronic devices. When nanotubes are placed in a grid, the intersections of the nanotubes become bits of information that can be stored non-volatilely. Semiconducting nanotubes also can be used as single molecule transistors.

1.5.6 Nanothermometer. A carbon nanotube can be partially filled with gallium metal. When the temperature is changed, the gallium metal expands or contracts to fill or empty the carbon nanotube. The gallium level in the carbon nanotube varies almost linearly with temperature.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction: The research in the area of carbon nanotubes has increased tremendously in last few years. A brief review of research is concerned with predicting the optimum results for enhancing the properties of carbon nanotubes.

Toshiaki Natsuki *et al*.**[21]** presented a review for prediction of elastic properties for single-walled carbon nanotubes. A SWNT is regarded as a continuum-shell model which is composed of the discrete molecular structures linked by the carbon-to-carbon bonds. The elastic properties were investigated for the SWNTs as a function of the nanotube size. The theoretical prediction on elastic properties agreed reasonably with the existing experiment and theoretical results.

Antonio, Guilherme *et al*.**[22]** presented a review for molecular mechanics applied to single-walled carbon nanotubes .Single-walled carbon nanotubes, with stiffness of 1.0 TPa and strength of 60 GPa, are a natural choice for high strength materials. A problem, however, arises when experimental data are compiled. The large variability of experimental data leads to the development of numerical models denominated molecular mechanics, which is a "symbiotic" association of molecular dynamics and solid mechanics. This paper deals with molecular mechanics simulations of single-walled carbon nanotubes. To be able to evaluate the molecular mechanics model, the three major carbon nanotube configurations (armchair, zigzag and chiral) were simulated. It was proven that the carbon nanotube configuration has influence on stiffness. By varying the radius, hence the curvature, the Young's modulus changed from 0.95 TPa to 5.5 TPa. The numerical simulations were in good agreement with those presented in the literature.

L Boldrin *et al*.**[23]** presented a review for effective mechanical properties of hexagonal boron nitride nanosheets. They propose an analytical formulation to extract from energy equivalence principles the equivalent thickness and in-plane mechanical properties (tensile and shear rigidity, and Poisson's ratio) of hexagonal boron nitride nanosheets. The model developed provides not only very good agreement with existing data available in the open literature from experimental, density functional theory (DFT) and molecular dynamics (MD) simulations, but also highlights the specific deformation mechanisms existing in boron nitride sheets, and their difference with carbon-based graphitic systems.

Michele Meo *et al*.**[24]** presented a review for prediction of Young's modulus of single wall carbon nanotubes by molecular-mechanics based finite element modeling. The aim of this paper is to propose a Single Walled Carbon Nanotube (SWCNT) finite element (FE) model, based on the use of nonlinear and torsional spring elements, to evaluate its mechanical properties. The choice of the spring elements to build the FE model, was based on the observation that other elements as beam, truss or shell are not very applicable because of the complex interaction of many atoms and the absence of rotational degrees of freedom. Moreover, it was also possible to model the bond interaction without introducing any non-physical variable, such as area and inertia of atoms linkage when using beam elements.With the proposed model, the influence of tube diameter and chirality on the Young's modulus of SWCNTs was investigated. In particular, armchair, zig-zag and chiral nanotubes, with different size, were tested under uniaxial load.The results show that good agreement was achieved with existing experimental results. The presented results demonstrate that the proposed FE model may also provide a valuable numerical tool for the prediction of the strength behaviour of single walled carbon nanotubes.

Jin-Liang *et al*.**[25]** presented a review for a comparative study of Young's modulus of single-walled carbon nanotube by CPMD, MD and first principle simulations. Carbon nanotubes(CNTs), due to their exceptional magnetic, electrical and mechanical properties, are promising candidates for several technical applications ranging from nanoelectronic devices to composites. Young's modulus holds the special status in material properties and micro/nano-electromechanical systems (MEMS/NEMS) design. The excellently regular

structures of CNTs facilitate accurate simulation of CNTs' behavior by applying a variety of theoretical methods. Here, three representative numerical methods, i.e., Car–Parrinello molecular dynamics (CPMD), density functional theory (DFT) and molecular dynamics (MD), were applied to calculate Young's modulus of single-walled carbon nanotube (SWCNT) with chirality (3,3). The comparative studies showed that the most accurate result is offered by time consuming DFT simulation. MD simulation produced a less accurate result due to neglecting electronic motions.

Y. Jin *et al*.**[26]** presented a review for simulation of elastic properties of single-walled carbon nanotubes. In this paper, selected effective elastic moduli of single-walled carbon nanotubes are simulated numerically. This effective macroscopic behavior is studied using molecular dynamics (MD) simulations in which the dynamic response and mutual force interaction among atoms of the nanostructures are obtained when subjected to small-strain deformation. Both force and energy approaches that link the behavior at the atomic and macroscopic scales of the nanotubes are used to predict the elastic moduli under different deformation modes. A comparison of the elastic constants obtained from MD simulation with available experimental data is made.

J. Cho *et al*.**[27]** presented a review for mechanical characterization of graphite/epoxy nano composites by multi-scale analysis. Mechanical properties of Nano composites consisting of epoxy matrix reinforced with randomly oriented graphite platelets were studied in conjunction with molecular mechanics. Elastic constants of graphite Nano platelets, which are the inclusion phase in the micromechanical model, were calculated based on their molecular force field. The calculated elastic constants compared well with both experimental data and other published theoretical predictions. The results of the micromechanical analysis, using the graphite platelet moduli calculated by molecular mechanics, were found to be insensitive to the variation of out-of plane modulus. The calculations confirm that the modulus of the Nano composites studied here is strongly dependent on the aspect ratio of the reinforcing particles, but not on their size. The predicted moduli compare favorably with experimental results of several Nano composites with graphite particles of various aspect ratios and size.

Kaveh Saffar *et al*.**[28]** presented a review for a Finite Element Model for estimating Young's Modulus of Carbon Nanotube Reinforced Composites Incorporating Elastic Cross-Links.The presence of chemical bonding between functionalized carbon nanotubes and matrix in carbon nanotube reinforced composites is modeled by elastic beam elements representing covalent bonding characteristics. Neglecting other reinforcing mechanisms in the composite such as relatively weak interatomic Van der Waals forces, this model shows close results to the Rule of Mixtures model's prediction for effective Young's modulus of a Representative Volume Element of composite for small volume fractions (~1%) and high aspect ratios (L/D>200) of CNT.

K.I. Tserpes *et al*.**[29]** presented a review for finite element modeling of single-walled carbon nanotubes. A three-dimensional finite element (FE) model for armchair, zigzag and chiral single-walled carbon nanotubes (SWCNTs) is proposed. The model development is based on the assumption that carbon nanotubes, when subjected to loading, behave like space-frame structures. The bonds between carbon atoms are considered as connecting load-carrying members, while the carbon atoms as joints of the members. To create the FE models, nodes are placed at the locations of carbon atoms and the bonds between them are modeled using three-dimensional elastic beam elements. The elastic moduli of beam elements are determined by using a linkage between molecular and continuum mechanics. In order to evaluate the FE model and demonstrate its performance, the influence of tube wall thickness, diameter and chirality on the elastic moduli (Young's modulus) of SWCNTs is investigated. The investigation includes armchair, zigzag and chiral SWCNTs. It is found that the choice of wall thickness significantly affects the calculation of Young's modulus. For the values of wall thickness used in the literature, the obtained values of Young's modulus agree very well with the corresponding theoretical results and many experimental measurements. Dependence of elastic moduli to diameter and chirality of the nanotubes is also obtained. The Young's modulus of chiral SWCNTs is found to be larger than that of armchair and zigzag SWCNT.

Xiaoxing Lu *et al*.**[30]** presented a review for mechanical property evaluation of single-walled carbon nanotubes by finite element modeling. Computational simulation for predicting mechanical properties of carbon nanotubes (CNTs) has been adopted as a powerful tool

relative to the experimental difficulty. Based on molecular mechanics, an improved 3D finite element (FE) model for armchair, zigzag and chiral single-walled carbon nanotubes (SWNTs) has been developed. The bending stiffness of the graphene layer has been considered. The potentials associated with the atomic interactions within a SWNT were evaluated by the strain energies of beam elements which serve as structural substitutions of covalent bonds. The out-of-plane deformation of the bonds was distinguished from the in-plane deformation by considering an elliptical cross-section for the beam elements. The elastic stiffness of graphene has been studied and the rolling energy per atom has been calculated through the analysis of rolling a graphene sheet into a SWNT to validate the proposed FE model. The effects of diameters and helicity on Young's modulus and the shear modulus of SWNTs were investigated. The simulation results from this work are comparable to both experimental tests and theoretical studies from the literatures.

Wendy D *et al*.**[31]** presented a review for a Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. And presented the derivation of a new molecular mechanical force field for simulating the structures, conformational energies, and interaction energies of proteins, nucleic acids, and many related organic molecules in condensed phases. This effective two-body force field is the successor to the Weiner, force field and was developed with some of the same philosophies, such as the use of a simple diagonal potential function and electrostatic potential fit atom centered charges. The new van der Waals parameters have been derived from liquid simulations and include hydrogen parameters which take into account the effects of any geminal electronegative atoms. The bonded parameters developed by Weiner, were modified as necessary to reproduce experimental vibrational frequencies and structures.

K.V. Zakharchenko *et al*.**[32]** presented a review for finite temperature lattice properties of graphene beyond the quasiharmonic approximation. The thermal and mechanical stability of graphene is important for many potential applications in nanotechnology. We calculate the temperature dependence of lattice parameter, elastic properties and heat capacity by means of atomistic Monte Carlo simulations that allow to go beyond the quasiharmonic approximation.

Junmei Wang *et al*.**[33]** presented a review for development and testing of a General Amber Force Field. We describe here a general Amber force field (GAFF) for organic molecules. GAFF is designed to be compatible with existing Amber force fields for proteins and nucleic acids and has parameters for most organic and pharmaceutical molecules that are composed of H, C, N, O, S, P and halogens. It uses a simple functional form and a limited number of atom types, but incorporates both empirical and heuristic models to estimate force constants and partial atomic charge.

Yeau-Ren *et al*.**[34]** presented a review for effects of temperature and vacancy defects on tensile deformation of single-walled carbon nanotubes. This study adopts the Tersoff–Brenner interaction potential function in a series of molecular dynamic (MD) simulations which investigate the mechanical properties under tensile loading of (10,0) zigzag, (8,3) chiral and (6,6) armchair single-walled carbon nanotubes (SWCNTs) of similar radii. The Young's modulus values of the (10,0), (8,3) and (6,6) nanotubes are determined to be approximately 0.92, 0.95, and 1.03 TPa, respectively. Of these nanotubes, the results reveal that the (6,6) nanotube possesses the best tensile strength and toughness properties under tension. Although it is noted that under small tensions, the mechanical properties such as Young's modulus are essentially insensitive to helicity, under larger plastic deformations, they may be influenced by helicity effects. Finally, the simulations demonstrate that the values of the majority of the considered mechanical properties decrease with increasing temperature and increasing vacancy percentage.

Toshiaki *et al*.**[35]** presented a review stress simulation of carbon nanotubes in tension and compression. Based on a continuum shell model, a structural mechanics approach is presented to simulate stress–strain behavior of carbon nanotubes (CNTs). The nanoscale continuum theory is established to directly incorporate the Morse potential function into the constitutive model of CNTs. According to the present model, the mechanical properties of both zigzag and armchair tubes are investigated. The result shows that the atomic structures of CNTs have a significant influence on the stress–strain behavior. The armchair zigzag tube exhibits larger stress–strain response than the zigzag tube under tensile loading, but its relationship turns over between the tension and compression deformations. The theoretical approach supplies a

set of very simple formulas and able be serve as a good approximation on the mechanical properties for CNTs.

T. Belytschko *et al*.**[36]** presented a review for effects of defects on the Strength of nanotubes: experimental-computational comparisons. The failure stresses and strains of nanotubes given by theoretical or numerical predictions are much higher than observed in experiments. We show that defects can explain part of this discrepancy: for an n-atom defect with 2 <=n<=8 , the range of failure stresses for a molecular mechanics calculation is found to be 36GPa to 64. This compares quite well with upper end of the experimental failure stresses, 11GPa to 63. The computed failure strains are 4% to 8%, whereas the experimental values are 2% to 13%. The under prediction of failure strains can be explained by the slippage that occurred in the experiments. The failure processes of nanotubes are clearly brittle in both the experiments and our calculations.

2.2 Gaps in literature:-

1. For single wall carbon nanotubes, different values of force constants are used in different research papers for calculating young's modulus, but no one had specified the range of constants or the finest value of the constants in order to predict the optimum value of young's modulus.
2. No temperature consideration was taken into account by most of the researchers in calculating young's modulus of single wall carbon nanotubes. However, the effect of temperature variation plays a significant role in finding the elastic properties of the carbon nanotubes.
3. It would also be interesting to see that the bond length and thickness are the important factor that needs to be studied very carefully for predicting the elastic properties of carbon nanotubes.

CHAPTER 3

3.1 PROBLEM FORMULATION:

After studying the various effects of parameters on the mechanical strength of nanotubes from various research papers mentioned in the study it is found that there is variation in the results obtained for the elastic properties of carbon nanotubes. The effort is to predict optimum value of young's modulus by examining certain parameters (force constants, temperature effects, bond length variation and thickness) which favors the conditions for enhancing the properties of nanotubes. The present investigation validates the majority of the predictions of simpler theories, and reveals the limits of their applicability.

PLAN (A):- Examining the effects of various force constants on the young's modulus of carbon nanotubes for obtaining the optimum values.

PLAN (B):- Examining the temperature variation effects on bond length extremities of carbon nanotubes for determining the young's modulus.

PLAN (C):- Evaluating the finest values of young's modulus by varying the thickness so that the properties can be improved.

3.2 Methodology:-

Based on a link between molecular and solid mechanics, an analytical method was approached for modeling the elastic properties of single-walled carbon nanotubes (SWNTs). The elastic properties were investigated for the SWNTs as a function of the nanotube size in terms of the chiral vector integers. The theoretical prediction on elastic properties agreed reasonably with the existing experiment and theoretical results. The present formulas are able to serve as a good approximation of the elastic properties for SWNTs.

3.2.1 Structure of carbon nanotube

A SWNT is formed by folding a single graphene sheet to form a hollow tube composed of carbon hexagons. The fundamental carbon nanotube is classified into three categories of zigzag, armchair and chiral in terms of the chiral vector integers(n,m). The symmetry groups of carbon nanotubes are denoted the zigzag nanotube (m=0) and armchair nanotube (n=m). The integers (n,m) uniquely determine the diameter of SWNT. The relationship between diameter(D_1) and the integers(n,m) is [21]

$$D_1 = \frac{\sqrt{3}b}{\pi}\sqrt{(n^2 + m^2 + mn)}$$

For the SWCNT, the bond length (b) is equal to 1.42 Å.

Considering the layer thickness(t), the effective diameter of SWNT(D_2), is given by

$$D_2 = \frac{\sqrt{3}b}{\pi}\sqrt{(n^2 + m^2 + mn)} + t$$

3.2.2 Theoretical approach:

A SWNT can be regarded as a two dimensional continuum-shell model which is composed of the discrete molecular structures linked by the carbon to carbon bonds. Fig.13 shows the unrolled graphene sheet of SWNTs subjected to axial tension in the Cartesian coordinate system. The molecular mechanics model is substituted with a frame structure model so as to form an equivalent-continuum model. Subsequently, the SWNT can be analyzed based on the solid mechanics theory. For the frame structure model, the spring constant (k_1) is used for modeling the axial deformation of the carbon-to-carbon bond, and the bending constant (k_2) for the angular distortion of the bond angles.

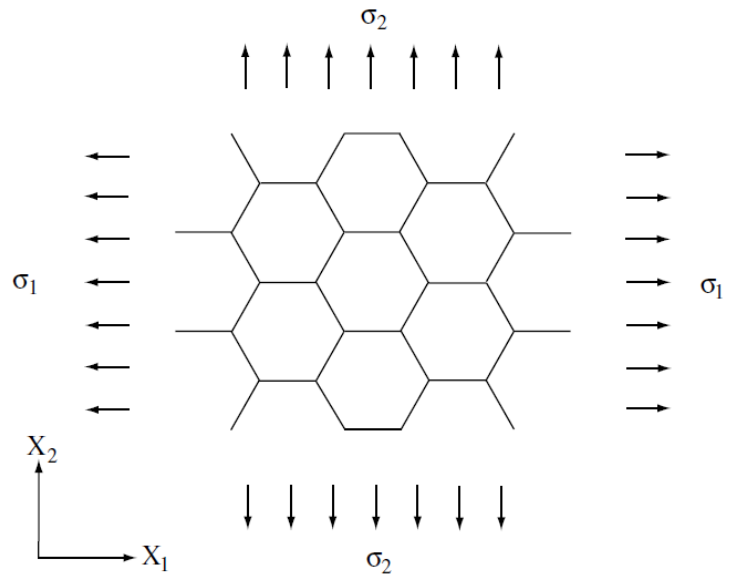

Fig.13 (The unrolled graphene sheet of SWNTs)[21]

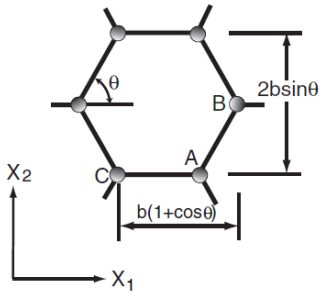

Fig.14 (Zoom in view of nanotube)

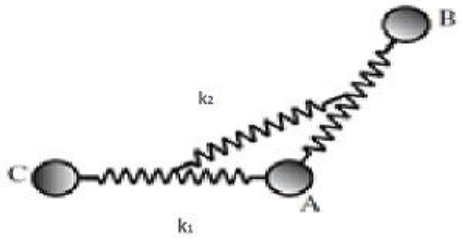

Fig.15 (Element of a frame structure model)[21]

3.2.3 Elastic modulus for the zigzag nanotube:

According to linear elastic theory, a superposition technique can be used to present a solution. For the zigzag tube, force and deformation of a truss of the framework are analyzed. The stretch and the angular deformation of the truss are caused by the axial force and the bending moment, respectively. Consider the force and the moment acting the Truss AB. When a SWNT rolled by graphene sheet is subjected to the tension stress,(σ_1) the force (F_1)and the moment (M) is given as

$$F_1 = \sigma_1 t b \sin\theta$$

$$M = M_1 + M_2 = F_1 b \sin\theta,$$

Based on the elastic theory, we obtain the equilibrium equations about extension and angle variation of the truss, given by

$$F_1 \cos\theta = \mathrm{k}_1 \delta^1_{AB}, \qquad 2F_1 = \mathrm{k}_1 \delta^1_{\mathrm{AC}},$$

$$\mathrm{M}_\mathrm{i} = \mathrm{k}_2 \Delta\theta + \mathrm{k}_2 (2\Delta\theta), \;\; \mathrm{i} = (\mathrm{a}, \mathrm{b})$$

where δ^1_{AB} and δ^1_{AC}, in above Eq. are the deformations of trusses. Each truss connects with other four trusses and associates with four bond angles. In above Eq., $\Delta\theta$ and $(2\Delta\theta)$ are the angle variations between Truss AB and the two nearest neighbor trusses. One of them has twice the angle variation of $\Delta\theta$ because of the symmetry of the hexagonal structure.

The strain in the direction of X_1 is defined as, respectively,

$$\epsilon_1 = \frac{\delta \sin\theta + \delta^1_{AB} cos\theta + \delta^1_{AC}}{\mathrm{b}(1 + \cos\theta)}$$

For a SWNT with the effective diameter (D_2), the elastic modulus of a zigzag nanotube can be given as

$$\mathrm{E}_1 = \frac{4\mathrm{D}_1 t}{\mathrm{D}_2^2} \left(\frac{\sigma_1}{\epsilon_1}\right)$$

where $\frac{\sigma_1}{\epsilon_1}$ is defined as Young's modulus of graphene sheet in the X-direction. Substituting values in above Eq., we obtain

$$\mathrm{E}_1 = \frac{24\mathrm{D}_1(1 + \cos\theta)}{\mathrm{D}_2^2 \sin\theta} \left[\frac{\mathrm{k}_1 \mathrm{k}_2}{\mathrm{b}^2 \mathrm{k}_1 \sin^2\theta + 6k_2(\cos^2\theta + 2)}\right]$$

Putting $\theta = \frac{\pi}{3}$, in above Eq.,

The elastic modulus for the zigzag nanotube as follows:-

$$E_1 = \frac{32\sqrt{3}\mathrm{D}_1}{D_2^2} \left[\frac{\mathrm{k}_1 k_2}{b^2 \mathrm{k}_1 + 18k_2}\right]$$

3.2.4 Elastic modulus for the armchair nanotube:-

For an armchair nanotube, the analysis approach is similar to those for a zigzag nanotube. The analysis of force and deformation of a truss. When a SWNT is subjected to the tension stress(σ_2), the force and the moment is given as

$$\mathrm{F}_2 = \sigma_2 tb(1 + cos\theta),$$
$$\mathrm{M} = \mathrm{M}_1 + \mathrm{M}_2 = \mathrm{F}_2 \mathrm{b}\cos\theta$$

The equilibrium equations about extension and angle variation of truss are given by

$$F_2 \sin\theta = \mathrm{k}_1 \delta_{AB}^1,$$
$$\mathrm{M}_\mathrm{i} = \mathrm{k}_2 \Delta\theta + \mathrm{k}_2(2\Delta\theta), \qquad (\mathrm{i} = \mathrm{A}, \mathrm{B})$$

The strain in the direction of X1 is defined as:-

$$\epsilon_1 = \frac{\delta_{\mathrm{AB}}^1 \cos\theta - \delta \sin\theta}{\mathrm{b}(1 + \cos\theta)}$$

Thus, the elastic modulus of an armchair nanotube can be given as follows:

$$\mathrm{E}_2 = \frac{24\mathrm{D}_1 \sin\theta}{\mathrm{D}_2^2\ (1 + \cos\theta)} \left[\frac{\mathrm{k}_1 k_2}{\mathrm{b}^2 \mathrm{k}_1 \cos^2\theta + 6k_2 \sin^2\theta}\right]$$

Putting $\theta = \frac{\pi}{3}$, in above Eq. the elastic modulus for the zigzag nanotube as follows:-

$$E_2 = \frac{32\sqrt{3}\mathrm{D}_1}{D_2^2} \left[\frac{\mathrm{k}_1 k_2}{b^2 \mathrm{k}_1 + 18k_2}\right]$$

CHAPTER 4

Analysis

It has been analyzed that there is variance in the parameters which results in differing the values of young's modulus of carbon nanotubes. Now, the various values of force constants have been analyzed to predict the optimum values of young's modulus. Also, the effect of increased temperature at the extreme points of bond length is also considered by examining various parameters (force constants, bond length variation and thickness) which favours the conditions for enhancing the properties of nanotubes.

STEP 1:- Analysis on the various force constants for evaluating the values young's modulus of carbon nanotubes has been done.

STEP 2:-Analysis on the extreme points of bond length with rising of temperature, in accordance with the best range of force constants. And also, by varying the thickness, the Young's Modulus has been obtained.

The units of different parameters used in the analysis are:-

1. diameter(D_1) in angstrom(Å)
2. effective diameter(D_2) in angstrom(Å)
3. thickness(t) in angstrom(Å)
4. bond length(b) in angstrom(Å)
5. k_1 in $\frac{\text{kcal}}{\text{mole Å}^2}$
6. k_2 in $\frac{\text{kcal}}{\text{mole}\,rad^2}$
7. E in terapascal (TPa)

Important conversions used in the analysis:-

1. 1 degree = 0.01745 radians
2. 1 TPa = 143.93 kcal $mole^{-1}Å^{-3}$
3. 10 Å = 1 nm
4. 1 kc = 4187 joules = 4187 Nm = kg $m^2\ s^{-2}$
5. 1 N/m = 1.43 kcal $mole^{-1}$ $Å^{-2}$

4.1 ZIG-ZAG (m, n=0) (k_1=634, k_2=126):-

Table 4.1 Summary of Young's modulus variation in accordance with $k_1 = 634$ & $k_2 = 126$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	0	3.916421	7.316421	634	126	0.634634
3.4	1.42	6	0	4.699705	8.099705	634	126	0.621389
3.4	1.42	7	0	5.482989	8.882989	634	126	0.602741
3.4	1.42	8	0	6.266273	9.666273	634	126	0.581732
3.4	1.42	9	0	7.049557	10.44956	634	126	0.560013
3.4	1.42	10	0	7.832841	11.23284	634	126	0.538483
3.4	1.42	11	0	8.616125	12.01613	634	126	0.517624
3.4	1.42	12	0	9.399409	12.79941	634	126	0.497682
3.4	1.42	13	0	10.18269	13.58269	634	126	0.478765
3.4	1.42	14	0	10.96598	14.36598	634	126	0.460902
3.4	1.42	15	0	11.74926	15.14926	634	126	0.444078
3.4	1.42	16	0	12.53255	15.93255	634	126	0.428253
3.4	1.42	17	0	13.31583	16.71583	634	126	0.413375
3.4	1.42	18	0	14.09911	17.49911	634	126	0.399385
3.4	1.42	19	0	14.8824	18.2824	634	126	0.386223
3.4	1.42	20	0	15.66568	19.06568	634	126	0.373832
3.4	1.42	21	0	16.44897	19.84897	634	126	0.362155
3.4	1.42	22	0	17.23225	20.63225	634	126	0.35114
3.4	1.42	23	0	18.01553	21.41553	634	126	0.340738
3.4	1.42	24	0	18.79882	22.19882	634	126	0.330904
3.4	1.42	25	0	19.5821	22.9821	634	126	0.321597
3.4	1.42	26	0	20.36539	23.76539	634	126	0.312777
3.4	1.42	27	0	21.14867	24.54867	634	126	0.30441
3.4	1.42	28	0	21.93196	25.33196	634	126	0.296464
3.4	1.42	29	0	22.71524	26.11524	634	126	0.288909
3.4	1.42	30	0	23.49852	26.89852	634	126	0.281718
3.4	1.42	31	0	24.28181	27.68181	634	126	0.274868
3.4	1.42	32	0	25.06509	28.46509	634	126	0.268334
3.4	1.42	33	0	25.84838	29.24838	634	126	0.262097
3.4	1.42	34	0	26.63166	30.03166	634	126	0.256136
3.4	1.42	35	0	27.41494	30.81494	634	126	0.250436
3.4	1.42	36	0	28.19823	31.59823	634	126	0.244979
3.4	1.42	37	0	28.98151	32.38151	634	126	0.23975
3.4	1.42	38	0	29.7648	33.1648	634	126	0.234736
3.4	1.42	39	0	30.54808	33.94808	634	126	0.229924
3.4	1.42	40	0	31.33136	34.73136	634	126	0.225303

4.2 ARM-CHAIR (m=n) (k_1=634, k_2=126):-

Table 4.2 Summary of Young's modulus variation in accordance with $k_1 = 634$ & $k_2 = 126$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	5	6.783439	10.18344	634	126	0.567404
3.4	1.42	6	6	8.140127	11.54013	634	126	0.530202
3.4	1.42	7	7	9.496815	12.89682	634	126	0.495273
3.4	1.42	8	8	10.8535	14.2535	634	126	0.463402
3.4	1.42	9	9	12.21019	15.61019	634	126	0.434648
3.4	1.42	10	10	13.56688	16.96688	634	126	0.408797
3.4	1.42	11	11	14.92357	18.32357	634	126	0.385553
3.4	1.42	12	12	16.28025	19.68025	634	126	0.364612
3.4	1.42	13	13	17.63694	21.03694	634	126	0.345692
3.4	1.42	14	14	18.99363	22.39363	634	126	0.328542
3.4	1.42	15	15	20.35032	23.75032	634	126	0.312942
3.4	1.42	16	16	21.70701	25.10701	634	126	0.298704
3.4	1.42	17	17	23.06369	26.46369	634	126	0.285667
3.4	1.42	18	18	24.42038	27.82038	634	126	0.273689
3.4	1.42	19	19	25.77707	29.17707	634	126	0.262653
3.4	1.42	20	20	27.13376	30.53376	634	126	0.252453
3.4	1.42	21	21	28.49045	31.89045	634	126	0.243002
3.4	1.42	22	22	29.84713	33.24713	634	126	0.234221
3.4	1.42	23	23	31.20382	34.60382	634	126	0.226043
3.4	1.42	24	24	32.56051	35.96051	634	126	0.218409
3.4	1.42	25	25	33.9172	37.3172	634	126	0.211268
3.4	1.42	26	26	35.27389	38.67389	634	126	0.204573
3.4	1.42	27	27	36.63057	40.03057	634	126	0.198286
3.4	1.42	28	28	37.98726	41.38726	634	126	0.19237
3.4	1.42	29	29	39.34395	42.74395	634	126	0.186793
3.4	1.42	30	30	40.70064	44.10064	634	126	0.181528
3.4	1.42	31	31	42.05732	45.45732	634	126	0.176549
3.4	1.42	32	32	43.41401	46.81401	634	126	0.171834
3.4	1.42	33	33	44.7707	48.1707	634	126	0.167363
3.4	1.42	34	34	46.12739	49.52739	634	126	0.163117
3.4	1.42	35	35	47.48408	50.88408	634	126	0.15908
3.4	1.42	36	36	48.84076	52.24076	634	126	0.155237
3.4	1.42	37	37	50.19745	53.59745	634	126	0.151574
3.4	1.42	38	38	51.55414	54.95414	634	126	0.148079
3.4	1.42	39	39	52.91083	56.31083	634	126	0.144741
3.4	1.42	40	40	54.26752	57.66752	634	126	0.14155

4.3 ZIG-ZAG (m, n=0) (k_1 =1140, k_2=126):-

Table 4.3 Summary of Young's modulus variation in accordance with $k_1 = 1140$ & $k_2 = 126$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	0	3.916421	7.316421	1140	126	0.886185
3.4	1.42	6	0	4.699705	8.099705	1140	126	0.86769
3.4	1.42	7	0	5.482989	8.882989	1140	126	0.84165
3.4	1.42	8	0	6.266273	9.666273	1140	126	0.812314
3.4	1.42	9	0	7.049557	10.44956	1140	126	0.781985
3.4	1.42	10	0	7.832841	11.23284	1140	126	0.751922
3.4	1.42	11	0	8.616125	12.01613	1140	126	0.722796
3.4	1.42	12	0	9.399409	12.79941	1140	126	0.69495
3.4	1.42	13	0	10.18269	13.58269	1140	126	0.668534
3.4	1.42	14	0	10.96598	14.36598	1140	126	0.64359
3.4	1.42	15	0	11.74926	15.14926	1140	126	0.620098
3.4	1.42	16	0	12.53255	15.93255	1140	126	0.598
3.4	1.42	17	0	13.31583	16.71583	1140	126	0.577225
3.4	1.42	18	0	14.09911	17.49911	1140	126	0.557689
3.4	1.42	19	0	14.8824	18.2824	1140	126	0.539311
3.4	1.42	20	0	15.66568	19.06568	1140	126	0.522008
3.4	1.42	21	0	16.44897	19.84897	1140	126	0.505703
3.4	1.42	22	0	17.23225	20.63225	1140	126	0.490322
3.4	1.42	23	0	18.01553	21.41553	1140	126	0.475797
3.4	1.42	24	0	18.79882	22.19882	1140	126	0.462065
3.4	1.42	25	0	19.5821	22.9821	1140	126	0.449068
3.4	1.42	26	0	20.36539	23.76539	1140	126	0.436753
3.4	1.42	27	0	21.14867	24.54867	1140	126	0.425069
3.4	1.42	28	0	21.93196	25.33196	1140	126	0.413973
3.4	1.42	29	0	22.71524	26.11524	1140	126	0.403424
3.4	1.42	30	0	23.49852	26.89852	1140	126	0.393384
3.4	1.42	31	0	24.28181	27.68181	1140	126	0.383817
3.4	1.42	32	0	25.06509	28.46509	1140	126	0.374694
3.4	1.42	33	0	25.84838	29.24838	1140	126	0.365984
3.4	1.42	34	0	26.63166	30.03166	1140	126	0.357661
3.4	1.42	35	0	27.41494	30.81494	1140	126	0.349701
3.4	1.42	36	0	28.19823	31.59823	1140	126	0.342081
3.4	1.42	37	0	28.98151	32.38151	1140	126	0.33478
3.4	1.42	38	0	29.7648	33.1648	1140	126	0.327779
3.4	1.42	39	0	30.54808	33.94808	1140	126	0.32106
3.4	1.42	40	0	31.33136	34.73136	1140	126	0.314607

4.4 ARMCHAIR (m=n) k_1=1140, k_2=126):-

Table 4.4 Summary of Young's modulus variation in accordance with $k_1 = 1140$ & $k_2 = 126$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	Ez(TPa)
3.4	1.42	5	5	6.783439	10.18344	1140	126	0.792307
3.4	1.42	6	6	8.140127	11.54013	1140	126	0.740359
3.4	1.42	7	7	9.496815	12.89682	1140	126	0.691585
3.4	1.42	8	8	10.8535	14.2535	1140	126	0.647082
3.4	1.42	9	9	12.21019	15.61019	1140	126	0.60693
3.4	1.42	10	10	13.56688	16.96688	1140	126	0.570832
3.4	1.42	11	11	14.92357	18.32357	1140	126	0.538375
3.4	1.42	12	12	16.28025	19.68025	1140	126	0.509134
3.4	1.42	13	13	17.63694	21.03694	1140	126	0.482715
3.4	1.42	14	14	18.99363	22.39363	1140	126	0.458766
3.4	1.42	15	15	20.35032	23.75032	1140	126	0.436983
3.4	1.42	16	16	21.70701	25.10701	1140	126	0.417102
3.4	1.42	17	17	23.06369	26.46369	1140	126	0.398897
3.4	1.42	18	18	24.42038	27.82038	1140	126	0.382172
3.4	1.42	19	19	25.77707	29.17707	1140	126	0.366761
3.4	1.42	20	20	27.13376	30.53376	1140	126	0.352519
3.4	1.42	21	21	28.49045	31.89045	1140	126	0.339321
3.4	1.42	22	22	29.84713	33.24713	1140	126	0.32706
3.4	1.42	23	23	31.20382	34.60382	1140	126	0.31564
3.4	1.42	24	24	32.56051	35.96051	1140	126	0.304981
3.4	1.42	25	25	33.9172	37.3172	1140	126	0.295008
3.4	1.42	26	26	35.27389	38.67389	1140	126	0.285661
3.4	1.42	27	27	36.63057	40.03057	1140	126	0.276881
3.4	1.42	28	28	37.98726	41.38726	1140	126	0.268619
3.4	1.42	29	29	39.34395	42.74395	1140	126	0.260832
3.4	1.42	30	30	40.70064	44.10064	1140	126	0.25348
3.4	1.42	31	31	42.05732	45.45732	1140	126	0.246528
3.4	1.42	32	32	43.41401	46.81401	1140	126	0.239944
3.4	1.42	33	33	44.7707	48.1707	1140	126	0.233701
3.4	1.42	34	34	46.12739	49.52739	1140	126	0.227772
3.4	1.42	35	35	47.48408	50.88408	1140	126	0.222135
3.4	1.42	36	36	48.84076	52.24076	1140	126	0.216768
3.4	1.42	37	37	50.19745	53.59745	1140	126	0.211654
3.4	1.42	38	38	51.55414	54.95414	1140	126	0.206774
3.4	1.42	39	39	52.91083	56.31083	1140	126	0.202113
3.4	1.42	40	40	54.26752	57.66752	1140	126	0.197656

4.5 ZIG-ZAG (m, n=0) (k_1= 938, k_2=126):-

Table 4.5 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 126$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	0	3.916421	7.316421	938	126	0.800563
3.4	1.42	6	0	4.699705	8.099705	938	126	0.783855
3.4	1.42	7	0	5.482989	8.882989	938	126	0.760331
3.4	1.42	8	0	6.266273	9.666273	938	126	0.733829
3.4	1.42	9	0	7.049557	10.44956	938	126	0.706431
3.4	1.42	10	0	7.832841	11.23284	938	126	0.679272
3.4	1.42	11	0	8.616125	12.01613	938	126	0.65296
3.4	1.42	12	0	9.399409	12.79941	938	126	0.627805
3.4	1.42	13	0	10.18269	13.58269	938	126	0.603941
3.4	1.42	14	0	10.96598	14.36598	938	126	0.581408
3.4	1.42	15	0	11.74926	15.14926	938	126	0.560185
3.4	1.42	16	0	12.53255	15.93255	938	126	0.540223
3.4	1.42	17	0	13.31583	16.71583	938	126	0.521454
3.4	1.42	18	0	14.09911	17.49911	938	126	0.503806
3.4	1.42	19	0	14.8824	18.2824	938	126	0.487203
3.4	1.42	20	0	15.66568	19.06568	938	126	0.471572
3.4	1.42	21	0	16.44897	19.84897	938	126	0.456843
3.4	1.42	22	0	17.23225	20.63225	938	126	0.442948
3.4	1.42	23	0	18.01553	21.41553	938	126	0.429826
3.4	1.42	24	0	18.79882	22.19882	938	126	0.417421
3.4	1.42	25	0	19.5821	22.9821	938	126	0.40568
3.4	1.42	26	0	20.36539	23.76539	938	126	0.394554
3.4	1.42	27	0	21.14867	24.54867	938	126	0.384
3.4	1.42	28	0	21.93196	25.33196	938	126	0.373976
3.4	1.42	29	0	22.71524	26.11524	938	126	0.364446
3.4	1.42	30	0	23.49852	26.89852	938	126	0.355375
3.4	1.42	31	0	24.28181	27.68181	938	126	0.346734
3.4	1.42	32	0	25.06509	28.46509	938	126	0.338492
3.4	1.42	33	0	25.84838	29.24838	938	126	0.330623
3.4	1.42	34	0	26.63166	30.03166	938	126	0.323105
3.4	1.42	35	0	27.41494	30.81494	938	126	0.315914
3.4	1.42	36	0	28.19823	31.59823	938	126	0.30903
3.4	1.42	37	0	28.98151	32.38151	938	126	0.302434
3.4	1.42	38	0	29.7648	33.1648	938	126	0.296109
3.4	1.42	39	0	30.54808	33.94808	938	126	0.29004
3.4	1.42	40	0	31.33136	34.73136	938	126	0.28421

4.6 ARMCHAIR(m=n)(k_1=938,k_2=126):-

Table 4.6 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 126$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	5	6.783439	10.18344	938	126	0.715756
3.4	1.42	6	6	8.140127	11.54013	938	126	0.668827
3.4	1.42	7	7	9.496815	12.89682	938	126	0.624765
3.4	1.42	8	8	10.8535	14.2535	938	126	0.584562
3.4	1.42	9	9	12.21019	15.61019	938	126	0.548289
3.4	1.42	10	10	13.56688	16.96688	938	126	0.515679
3.4	1.42	11	11	14.92357	18.32357	938	126	0.486358
3.4	1.42	12	12	16.28025	19.68025	938	126	0.459942
3.4	1.42	13	13	17.63694	21.03694	938	126	0.436076
3.4	1.42	14	14	18.99363	22.39363	938	126	0.414441
3.4	1.42	15	15	20.35032	23.75032	938	126	0.394763
3.4	1.42	16	16	21.70701	25.10701	938	126	0.376803
3.4	1.42	17	17	23.06369	26.46369	938	126	0.360356
3.4	1.42	18	18	24.42038	27.82038	938	126	0.345247
3.4	1.42	19	19	25.77707	29.17707	938	126	0.331325
3.4	1.42	20	20	27.13376	30.53376	938	126	0.318459
3.4	1.42	21	21	28.49045	31.89045	938	126	0.306536
3.4	1.42	22	22	29.84713	33.24713	938	126	0.295459
3.4	1.42	23	23	31.20382	34.60382	938	126	0.285143
3.4	1.42	24	24	32.56051	35.96051	938	126	0.275514
3.4	1.42	25	25	33.9172	37.3172	938	126	0.266505
3.4	1.42	26	26	35.27389	38.67389	938	126	0.25806
3.4	1.42	27	27	36.63057	40.03057	938	126	0.250129
3.4	1.42	28	28	37.98726	41.38726	938	126	0.242666
3.4	1.42	29	29	39.34395	42.74395	938	126	0.235631
3.4	1.42	30	30	40.70064	44.10064	938	126	0.228989
3.4	1.42	31	31	42.05732	45.45732	938	126	0.222709
3.4	1.42	32	32	43.41401	46.81401	938	126	0.216761
3.4	1.42	33	33	44.7707	48.1707	938	126	0.211121
3.4	1.42	34	34	46.12739	49.52739	938	126	0.205765
3.4	1.42	35	35	47.48408	50.88408	938	126	0.200673
3.4	1.42	36	36	48.84076	52.24076	938	126	0.195825
3.4	1.42	37	37	50.19745	53.59745	938	126	0.191204
3.4	1.42	38	38	51.55414	54.95414	938	126	0.186796
3.4	1.42	39	39	52.91083	56.31083	938	126	0.182585
3.4	1.42	40	40	54.26752	57.66752	938	126	0.178559

4.7 ZIGZAG(m,n=0)(k_1=804,k_2=140):-

Table 4.7 Summary of Young's modulus variation in accordance with $k_1 = 804$ & $k_2 = 140$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	0	3.916421	7.316421	804	140	0.765792
3.4	1.42	6	0	4.699705	8.099705	804	140	0.749809
3.4	1.42	7	0	5.482989	8.882989	804	140	0.727307
3.4	1.42	8	0	6.266273	9.666273	804	140	0.701956
3.4	1.42	9	0	7.049557	10.44956	804	140	0.675748
3.4	1.42	10	0	7.832841	11.23284	804	140	0.649769
3.4	1.42	11	0	8.616125	12.01613	804	140	0.6246
3.4	1.42	12	0	9.399409	12.79941	804	140	0.600536
3.4	1.42	13	0	10.18269	13.58269	804	140	0.57771
3.4	1.42	14	0	10.96598	14.36598	804	140	0.556155
3.4	1.42	15	0	11.74926	15.14926	804	140	0.535854
3.4	1.42	16	0	12.53255	15.93255	804	140	0.516758
3.4	1.42	17	0	13.31583	16.71583	804	140	0.498805
3.4	1.42	18	0	14.09911	17.49911	804	140	0.481924
3.4	1.42	19	0	14.8824	18.2824	804	140	0.466042
3.4	1.42	20	0	15.66568	19.06568	804	140	0.45109
3.4	1.42	21	0	16.44897	19.84897	804	140	0.437
3.4	1.42	22	0	17.23225	20.63225	804	140	0.423709
3.4	1.42	23	0	18.01553	21.41553	804	140	0.411157
3.4	1.42	24	0	18.79882	22.19882	804	140	0.399291
3.4	1.42	25	0	19.5821	22.9821	804	140	0.38806
3.4	1.42	26	0	20.36539	23.76539	804	140	0.377417
3.4	1.42	27	0	21.14867	24.54867	804	140	0.367321
3.4	1.42	28	0	21.93196	25.33196	804	140	0.357733
3.4	1.42	29	0	22.71524	26.11524	804	140	0.348617
3.4	1.42	30	0	23.49852	26.89852	804	140	0.33994
3.4	1.42	31	0	24.28181	27.68181	804	140	0.331674
3.4	1.42	32	0	25.06509	28.46509	804	140	0.32379
3.4	1.42	33	0	25.84838	29.24838	804	140	0.316263
3.4	1.42	34	0	26.63166	30.03166	804	140	0.309071
3.4	1.42	35	0	27.41494	30.81494	804	140	0.302192
3.4	1.42	36	0	28.19823	31.59823	804	140	0.295607
3.4	1.42	37	0	28.98151	32.38151	804	140	0.289298
3.4	1.42	38	0	29.7648	33.1648	804	140	0.283248
3.4	1.42	39	0	30.54808	33.94808	804	140	0.277442
3.4	1.42	40	0	31.33136	34.73136	804	140	0.271866

4.8 ARMCHAIR (m=n)(k_1=804,k_2=140):-

Table 4.8 Summary of Young's modulus variation in accordance with $k_1 = 804$ & $k_2 = 140$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	5	6.783439	10.18344	804	140	0.684667
3.4	1.42	6	6	8.140127	11.54013	804	140	0.639777
3.4	1.42	7	7	9.496815	12.89682	804	140	0.597629
3.4	1.42	8	8	10.8535	14.2535	804	140	0.559172
3.4	1.42	9	9	12.21019	15.61019	804	140	0.524475
3.4	1.42	10	10	13.56688	16.96688	804	140	0.493281
3.4	1.42	11	11	14.92357	18.32357	804	140	0.465234
3.4	1.42	12	12	16.28025	19.68025	804	140	0.439965
3.4	1.42	13	13	17.63694	21.03694	804	140	0.417135
3.4	1.42	14	14	18.99363	22.39363	804	140	0.39644
3.4	1.42	15	15	20.35032	23.75032	804	140	0.377617
3.4	1.42	16	16	21.70701	25.10701	804	140	0.360436
3.4	1.42	17	17	23.06369	26.46369	804	140	0.344704
3.4	1.42	18	18	24.42038	27.82038	804	140	0.330252
3.4	1.42	19	19	25.77707	29.17707	804	140	0.316934
3.4	1.42	20	20	27.13376	30.53376	804	140	0.304627
3.4	1.42	21	21	28.49045	31.89045	804	140	0.293222
3.4	1.42	22	22	29.84713	33.24713	804	140	0.282626
3.4	1.42	23	23	31.20382	34.60382	804	140	0.272759
3.4	1.42	24	24	32.56051	35.96051	804	140	0.263547
3.4	1.42	25	25	33.9172	37.3172	804	140	0.25493
3.4	1.42	26	26	35.27389	38.67389	804	140	0.246852
3.4	1.42	27	27	36.63057	40.03057	804	140	0.239265
3.4	1.42	28	28	37.98726	41.38726	804	140	0.232126
3.4	1.42	29	29	39.34395	42.74395	804	140	0.225397
3.4	1.42	30	30	40.70064	44.10064	804	140	0.219043
3.4	1.42	31	31	42.05732	45.45732	804	140	0.213036
3.4	1.42	32	32	43.41401	46.81401	804	140	0.207347
3.4	1.42	33	33	44.7707	48.1707	804	140	0.201951
3.4	1.42	34	34	46.12739	49.52739	804	140	0.196828
3.4	1.42	35	35	47.48408	50.88408	804	140	0.191957
3.4	1.42	36	36	48.84076	52.24076	804	140	0.187319
3.4	1.42	37	37	50.19745	53.59745	804	140	0.182899
3.4	1.42	38	38	51.55414	54.95414	804	140	0.178682
3.4	1.42	39	39	52.91083	56.31083	804	140	0.174654
3.4	1.42	40	40	54.26752	57.66752	804	140	0.170803

4.9 ZIG-ZAG(m, n=0)(k_1=1068,k_2=200):-

Table 4.9 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	0	3.916421	7.316421	1068	200	1.04597
3.4	1.42	6	0	4.699705	8.099705	1068	200	1.02414
3.4	1.42	7	0	5.482989	8.882989	1068	200	0.993405
3.4	1.42	8	0	6.266273	9.666273	1068	200	0.958779
3.4	1.42	9	0	7.049557	10.44956	1068	200	0.922982
3.4	1.42	10	0	7.832841	11.23284	1068	200	0.887498
3.4	1.42	11	0	8.616125	12.01613	1068	200	0.85312
3.4	1.42	12	0	9.399409	12.79941	1068	200	0.820253
3.4	1.42	13	0	10.18269	13.58269	1068	200	0.789075
3.4	1.42	14	0	10.96598	14.36598	1068	200	0.759634
3.4	1.42	15	0	11.74926	15.14926	1068	200	0.731905
3.4	1.42	16	0	12.53255	15.93255	1068	200	0.705824
3.4	1.42	17	0	13.31583	16.71583	1068	200	0.681302
3.4	1.42	18	0	14.09911	17.49911	1068	200	0.658244
3.4	1.42	19	0	14.8824	18.2824	1068	200	0.636552
3.4	1.42	20	0	15.66568	19.06568	1068	200	0.616129
3.4	1.42	21	0	16.44897	19.84897	1068	200	0.596884
3.4	1.42	22	0	17.23225	20.63225	1068	200	0.57873
3.4	1.42	23	0	18.01553	21.41553	1068	200	0.561586
3.4	1.42	24	0	18.79882	22.19882	1068	200	0.545379
3.4	1.42	25	0	19.5821	22.9821	1068	200	0.530038
3.4	1.42	26	0	20.36539	23.76539	1068	200	0.515502
3.4	1.42	27	0	21.14867	24.54867	1068	200	0.501712
3.4	1.42	28	0	21.93196	25.33196	1068	200	0.488615
3.4	1.42	29	0	22.71524	26.11524	1068	200	0.476164
3.4	1.42	30	0	23.49852	26.89852	1068	200	0.464313
3.4	1.42	31	0	24.28181	27.68181	1068	200	0.453022
3.4	1.42	32	0	25.06509	28.46509	1068	200	0.442254
3.4	1.42	33	0	25.84838	29.24838	1068	200	0.431973
3.4	1.42	34	0	26.63166	30.03166	1068	200	0.42215
3.4	1.42	35	0	27.41494	30.81494	1068	200	0.412755
3.4	1.42	36	0	28.19823	31.59823	1068	200	0.40376
3.4	1.42	37	0	28.98151	32.38151	1068	200	0.395143
3.4	1.42	38	0	29.7648	33.1648	1068	200	0.386879
3.4	1.42	39	0	30.54808	33.94808	1068	200	0.378949
3.4	1.42	40	0	31.33136	34.73136	1068	200	0.371332

4.10 ARM-CHAIR (m, n)m=n(k_1 =1068,k_2=200):-

Table 4.10 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	5	6.783439	10.18344	1068	200	0.935165
3.4	1.42	6	6	8.140127	11.54013	1068	200	0.873851
3.4	1.42	7	7	9.496815	12.89682	1068	200	0.816282
3.4	1.42	8	8	10.8535	14.2535	1068	200	0.763755
3.4	1.42	9	9	12.21019	15.61019	1068	200	0.716363
3.4	1.42	10	10	13.56688	16.96688	1068	200	0.673757
3.4	1.42	11	11	14.92357	18.32357	1068	200	0.635448
3.4	1.42	12	12	16.28025	19.68025	1068	200	0.600934
3.4	1.42	13	13	17.63694	21.03694	1068	200	0.569751
3.4	1.42	14	14	18.99363	22.39363	1068	200	0.541485
3.4	1.42	15	15	20.35032	23.75032	1068	200	0.515774
3.4	1.42	16	16	21.70701	25.10701	1068	200	0.492308
3.4	1.42	17	17	23.06369	26.46369	1068	200	0.47082
3.4	1.42	18	18	24.42038	27.82038	1068	200	0.45108
3.4	1.42	19	19	25.77707	29.17707	1068	200	0.43289
3.4	1.42	20	20	27.13376	30.53376	1068	200	0.41608
3.4	1.42	21	21	28.49045	31.89045	1068	200	0.400503
3.4	1.42	22	22	29.84713	33.24713	1068	200	0.38603
3.4	1.42	23	23	31.20382	34.60382	1068	200	0.372552
3.4	1.42	24	24	32.56051	35.96051	1068	200	0.35997
3.4	1.42	25	25	33.9172	37.3172	1068	200	0.3482
3.4	1.42	26	26	35.27389	38.67389	1068	200	0.337167
3.4	1.42	27	27	36.63057	40.03057	1068	200	0.326804
3.4	1.42	28	28	37.98726	41.38726	1068	200	0.317053
3.4	1.42	29	29	39.34395	42.74395	1068	200	0.307862
3.4	1.42	30	30	40.70064	44.10064	1068	200	0.299184
3.4	1.42	31	31	42.05732	45.45732	1068	200	0.290979
3.4	1.42	32	32	43.41401	46.81401	1068	200	0.283208
3.4	1.42	33	33	44.7707	48.1707	1068	200	0.275839
3.4	1.42	34	34	46.12739	49.52739	1068	200	0.268841
3.4	1.42	35	35	47.48408	50.88408	1068	200	0.262187
3.4	1.42	36	36	48.84076	52.24076	1068	200	0.255853
3.4	1.42	37	37	50.19745	53.59745	1068	200	0.249816
3.4	1.42	38	38	51.55414	54.95414	1068	200	0.244056
3.4	1.42	39	39	52.91083	56.31083	1068	200	0.238555
3.4	1.42	40	40	54.26752	57.66752	1068	200	0.233295

4.11 ZIG-ZAG (m, n=0)(k_1=1132,k_2=126):-

Table 4.11 Summary of Young's modulus variation in accordance with $k_1 = 1132$ & $k_2 = 126$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	0	3.916421	7.316421	1132	126	0.883086
3.4	1.42	6	0	4.699705	8.099705	1132	126	0.864656
3.4	1.42	7	0	5.482989	8.882989	1132	126	0.838707
3.4	1.42	8	0	6.266273	9.666273	1132	126	0.809473
3.4	1.42	9	0	7.049557	10.44956	1132	126	0.77925
3.4	1.42	10	0	7.832841	11.23284	1132	126	0.749292
3.4	1.42	11	0	8.616125	12.01613	1132	126	0.720268
3.4	1.42	12	0	9.399409	12.79941	1132	126	0.692519
3.4	1.42	13	0	10.18269	13.58269	1132	126	0.666196
3.4	1.42	14	0	10.96598	14.36598	1132	126	0.641339
3.4	1.42	15	0	11.74926	15.14926	1132	126	0.617929
3.4	1.42	16	0	12.53255	15.93255	1132	126	0.595909
3.4	1.42	17	0	13.31583	16.71583	1132	126	0.575206
3.4	1.42	18	0	14.09911	17.49911	1132	126	0.555739
3.4	1.42	19	0	14.8824	18.2824	1132	126	0.537425
3.4	1.42	20	0	15.66568	19.06568	1132	126	0.520182
3.4	1.42	21	0	16.44897	19.84897	1132	126	0.503934
3.4	1.42	22	0	17.23225	20.63225	1132	126	0.488607
3.4	1.42	23	0	18.01553	21.41553	1132	126	0.474133
3.4	1.42	24	0	18.79882	22.19882	1132	126	0.460449
3.4	1.42	25	0	19.5821	22.9821	1132	126	0.447498
3.4	1.42	26	0	20.36539	23.76539	1132	126	0.435225
3.4	1.42	27	0	21.14867	24.54867	1132	126	0.423583
3.4	1.42	28	0	21.93196	25.33196	1132	126	0.412526
3.4	1.42	29	0	22.71524	26.11524	1132	126	0.402013
3.4	1.42	30	0	23.49852	26.89852	1132	126	0.392008
3.4	1.42	31	0	24.28181	27.68181	1132	126	0.382475
3.4	1.42	32	0	25.06509	28.46509	1132	126	0.373383
3.4	1.42	33	0	25.84838	29.24838	1132	126	0.364704
3.4	1.42	34	0	26.63166	30.03166	1132	126	0.356411
3.4	1.42	35	0	27.41494	30.81494	1132	126	0.348478
3.4	1.42	36	0	28.19823	31.59823	1132	126	0.340885
3.4	1.42	37	0	28.98151	32.38151	1132	126	0.333609
3.4	1.42	38	0	29.7648	33.1648	1132	126	0.326632
3.4	1.42	39	0	30.54808	33.94808	1132	126	0.319937
3.4	1.42	40	0	31.33136	34.73136	1132	126	0.313507

4.12 ARMCHAIR(m=n)(k_1=1132,k_2=126):-

Table 4.12 Summary of Young's modulus variation in accordance with $k_1 = 1132$ & $k_2 = 126$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	5	6.783439	10.18344	1132	126	0.789536
3.4	1.42	6	6	8.140127	11.54013	1132	126	0.73777
3.4	1.42	7	7	9.496815	12.89682	1132	126	0.689166
3.4	1.42	8	8	10.8535	14.2535	1132	126	0.644819
3.4	1.42	9	9	12.21019	15.61019	1132	126	0.604807
3.4	1.42	10	10	13.56688	16.96688	1132	126	0.568836
3.4	1.42	11	11	14.92357	18.32357	1132	126	0.536492
3.4	1.42	12	12	16.28025	19.68025	1132	126	0.507354
3.4	1.42	13	13	17.63694	21.03694	1132	126	0.481027
3.4	1.42	14	14	18.99363	22.39363	1132	126	0.457162
3.4	1.42	15	15	20.35032	23.75032	1132	126	0.435455
3.4	1.42	16	16	21.70701	25.10701	1132	126	0.415644
3.4	1.42	17	17	23.06369	26.46369	1132	126	0.397502
3.4	1.42	18	18	24.42038	27.82038	1132	126	0.380835
3.4	1.42	19	19	25.77707	29.17707	1132	126	0.365478
3.4	1.42	20	20	27.13376	30.53376	1132	126	0.351286
3.4	1.42	21	21	28.49045	31.89045	1132	126	0.338134
3.4	1.42	22	22	29.84713	33.24713	1132	126	0.325916
3.4	1.42	23	23	31.20382	34.60382	1132	126	0.314536
3.4	1.42	24	24	32.56051	35.96051	1132	126	0.303914
3.4	1.42	25	25	33.9172	37.3172	1132	126	0.293977
3.4	1.42	26	26	35.27389	38.67389	1132	126	0.284661
3.4	1.42	27	27	36.63057	40.03057	1132	126	0.275912
3.4	1.42	28	28	37.98726	41.38726	1132	126	0.26768
3.4	1.42	29	29	39.34395	42.74395	1132	126	0.25992
3.4	1.42	30	30	40.70064	44.10064	1132	126	0.252594
3.4	1.42	31	31	42.05732	45.45732	1132	126	0.245666
3.4	1.42	32	32	43.41401	46.81401	1132	126	0.239105
3.4	1.42	33	33	44.7707	48.1707	1132	126	0.232884
3.4	1.42	34	34	46.12739	49.52739	1132	126	0.226975
3.4	1.42	35	35	47.48408	50.88408	1132	126	0.221358
3.4	1.42	36	36	48.84076	52.24076	1132	126	0.21601
3.4	1.42	37	37	50.19745	53.59745	1132	126	0.210913
3.4	1.42	38	38	51.55414	54.95414	1132	126	0.20605
3.4	1.42	39	39	52.91083	56.31083	1132	126	0.201406
3.4	1.42	40	40	54.26752	57.66752	1132	126	0.196965

4.13 ZIGZAG(m,n=0)(k_1=938,k_2=200):-

Table 4.13 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	0	3.916421	7.316421	938	200	0.962504
3.4	1.42	6	0	4.699705	8.099705	938	200	0.942416
3.4	1.42	7	0	5.482989	8.882989	938	200	0.914133
3.4	1.42	8	0	6.266273	9.666273	938	200	0.88227
3.4	1.42	9	0	7.049557	10.44956	938	200	0.84933
3.4	1.42	10	0	7.832841	11.23284	938	200	0.816677
3.4	1.42	11	0	8.616125	12.01613	938	200	0.785043
3.4	1.42	12	0	9.399409	12.79941	938	200	0.754799
3.4	1.42	13	0	10.18269	13.58269	938	200	0.726108
3.4	1.42	14	0	10.96598	14.36598	938	200	0.699016
3.4	1.42	15	0	11.74926	15.14926	938	200	0.673501
3.4	1.42	16	0	12.53255	15.93255	938	200	0.6495
3.4	1.42	17	0	13.31583	16.71583	938	200	0.626935
3.4	1.42	18	0	14.09911	17.49911	938	200	0.605717
3.4	1.42	19	0	14.8824	18.2824	938	200	0.585756
3.4	1.42	20	0	15.66568	19.06568	938	200	0.566963
3.4	1.42	21	0	16.44897	19.84897	938	200	0.549254
3.4	1.42	22	0	17.23225	20.63225	938	200	0.532548
3.4	1.42	23	0	18.01553	21.41553	938	200	0.516773
3.4	1.42	24	0	18.79882	22.19882	938	200	0.501858
3.4	1.42	25	0	19.5821	22.9821	938	200	0.487742
3.4	1.42	26	0	20.36539	23.76539	938	200	0.474366
3.4	1.42	27	0	21.14867	24.54867	938	200	0.461676
3.4	1.42	28	0	21.93196	25.33196	938	200	0.449625
3.4	1.42	29	0	22.71524	26.11524	938	200	0.438167
3.4	1.42	30	0	23.49852	26.89852	938	200	0.427262
3.4	1.42	31	0	24.28181	27.68181	938	200	0.416872
3.4	1.42	32	0	25.06509	28.46509	938	200	0.406963
3.4	1.42	33	0	25.84838	29.24838	938	200	0.397503
3.4	1.42	34	0	26.63166	30.03166	938	200	0.388463
3.4	1.42	35	0	27.41494	30.81494	938	200	0.379817
3.4	1.42	36	0	28.19823	31.59823	938	200	0.371541
3.4	1.42	37	0	28.98151	32.38151	938	200	0.363611
3.4	1.42	38	0	29.7648	33.1648	938	200	0.356007
3.4	1.42	39	0	30.54808	33.94808	938	200	0.34871
3.4	1.42	40	0	31.33136	34.73136	938	200	0.341701

4.14 ARMCHAIR(m=n)(k_1=938,k_2=200):-

Table 4.14 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	5	6.783439	10.18344	938	200	0.860541
3.4	1.42	6	6	8.140127	11.54013	938	200	0.804119
3.4	1.42	7	7	9.496815	12.89682	938	200	0.751144
3.4	1.42	8	8	10.8535	14.2535	938	200	0.702809
3.4	1.42	9	9	12.21019	15.61019	938	200	0.659199
3.4	1.42	10	10	13.56688	16.96688	938	200	0.619992
3.4	1.42	11	11	14.92357	18.32357	938	200	0.58474
3.4	1.42	12	12	16.28025	19.68025	938	200	0.552981
3.4	1.42	13	13	17.63694	21.03694	938	200	0.524286
3.4	1.42	14	14	18.99363	22.39363	938	200	0.498275
3.4	1.42	15	15	20.35032	23.75032	938	200	0.474616
3.4	1.42	16	16	21.70701	25.10701	938	200	0.453023
3.4	1.42	17	17	23.06369	26.46369	938	200	0.43325
3.4	1.42	18	18	24.42038	27.82038	938	200	0.415085
3.4	1.42	19	19	25.77707	29.17707	938	200	0.398346
3.4	1.42	20	20	27.13376	30.53376	938	200	0.382877
3.4	1.42	21	21	28.49045	31.89045	938	200	0.368543
3.4	1.42	22	22	29.84713	33.24713	938	200	0.355226
3.4	1.42	23	23	31.20382	34.60382	938	200	0.342823
3.4	1.42	24	24	32.56051	35.96051	938	200	0.331245
3.4	1.42	25	25	33.9172	37.3172	938	200	0.320415
3.4	1.42	26	26	35.27389	38.67389	938	200	0.310262
3.4	1.42	27	27	36.63057	40.03057	938	200	0.300726
3.4	1.42	28	28	37.98726	41.38726	938	200	0.291753
3.4	1.42	29	29	39.34395	42.74395	938	200	0.283295
3.4	1.42	30	30	40.70064	44.10064	938	200	0.27531
3.4	1.42	31	31	42.05732	45.45732	938	200	0.267759
3.4	1.42	32	32	43.41401	46.81401	938	200	0.260608
3.4	1.42	33	33	44.7707	48.1707	938	200	0.253827
3.4	1.42	34	34	46.12739	49.52739	938	200	0.247388
3.4	1.42	35	35	47.48408	50.88408	938	200	0.241265
3.4	1.42	36	36	48.84076	52.24076	938	200	0.235436
3.4	1.42	37	37	50.19745	53.59745	938	200	0.229881
3.4	1.42	38	38	51.55414	54.95414	938	200	0.224581
3.4	1.42	39	39	52.91083	56.31083	938	200	0.219518
3.4	1.42	40	40	54.26752	57.66752	938	200	0.214678

4.15 ZIG-ZAG (m,n=0)(k_1=960,k_2=180):-

Table 4.15 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.34	5	0	3.695777	7.095777	960	180	0.984004
3.4	1.34	6	0	4.434933	7.834933	960	180	0.968517
3.4	1.34	7	0	5.174088	8.574088	960	180	0.943515
3.4	1.34	8	0	5.913244	9.313244	960	180	0.913934
3.4	1.34	9	0	6.652399	10.0524	960	180	0.88253
3.4	1.34	10	0	7.391554	10.79155	960	180	0.850861
3.4	1.34	11	0	8.13071	11.53071	960	180	0.819799
3.4	1.34	12	0	8.869865	12.26987	960	180	0.78982
3.4	1.34	13	0	9.609021	13.00902	960	180	0.761168
3.4	1.34	14	0	10.34818	13.74818	960	180	0.733947
3.4	1.34	15	0	11.08733	14.48733	960	180	0.708176
3.4	1.34	16	0	11.82649	15.22649	960	180	0.683828
3.4	1.34	17	0	12.56564	15.96564	960	180	0.66085
3.4	1.34	18	0	13.3048	16.7048	960	180	0.63917
3.4	1.34	19	0	14.04395	17.44395	960	180	0.618715
3.4	1.34	20	0	14.78311	18.18311	960	180	0.599405
3.4	1.34	21	0	15.52226	18.92226	960	180	0.581165
3.4	1.34	22	0	16.26142	19.66142	960	180	0.563923
3.4	1.34	23	0	17.00058	20.40058	960	180	0.547608
3.4	1.34	24	0	17.73973	21.13973	960	180	0.532156
3.4	1.34	25	0	18.47889	21.87889	960	180	0.517507
3.4	1.34	26	0	19.21804	22.61804	960	180	0.503605
3.4	1.34	27	0	19.9572	23.3572	960	180	0.490398
3.4	1.34	28	0	20.69635	24.09635	960	180	0.477839
3.4	1.34	29	0	21.43551	24.83551	960	180	0.465885
3.4	1.34	30	0	22.17466	25.57466	960	180	0.454494
3.4	1.34	31	0	22.91382	26.31382	960	180	0.44363
3.4	1.34	32	0	23.65297	27.05297	960	180	0.433258
3.4	1.34	33	0	24.39213	27.79213	960	180	0.423347
3.4	1.34	34	0	25.13128	28.53128	960	180	0.413869
3.4	1.34	35	0	25.87044	29.27044	960	180	0.404796
3.4	1.34	36	0	26.6096	30.0096	960	180	0.396104
3.4	1.34	37	0	27.34875	30.74875	960	180	0.387769
3.4	1.34	38	0	28.08791	31.48791	960	180	0.379772
3.4	1.34	39	0	28.82706	32.22706	960	180	0.372092
3.4	1.34	40	0	29.56622	32.96622	960	180	0.364711

4.16 ARMCHAIR(b=1.34)(k_1=960,k_2=180):

Table 4.16 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.34	5	5	6.401274	9.801274	960	180	0.893289
3.4	1.34	6	6	7.681529	11.08153	960	180	0.83857
3.4	1.34	7	7	8.961783	12.36178	960	180	0.786182
3.4	1.34	8	8	10.24204	13.64204	960	180	0.737766
3.4	1.34	9	9	11.52229	14.92229	960	180	0.693679
3.4	1.34	10	10	12.80255	16.20255	960	180	0.653763
3.4	1.34	11	11	14.0828	17.4828	960	180	0.617672
3.4	1.34	12	12	15.36306	18.76306	960	180	0.585007
3.4	1.34	13	13	16.64331	20.04331	960	180	0.555382
3.4	1.34	14	14	17.92357	21.32357	960	180	0.52844
3.4	1.34	15	15	19.20382	22.60382	960	180	0.503866
3.4	1.34	16	16	20.48408	23.88408	960	180	0.481383
3.4	1.34	17	17	21.76433	25.16433	960	180	0.46075
3.4	1.34	18	18	23.04459	26.44459	960	180	0.44176
3.4	1.34	19	19	24.32484	27.72484	960	180	0.424231
3.4	1.34	20	20	25.6051	29.0051	960	180	0.408008
3.4	1.34	21	21	26.88535	30.28535	960	180	0.392954
3.4	1.34	22	22	28.16561	31.56561	960	180	0.37895
3.4	1.34	23	23	29.44586	32.84586	960	180	0.365893
3.4	1.34	24	24	30.72611	34.12611	960	180	0.353692
3.4	1.34	25	25	32.00637	35.40637	960	180	0.342267
3.4	1.34	26	26	33.28662	36.68662	960	180	0.331547
3.4	1.34	27	27	34.56688	37.96688	960	180	0.321471
3.4	1.34	28	28	35.84713	39.24713	960	180	0.311982
3.4	1.34	29	29	37.12739	40.52739	960	180	0.303032
3.4	1.34	30	30	38.40764	41.80764	960	180	0.294576
3.4	1.34	31	31	39.6879	43.0879	960	180	0.286575
3.4	1.34	32	32	40.96815	44.36815	960	180	0.278994
3.4	1.34	33	33	42.24841	45.64841	960	180	0.2718
3.4	1.34	34	34	43.52866	46.92866	960	180	0.264966
3.4	1.34	35	35	44.80892	48.20892	960	180	0.258464
3.4	1.34	36	36	46.08917	49.48917	960	180	0.252272
3.4	1.34	37	37	47.36943	50.76943	960	180	0.246368
3.4	1.34	38	38	48.64968	52.04968	960	180	0.240732
3.4	1.34	39	39	49.92994	53.32994	960	180	0.235348
3.4	1.34	40	40	51.21019	54.61019	960	180	0.230197

4.17 ZIG-ZAG (m, n=0) (k_1=700,k_2=100):-

Table 4.17 Summary of Young's modulus variation in accordance with $k_1 = 700$ & $k_2 = 100$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	0	3.916421	7.316421	700	100	0.614107
3.4	1.42	6	0	4.699705	8.099705	700	100	0.60129
3.4	1.42	7	0	5.482989	8.882989	700	100	0.583245
3.4	1.42	8	0	6.266273	9.666273	700	100	0.562916
3.4	1.42	9	0	7.049557	10.44956	700	100	0.541899
3.4	1.42	10	0	7.832841	11.23284	700	100	0.521065
3.4	1.42	11	0	8.616125	12.01613	700	100	0.500882
3.4	1.42	12	0	9.399409	12.79941	700	100	0.481585
3.4	1.42	13	0	10.18269	13.58269	700	100	0.463279
3.4	1.42	14	0	10.96598	14.36598	700	100	0.445994
3.4	1.42	15	0	11.74926	15.14926	700	100	0.429714
3.4	1.42	16	0	12.53255	15.93255	700	100	0.414401
3.4	1.42	17	0	13.31583	16.71583	700	100	0.400004
3.4	1.42	18	0	14.09911	17.49911	700	100	0.386466
3.4	1.42	19	0	14.8824	18.2824	700	100	0.373731
3.4	1.42	20	0	15.66568	19.06568	700	100	0.36174
3.4	1.42	21	0	16.44897	19.84897	700	100	0.350441
3.4	1.42	22	0	17.23225	20.63225	700	100	0.339782
3.4	1.42	23	0	18.01553	21.41553	700	100	0.329717
3.4	1.42	24	0	18.79882	22.19882	700	100	0.320201
3.4	1.42	25	0	19.5821	22.9821	700	100	0.311194
3.4	1.42	26	0	20.36539	23.76539	700	100	0.30266
3.4	1.42	27	0	21.14867	24.54867	700	100	0.294564
3.4	1.42	28	0	21.93196	25.33196	700	100	0.286875
3.4	1.42	29	0	22.71524	26.11524	700	100	0.279564
3.4	1.42	30	0	23.49852	26.89852	700	100	0.272606
3.4	1.42	31	0	24.28181	27.68181	700	100	0.265977
3.4	1.42	32	0	25.06509	28.46509	700	100	0.259655
3.4	1.42	33	0	25.84838	29.24838	700	100	0.253619
3.4	1.42	34	0	26.63166	30.03166	700	100	0.247852
3.4	1.42	35	0	27.41494	30.81494	700	100	0.242335
3.4	1.42	36	0	28.19823	31.59823	700	100	0.237055
3.4	1.42	37	0	28.98151	32.38151	700	100	0.231995
3.4	1.42	38	0	29.7648	33.1648	700	100	0.227144
3.4	1.42	39	0	30.54808	33.94808	700	100	0.222487
3.4	1.42	40	0	31.33136	34.73136	700	100	0.218016

4.18 ARMCHAIR(m=n)(k_1=700,k_2=100):

Table 4.18 Summary of Young's modulus variation in accordance with $k_1 = 700$ & $k_2 = 100$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.42	5	5	6.783439	10.18344	700	100	0.549051
3.4	1.42	6	6	8.140127	11.54013	700	100	0.513053
3.4	1.42	7	7	9.496815	12.89682	700	100	0.479253
3.4	1.42	8	8	10.8535	14.2535	700	100	0.448414
3.4	1.42	9	9	12.21019	15.61019	700	100	0.420589
3.4	1.42	10	10	13.56688	16.96688	700	100	0.395574
3.4	1.42	11	11	14.92357	18.32357	700	100	0.373082
3.4	1.42	12	12	16.28025	19.68025	700	100	0.352819
3.4	1.42	13	13	17.63694	21.03694	700	100	0.334511
3.4	1.42	14	14	18.99363	22.39363	700	100	0.317915
3.4	1.42	15	15	20.35032	23.75032	700	100	0.30282
3.4	1.42	16	16	21.70701	25.10701	700	100	0.289043
3.4	1.42	17	17	23.06369	26.46369	700	100	0.276427
3.4	1.42	18	18	24.42038	27.82038	700	100	0.264837
3.4	1.42	19	19	25.77707	29.17707	700	100	0.254157
3.4	1.42	20	20	27.13376	30.53376	700	100	0.244288
3.4	1.42	21	21	28.49045	31.89045	700	100	0.235142
3.4	1.42	22	22	29.84713	33.24713	700	100	0.226645
3.4	1.42	23	23	31.20382	34.60382	700	100	0.218732
3.4	1.42	24	24	32.56051	35.96051	700	100	0.211345
3.4	1.42	25	25	33.9172	37.3172	700	100	0.204434
3.4	1.42	26	26	35.27389	38.67389	700	100	0.197957
3.4	1.42	27	27	36.63057	40.03057	700	100	0.191872
3.4	1.42	28	28	37.98726	41.38726	700	100	0.186147
3.4	1.42	29	29	39.34395	42.74395	700	100	0.180751
3.4	1.42	30	30	40.70064	44.10064	700	100	0.175656
3.4	1.42	31	31	42.05732	45.45732	700	100	0.170839
3.4	1.42	32	32	43.41401	46.81401	700	100	0.166276
3.4	1.42	33	33	44.7707	48.1707	700	100	0.16195
3.4	1.42	34	34	46.12739	49.52739	700	100	0.157841
3.4	1.42	35	35	47.48408	50.88408	700	100	0.153935
3.4	1.42	36	36	48.84076	52.24076	700	100	0.150216
3.4	1.42	37	37	50.19745	53.59745	700	100	0.146671
3.4	1.42	38	38	51.55414	54.95414	700	100	0.14329
3.4	1.42	39	39	52.91083	56.31083	700	100	0.14006
3.4	1.42	40	40	54.26752	57.66752	700	100	0.136971

4.19 ZIG-ZAG(m,n=0)(b=1.522)(k_1=632,k_2=126):-

Table 4.19 Summary of Young's modulus variation in accordance with $k_1 = 632$ & $k_2 = 126$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.522	5	0	4.197741	7.597741	632	126	0.597516
3.4	1.522	6	0	5.037289	8.437289	632	126	0.581426
3.4	1.522	7	0	5.876837	9.276837	632	126	0.561109
3.4	1.522	8	0	6.716386	10.11639	632	126	0.539247
3.4	1.522	9	0	7.555934	10.95593	632	126	0.517241
3.4	1.522	10	0	8.395482	11.79548	632	126	0.495812
3.4	1.522	11	0	9.23503	12.63503	632	126	0.475323
3.4	1.522	12	0	10.07458	13.47458	632	126	0.455932
3.4	1.522	13	0	10.91413	14.31413	632	126	0.437686
3.4	1.522	14	0	11.75367	15.15367	632	126	0.420573
3.4	1.522	15	0	12.59322	15.99322	632	126	0.404546
3.4	1.522	16	0	13.43277	16.83277	632	126	0.389545
3.4	1.522	17	0	14.27232	17.67232	632	126	0.375501
3.4	1.522	18	0	15.11187	18.51187	632	126	0.362344
3.4	1.522	19	0	15.95142	19.35142	632	126	0.350007
3.4	1.522	20	0	16.79096	20.19096	632	126	0.338427
3.4	1.522	21	0	17.63051	21.03051	632	126	0.327543
3.4	1.522	22	0	18.47006	21.87006	632	126	0.317301
3.4	1.522	23	0	19.30961	22.70961	632	126	0.30765
3.4	1.522	24	0	20.14916	23.54916	632	126	0.298545
3.4	1.522	25	0	20.9887	24.3887	632	126	0.289942
3.4	1.522	26	0	21.82825	25.22825	632	126	0.281804
3.4	1.522	27	0	22.6678	26.0678	632	126	0.274097
3.4	1.522	28	0	23.50735	26.90735	632	126	0.266787
3.4	1.522	29	0	24.3469	27.7469	632	126	0.259847
3.4	1.522	30	0	25.18645	28.58645	632	126	0.25325
3.4	1.522	31	0	26.02599	29.42599	632	126	0.246972
3.4	1.522	32	0	26.86554	30.26554	632	126	0.240992
3.4	1.522	33	0	27.70509	31.10509	632	126	0.235288
3.4	1.522	34	0	28.54464	31.94464	632	126	0.229843
3.4	1.522	35	0	29.38419	32.78419	632	126	0.22464
3.4	1.522	36	0	30.22373	33.62373	632	126	0.219664
3.4	1.522	37	0	31.06328	34.46328	632	126	0.2149
3.4	1.522	38	0	31.90283	35.30283	632	126	0.210336
3.4	1.522	39	0	32.74238	36.14238	632	126	0.205959
3.4	1.522	40	0	33.58193	36.98193	632	126	0.201758

4.20 ARMCHAIR(b=1.522)(k_1=632,k_2=126):-

Table 4.20 Summary of Young's modulus variation in accordance with $k_1 = 632$ & $k_2 = 126$

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.522	5	5	7.270701	10.6707	632	126	0.524679
3.4	1.522	6	6	8.724841	12.12484	632	126	0.48765
3.4	1.522	7	7	10.17898	13.57898	632	126	0.4536
3.4	1.522	8	8	11.63312	15.03312	632	126	0.422962
3.4	1.522	9	9	13.08726	16.48726	632	126	0.395599
3.4	1.522	10	10	14.5414	17.9414	632	126	0.37119
3.4	1.522	11	11	15.99554	19.39554	632	126	0.34938
3.4	1.522	12	12	17.44968	20.84968	632	126	0.329831
3.4	1.522	13	13	18.90382	22.30382	632	126	0.312244
3.4	1.522	14	14	20.35796	23.75796	632	126	0.29636
3.4	1.522	15	15	21.8121	25.2121	632	126	0.281957
3.4	1.522	16	16	23.26624	26.66624	632	126	0.268847
3.4	1.522	17	17	24.72038	28.12038	632	126	0.256872
3.4	1.522	18	18	26.17452	29.57452	632	126	0.245893
3.4	1.522	19	19	27.62866	31.02866	632	126	0.235796
3.4	1.522	20	20	29.0828	32.4828	632	126	0.226481
3.4	1.522	21	21	30.53694	33.93694	632	126	0.217863
3.4	1.522	22	22	31.99108	35.39108	632	126	0.209867
3.4	1.522	23	23	33.44522	36.84522	632	126	0.20243
3.4	1.522	24	24	34.89936	38.29936	632	126	0.195496
3.4	1.522	25	25	36.3535	39.7535	632	126	0.189016
3.4	1.522	26	26	37.80764	41.20764	632	126	0.182948
3.4	1.522	27	27	39.26178	42.66178	632	126	0.177254
3.4	1.522	28	28	40.71592	44.11592	632	126	0.1719
3.4	1.522	29	29	42.17006	45.57006	632	126	0.166858
3.4	1.522	30	30	43.6242	47.0242	632	126	0.162102
3.4	1.522	31	31	45.07834	48.47834	632	126	0.157607
3.4	1.522	32	32	46.53248	49.93248	632	126	0.153353
3.4	1.522	33	33	47.98662	51.38662	632	126	0.149322
3.4	1.522	34	34	49.44076	52.84076	632	126	0.145496
3.4	1.522	35	35	50.8949	54.2949	632	126	0.14186
3.4	1.522	36	36	52.34904	55.74904	632	126	0.1384
3.4	1.522	37	37	53.80318	57.20318	632	126	0.135105
3.4	1.522	38	38	55.25732	58.65732	632	126	0.131962
3.4	1.522	39	39	56.71146	60.11146	632	126	0.128961
3.4	1.522	40	40	58.16561	61.56561	632	126	0.126094

4.21 ZIG-ZAG(b=1.35)(k_1=938,k_2=200):-

Table 4.21 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length(300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.35	5	0	3.72336	7.1234	938	200	0.9984
3.4	1.35	6	0	4.46803	7.868	938	200	0.98202
3.4	1.35	7	0	5.2127	8.6127	938	200	0.95614
3.4	1.35	8	0	5.95737	9.3574	938	200	0.92573
3.4	1.35	9	0	6.70204	10.102	938	200	0.89357
3.4	1.35	10	0	7.44672	10.847	938	200	0.8612
3.4	1.35	11	0	8.19139	11.591	938	200	0.82952
3.4	1.35	12	0	8.93606	12.336	938	200	0.79897
3.4	1.35	13	0	9.68073	13.081	938	200	0.76981
3.4	1.35	14	0	10.4254	13.825	938	200	0.74212
3.4	1.35	15	0	11.1701	14.57	938	200	0.71593
3.4	1.35	16	0	11.9147	15.315	938	200	0.6912
3.4	1.35	17	0	12.6594	16.059	938	200	0.66787
3.4	1.35	18	0	13.4041	16.804	938	200	0.64587
3.4	1.35	19	0	14.1488	17.549	938	200	0.62512
3.4	1.35	20	0	14.8934	18.293	938	200	0.60554
3.4	1.35	21	0	15.6381	19.038	938	200	0.58705
3.4	1.35	22	0	16.3828	19.783	938	200	0.56958
3.4	1.35	23	0	17.1274	20.527	938	200	0.55305
3.4	1.35	24	0	17.8721	21.272	938	200	0.53739
3.4	1.35	25	0	18.6168	22.017	938	200	0.52256
3.4	1.35	26	0	19.3615	22.761	938	200	0.50848
3.4	1.35	27	0	20.1061	23.506	938	200	0.49511
3.4	1.35	28	0	20.8508	24.251	938	200	0.4824
3.4	1.35	29	0	21.5955	24.995	938	200	0.4703
3.4	1.35	30	0	22.3401	25.74	938	200	0.45878
3.4	1.35	31	0	23.0848	26.485	938	200	0.44779
3.4	1.35	32	0	23.8295	27.229	938	200	0.43729
3.4	1.35	33	0	24.5742	27.974	938	200	0.42727
3.4	1.35	34	0	25.3188	28.719	938	200	0.41768
3.4	1.35	35	0	26.0635	29.464	938	200	0.40851
3.4	1.35	36	0	26.8082	30.208	938	200	0.39972
3.4	1.35	37	0	27.5528	30.953	938	200	0.39129
3.4	1.35	38	0	28.2975	31.698	938	200	0.38321
3.4	1.35	39	0	29.0422	32.442	938	200	0.37545
3.4	1.35	40	0	29.7869	33.187	938	200	0.36799

4.22 ARMCHAIR(b=1.35)(k_1=938,k_2=200):

Table 4.22 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length(300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.35	5	5	6.44904	9.849	938	200	0.90458
3.4	1.35	6	6	7.73885	11.139	938	200	0.84866
3.4	1.35	7	7	9.02866	12.429	938	200	0.79527
3.4	1.35	8	8	10.3185	13.718	938	200	0.74601
3.4	1.35	9	9	11.6083	15.008	938	200	0.7012
3.4	1.35	10	10	12.8981	16.298	938	200	0.66068
3.4	1.35	11	11	14.1879	17.588	938	200	0.62406
3.4	1.35	12	12	15.4777	18.878	938	200	0.59094
3.4	1.35	13	13	16.7675	20.168	938	200	0.56092
3.4	1.35	14	14	18.0573	21.457	938	200	0.53363
3.4	1.35	15	15	19.3471	22.747	938	200	0.50875
3.4	1.35	16	16	20.6369	24.037	938	200	0.48599
3.4	1.35	17	17	21.9268	25.327	938	200	0.46511
3.4	1.35	18	18	23.2166	26.617	938	200	0.44589
3.4	1.35	19	19	24.5064	27.906	938	200	0.42816
3.4	1.35	20	20	25.7962	29.196	938	200	0.41176
3.4	1.35	21	21	27.086	30.486	938	200	0.39654
3.4	1.35	22	22	28.3758	31.776	938	200	0.38238
3.4	1.35	23	23	29.6656	33.066	938	200	0.36918
3.4	1.35	24	24	30.9554	34.355	938	200	0.35685
3.4	1.35	25	25	32.2452	35.645	938	200	0.3453
3.4	1.35	26	26	33.535	36.935	938	200	0.33447
3.4	1.35	27	27	34.8248	38.225	938	200	0.32429
3.4	1.35	28	28	36.1146	39.515	938	200	0.31471
3.4	1.35	29	29	37.4045	40.804	938	200	0.30567
3.4	1.35	30	30	38.6943	42.094	938	200	0.29712
3.4	1.35	31	31	39.9841	43.384	938	200	0.28904
3.4	1.35	32	32	41.2739	44.674	938	200	0.28139
3.4	1.35	33	33	42.5637	45.964	938	200	0.27412
3.4	1.35	34	34	43.8535	47.254	938	200	0.26722
3.4	1.35	35	35	45.1433	48.543	938	200	0.26066
3.4	1.35	36	36	46.4331	49.833	938	200	0.25441
3.4	1.35	37	37	47.7229	51.123	938	200	0.24845
3.4	1.35	38	38	49.0127	52.413	938	200	0.24276
3.4	1.35	39	39	50.3025	53.703	938	200	0.23732
3.4	1.35	40	40	51.5924	54.992	938	200	0.23212

4.23 ZIG-ZAG(b=1.5)(k_1=938,k_2=200):

Table 4.23 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length at (300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.5	5	0	4.13706	7.5371	938	200	0.92131
3.4	1.5	6	0	4.96448	8.3645	938	200	0.89766
3.4	1.5	7	0	5.79189	9.1919	938	200	0.86722
3.4	1.5	8	0	6.6193	10.019	938	200	0.83417
3.4	1.5	9	0	7.44672	10.847	938	200	0.80073
3.4	1.5	10	0	8.27413	11.674	938	200	0.76805
3.4	1.5	11	0	9.10154	12.502	938	200	0.73673
3.4	1.5	12	0	9.92895	13.329	938	200	0.70702
3.4	1.5	13	0	10.7564	14.156	938	200	0.67902
3.4	1.5	14	0	11.5838	14.984	938	200	0.65272
3.4	1.5	15	0	12.4112	15.811	938	200	0.62806
3.4	1.5	16	0	13.2386	16.639	938	200	0.60496
3.4	1.5	17	0	14.066	17.466	938	200	0.58331
3.4	1.5	18	0	14.8934	18.293	938	200	0.56302
3.4	1.5	19	0	15.7208	19.121	938	200	0.54398
3.4	1.5	20	0	16.5483	19.948	938	200	0.52609
3.4	1.5	21	0	17.3757	20.776	938	200	0.50927
3.4	1.5	22	0	18.2031	21.603	938	200	0.49344
3.4	1.5	23	0	19.0305	22.43	938	200	0.47851
3.4	1.5	24	0	19.8579	23.258	938	200	0.46442
3.4	1.5	25	0	20.6853	24.085	938	200	0.4511
3.4	1.5	26	0	21.5127	24.913	938	200	0.4385
3.4	1.5	27	0	22.3401	25.74	938	200	0.42656
3.4	1.5	28	0	23.1676	26.568	938	200	0.41524
3.4	1.5	29	0	23.995	27.395	938	200	0.40448
3.4	1.5	30	0	24.8224	28.222	938	200	0.39425
3.4	1.5	31	0	25.6498	29.05	938	200	0.38452
3.4	1.5	32	0	26.4772	29.877	938	200	0.37524
3.4	1.5	33	0	27.3046	30.705	938	200	0.36639
3.4	1.5	34	0	28.132	31.532	938	200	0.35794
3.4	1.5	35	0	28.9594	32.359	938	200	0.34987
3.4	1.5	36	0	29.7869	33.187	938	200	0.34215
3.4	1.5	37	0	30.6143	34.014	938	200	0.33475
3.4	1.5	38	0	31.4417	34.842	938	200	0.32766
3.4	1.5	39	0	32.2691	35.669	938	200	0.32086
3.4	1.5	40	0	33.0965	36.497	938	200	0.31434

4.24 ARMCHAIR (b=1.5)(k_1=938,k_2=200):

Table 4.24 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length at (300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.5	5	5	7.16561	10.566	938	200	0.81205
3.4	1.5	6	6	8.59873	11.999	938	200	0.75558
3.4	1.5	7	7	10.0318	13.432	938	200	0.70344
3.4	1.5	8	8	11.465	14.865	938	200	0.65639
3.4	1.5	9	9	12.8981	16.298	938	200	0.61429
3.4	1.5	10	10	14.3312	17.731	938	200	0.57667
3.4	1.5	11	11	15.7643	19.164	938	200	0.54301
3.4	1.5	12	12	17.1975	20.597	938	200	0.51281
3.4	1.5	13	13	18.6306	22.031	938	200	0.48562
3.4	1.5	14	14	20.0637	23.464	938	200	0.46104
3.4	1.5	15	15	21.4968	24.897	938	200	0.43874
3.4	1.5	16	16	22.9299	26.33	938	200	0.41843
3.4	1.5	17	17	24.3631	27.763	938	200	0.39987
3.4	1.5	18	18	25.7962	29.196	938	200	0.38284
3.4	1.5	19	19	27.2293	30.629	938	200	0.36718
3.4	1.5	20	20	28.6624	32.062	938	200	0.35273
3.4	1.5	21	21	30.0955	33.496	938	200	0.33935
3.4	1.5	22	22	31.5287	34.929	938	200	0.32693
3.4	1.5	23	23	32.9618	36.362	938	200	0.31538
3.4	1.5	24	24	34.3949	37.795	938	200	0.30461
3.4	1.5	25	25	35.828	39.228	938	200	0.29454
3.4	1.5	26	26	37.2611	40.661	938	200	0.28511
3.4	1.5	27	27	38.6943	42.094	938	200	0.27626
3.4	1.5	28	28	40.1274	43.527	938	200	0.26794
3.4	1.5	29	29	41.5605	44.961	938	200	0.2601
3.4	1.5	30	30	42.9936	46.394	938	200	0.2527
3.4	1.5	31	31	44.4268	47.827	938	200	0.24571
3.4	1.5	32	32	45.8599	49.26	938	200	0.23909
3.4	1.5	33	33	47.293	50.693	938	200	0.23282
3.4	1.5	34	34	48.7261	52.126	938	200	0.22687
3.4	1.5	35	35	50.1592	53.559	938	200	0.22121
3.4	1.5	36	36	51.5924	54.992	938	200	0.21582
3.4	1.5	37	37	53.0255	56.425	938	200	0.21069
3.4	1.5	38	38	54.4586	57.859	938	200	0.2058
3.4	1.5	39	39	55.8917	59.292	938	200	0.20113
3.4	1.5	40	40	57.3248	60.725	938	200	0.19667

4.25 ZIG-ZAG (b=1.3)(k_1=938,k_2=200):

Table 4.25 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.3	5	0	3.585455	6.985455	938	200	1.023717
3.4	1.3	6	0	4.302547	7.702547	938	200	1.010373
3.4	1.3	7	0	5.019638	8.419638	938	200	0.98653
3.4	1.3	8	0	5.736729	9.136729	938	200	0.957432
3.4	1.3	9	0	6.45382	9.85382	938	200	0.926046
3.4	1.3	10	0	7.170911	10.57091	938	200	0.894076
3.4	1.3	11	0	7.888002	11.288	938	200	0.862497
3.4	1.3	12	0	8.605093	12.00509	938	200	0.831858
3.4	1.3	13	0	9.322184	12.72218	938	200	0.802452
3.4	1.3	14	0	10.03928	13.43928	938	200	0.774418
3.4	1.3	15	0	10.75637	14.15637	938	200	0.747803
3.4	1.3	16	0	11.47346	14.87346	938	200	0.722596
3.4	1.3	17	0	12.19055	15.59055	938	200	0.698756
3.4	1.3	18	0	12.90764	16.30764	938	200	0.676222
3.4	1.3	19	0	13.62473	17.02473	938	200	0.654926
3.4	1.3	20	0	14.34182	17.74182	938	200	0.634794
3.4	1.3	21	0	15.05891	18.45891	938	200	0.615753
3.4	1.3	22	0	15.776	19.176	938	200	0.597731
3.4	1.3	23	0	16.4931	19.8931	938	200	0.580661
3.4	1.3	24	0	17.21019	20.61019	938	200	0.564478
3.4	1.3	25	0	17.92728	21.32728	938	200	0.549121
3.4	1.3	26	0	18.64437	22.04437	938	200	0.534536
3.4	1.3	27	0	19.36146	22.76146	938	200	0.52067
3.4	1.3	28	0	20.07855	23.47855	938	200	0.507475
3.4	1.3	29	0	20.79564	24.19564	938	200	0.494906
3.4	1.3	30	0	21.51273	24.91273	938	200	0.482923
3.4	1.3	31	0	22.22982	25.62982	938	200	0.471487
3.4	1.3	32	0	22.94692	26.34692	938	200	0.460564
3.4	1.3	33	0	23.66401	27.06401	938	200	0.450121
3.4	1.3	34	0	24.3811	27.7811	938	200	0.440128
3.4	1.3	35	0	25.09819	28.49819	938	200	0.430559
3.4	1.3	36	0	25.81528	29.21528	938	200	0.421388
3.4	1.3	37	0	26.53237	29.93237	938	200	0.41259
3.4	1.3	38	0	27.24946	30.64946	938	200	0.404145
3.4	1.3	39	0	27.96655	31.36655	938	200	0.396032
3.4	1.3	40	0	28.68364	32.08364	938	200	0.388232

4.26 ARMCHAIR (b=1.3)(k_1=938,k_2=200):

Table 4.26 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.3	5	5	6.210191	9.610191	938	200	0.936841
3.4	1.3	6	6	7.452229	10.85223	938	200	0.881603
3.4	1.3	7	7	8.694268	12.09427	938	200	0.828131
3.4	1.3	8	8	9.936306	13.33631	938	200	0.778357
3.4	1.3	9	9	11.17834	14.57834	938	200	0.732801
3.4	1.3	10	10	12.42038	15.82038	938	200	0.691395
3.4	1.3	11	11	13.66242	17.06242	938	200	0.65384
3.4	1.3	12	12	14.90446	18.30446	938	200	0.619765
3.4	1.3	13	13	16.1465	19.5465	938	200	0.588797
3.4	1.3	14	14	17.38854	20.78854	938	200	0.560583
3.4	1.3	15	15	18.63057	22.03057	938	200	0.53481
3.4	1.3	16	16	19.87261	23.27261	938	200	0.511199
3.4	1.3	17	17	21.11465	24.51465	938	200	0.489505
3.4	1.3	18	18	22.35669	25.75669	938	200	0.469518
3.4	1.3	19	19	23.59873	26.99873	938	200	0.451052
3.4	1.3	20	20	24.84076	28.24076	938	200	0.433947
3.4	1.3	21	21	26.0828	29.4828	938	200	0.418063
3.4	1.3	22	22	27.32484	30.72484	938	200	0.403277
3.4	1.3	23	23	28.56688	31.96688	938	200	0.389482
3.4	1.3	24	24	29.80892	33.20892	938	200	0.376584
3.4	1.3	25	25	31.05096	34.45096	938	200	0.3645
3.4	1.3	26	26	32.29299	35.69299	938	200	0.353157
3.4	1.3	27	27	33.53503	36.93503	938	200	0.342489
3.4	1.3	28	28	34.77707	38.17707	938	200	0.33244
3.4	1.3	29	29	36.01911	39.41911	938	200	0.322957
3.4	1.3	30	30	37.26115	40.66115	938	200	0.313994
3.4	1.3	31	31	38.50318	41.90318	938	200	0.305511
3.4	1.3	32	32	39.74522	43.14522	938	200	0.297471
3.4	1.3	33	33	40.98726	44.38726	938	200	0.289839
3.4	1.3	34	34	42.2293	45.6293	938	200	0.282586
3.4	1.3	35	35	43.47134	46.87134	938	200	0.275685
3.4	1.3	36	36	44.71338	48.11338	938	200	0.269111
3.4	1.3	37	37	45.95541	49.35541	938	200	0.26284
3.4	1.3	38	38	47.19745	50.59745	938	200	0.256854
3.4	1.3	39	39	48.43949	51.83949	938	200	0.251133
3.4	1.3	40	40	49.68153	53.08153	938	200	0.245659

4.27 ZIG-ZAG(b=1.55)(k_1=938,k_2=200):

Table 4.27 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.55	5	0	4.274966	7.674966	938	200	0.89568
3.4	1.55	6	0	5.129959	8.529959	938	200	0.870148
3.4	1.55	7	0	5.984953	9.384953	938	200	0.838629
3.4	1.55	8	0	6.839946	10.23995	938	200	0.805064
3.4	1.55	9	0	7.694939	11.09494	938	200	0.771487
3.4	1.55	10	0	8.549932	11.94993	938	200	0.738933
3.4	1.55	11	0	9.404926	12.80493	938	200	0.707904
3.4	1.55	12	0	10.25992	13.65992	938	200	0.678611
3.4	1.55	13	0	11.11491	14.51491	938	200	0.651104
3.4	1.55	14	0	11.96991	15.36991	938	200	0.625348
3.4	1.55	15	0	12.8249	16.2249	938	200	0.601261
3.4	1.55	16	0	13.67989	17.07989	938	200	0.578743
3.4	1.55	17	0	14.53488	17.93488	938	200	0.557683
3.4	1.55	18	0	15.38988	18.78988	938	200	0.537973
3.4	1.55	19	0	16.24487	19.64487	938	200	0.519507
3.4	1.55	20	0	17.09986	20.49986	938	200	0.502185
3.4	1.55	21	0	17.95486	21.35486	938	200	0.485917
3.4	1.55	22	0	18.80985	22.20985	938	200	0.470617
3.4	1.55	23	0	19.66484	23.06484	938	200	0.456208
3.4	1.55	24	0	20.51984	23.91984	938	200	0.44262
3.4	1.55	25	0	21.37483	24.77483	938	200	0.429788
3.4	1.55	26	0	22.22982	25.62982	938	200	0.417655
3.4	1.55	27	0	23.08482	26.48482	938	200	0.406168
3.4	1.55	28	0	23.93981	27.33981	938	200	0.395278
3.4	1.55	29	0	24.7948	28.1948	938	200	0.384942
3.4	1.55	30	0	25.6498	29.0498	938	200	0.375121
3.4	1.55	31	0	26.50479	29.90479	938	200	0.365777
3.4	1.55	32	0	27.35978	30.75978	938	200	0.356878
3.4	1.55	33	0	28.21478	31.61478	938	200	0.348393
3.4	1.55	34	0	29.06977	32.46977	938	200	0.340296
3.4	1.55	35	0	29.92476	33.32476	938	200	0.33256
3.4	1.55	36	0	30.77976	34.17976	938	200	0.325162
3.4	1.55	37	0	31.63475	35.03475	938	200	0.318082
3.4	1.55	38	0	32.48974	35.88974	938	200	0.3113
3.4	1.55	39	0	33.34474	36.74474	938	200	0.304797
3.4	1.55	40	0	34.19973	37.59973	938	200	0.298556

4.28 ARMCHAIR (b=1.55)(k_1=938,k_2=200):

Table 4.28 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.55	5	5	7.404459	10.80446	938	200	0.782817
3.4	1.55	6	6	8.88535	12.28535	938	200	0.726562
3.4	1.55	7	7	10.36624	13.76624	938	200	0.675093
3.4	1.55	8	8	11.84713	15.24713	938	200	0.628941
3.4	1.55	9	9	13.32803	16.72803	938	200	0.587827
3.4	1.55	10	10	14.80892	18.20892	938	200	0.551224
3.4	1.55	11	11	16.28981	19.68981	938	200	0.518569
3.4	1.55	12	12	17.7707	21.1707	938	200	0.489336
3.4	1.55	13	13	19.25159	22.65159	938	200	0.463065
3.4	1.55	14	14	20.73248	24.13248	938	200	0.43936
3.4	1.55	15	15	22.21338	25.61338	938	200	0.417882
3.4	1.55	16	16	23.69427	27.09427	938	200	0.398347
3.4	1.55	17	17	25.17516	28.57516	938	200	0.380512
3.4	1.55	18	18	26.65605	30.05605	938	200	0.364171
3.4	1.55	19	19	28.13694	31.53694	938	200	0.349149
3.4	1.55	20	20	29.61783	33.01783	938	200	0.335297
3.4	1.55	21	21	31.09873	34.49873	938	200	0.322485
3.4	1.55	22	22	32.57962	35.97962	938	200	0.310603
3.4	1.55	23	23	34.06051	37.46051	938	200	0.299555
3.4	1.55	24	24	35.5414	38.9414	938	200	0.289257
3.4	1.55	25	25	37.02229	40.42229	938	200	0.279637
3.4	1.55	26	26	38.50318	41.90318	938	200	0.27063
3.4	1.55	27	27	39.98408	43.38408	938	200	0.26218
3.4	1.55	28	28	41.46497	44.86497	938	200	0.254238
3.4	1.55	29	29	42.94586	46.34586	938	200	0.246759
3.4	1.55	30	30	44.42675	47.82675	938	200	0.239704
3.4	1.55	31	31	45.90764	49.30764	938	200	0.23304
3.4	1.55	32	32	47.38854	50.78854	938	200	0.226733
3.4	1.55	33	33	48.86943	52.26943	938	200	0.220757
3.4	1.55	34	34	50.35032	53.75032	938	200	0.215087
3.4	1.55	35	35	51.83121	55.23121	938	200	0.209699
3.4	1.55	36	36	53.3121	56.7121	938	200	0.204573
3.4	1.55	37	37	54.79299	58.19299	938	200	0.19969
3.4	1.55	38	38	56.27389	59.67389	938	200	0.195034
3.4	1.55	39	39	57.75478	61.15478	938	200	0.19059
3.4	1.55	40	40	59.23567	62.63567	938	200	0.186343

4.29 ZIG-ZAG (b=1.25)(k_1=938,k_2=200):

Table 4.29 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.25	5	0	3.447553	6.847553	938	200	1.048574
3.4	1.25	6	0	4.137064	7.537064	938	200	1.038597
3.4	1.25	7	0	4.826575	8.226575	938	200	1.017091
3.4	1.25	8	0	5.516085	8.916085	938	200	0.989559
3.4	1.25	9	0	6.205596	9.605596	938	200	0.959166
3.4	1.25	10	0	6.895107	10.29511	938	200	0.927766
3.4	1.25	11	0	7.584617	10.98462	938	200	0.896443
3.4	1.25	12	0	8.274128	11.67413	938	200	0.86583
3.4	1.25	13	0	8.963639	12.36364	938	200	0.836278
3.4	1.25	14	0	9.653149	13.05315	938	200	0.807974
3.4	1.25	15	0	10.34266	13.74266	938	200	0.780998
3.4	1.25	16	0	11.03217	14.43217	938	200	0.755365
3.4	1.25	17	0	11.72168	15.12168	938	200	0.731053
3.4	1.25	18	0	12.41119	15.81119	938	200	0.708016
3.4	1.25	19	0	13.1007	16.5007	938	200	0.686197
3.4	1.25	20	0	13.79021	17.19021	938	200	0.66553
3.4	1.25	21	0	14.47972	17.87972	938	200	0.645948
3.4	1.25	22	0	15.16923	18.56923	938	200	0.627386
3.4	1.25	23	0	15.85875	19.25875	938	200	0.609778
3.4	1.25	24	0	16.54826	19.94826	938	200	0.593064
3.4	1.25	25	0	17.23777	20.63777	938	200	0.577185
3.4	1.25	26	0	17.92728	21.32728	938	200	0.562086
3.4	1.25	27	0	18.61679	22.01679	938	200	0.547717
3.4	1.25	28	0	19.3063	22.7063	938	200	0.53403
3.4	1.25	29	0	19.99581	23.39581	938	200	0.520981
3.4	1.25	30	0	20.68532	24.08532	938	200	0.50853
3.4	1.25	31	0	21.37483	24.77483	938	200	0.496638
3.4	1.25	32	0	22.06434	25.46434	938	200	0.485272
3.4	1.25	33	0	22.75385	26.15385	938	200	0.474398
3.4	1.25	34	0	23.44336	26.84336	938	200	0.463986
3.4	1.25	35	0	24.13287	27.53287	938	200	0.45401
3.4	1.25	36	0	24.82238	28.22238	938	200	0.444442
3.4	1.25	37	0	25.51189	28.91189	938	200	0.43526
3.4	1.25	38	0	26.20141	29.60141	938	200	0.426441
3.4	1.25	39	0	26.89092	30.29092	938	200	0.417965
3.4	1.25	40	0	27.58043	30.98043	938	200	0.409813

4.30 ARMCHAIR (b=1.25)(k_1=938,k_2=200):

Table 4.30 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.25	5	5	5.971338	9.371338	938	200	0.969678
3.4	1.25	6	6	7.165605	10.56561	938	200	0.915426
3.4	1.25	7	7	8.359873	11.75987	938	200	0.862092
3.4	1.25	8	8	9.55414	12.95414	938	200	0.811958
3.4	1.25	9	9	10.74841	14.14841	938	200	0.765752
3.4	1.25	10	10	11.94268	15.34268	938	200	0.723533
3.4	1.25	11	11	13.13694	16.53694	938	200	0.685083
3.4	1.25	12	12	14.33121	17.73121	938	200	0.650078
3.4	1.25	13	13	15.52548	18.92548	938	200	0.618173
3.4	1.25	14	14	16.71975	20.11975	938	200	0.589039
3.4	1.25	15	15	17.91401	21.31401	938	200	0.562369
3.4	1.25	16	16	19.10828	22.50828	938	200	0.537893
3.4	1.25	17	17	20.30255	23.70255	938	200	0.515371
3.4	1.25	18	18	21.49682	24.89682	938	200	0.49459
3.4	1.25	19	19	22.69108	26.09108	938	200	0.475368
3.4	1.25	20	20	23.88535	27.28535	938	200	0.457543
3.4	1.25	21	21	25.07962	28.47962	938	200	0.440973
3.4	1.25	22	22	26.27389	29.67389	938	200	0.425534
3.4	1.25	23	23	27.46815	30.86815	938	200	0.411119
3.4	1.25	24	24	28.66242	32.06242	938	200	0.39763
3.4	1.25	25	25	29.85669	33.25669	938	200	0.384984
3.4	1.25	26	26	31.05096	34.45096	938	200	0.373105
3.4	1.25	27	27	32.24522	35.64522	938	200	0.361928
3.4	1.25	28	28	33.43949	36.83949	938	200	0.351392
3.4	1.25	29	29	34.63376	38.03376	938	200	0.341445
3.4	1.25	30	30	35.82803	39.22803	938	200	0.332039
3.4	1.25	31	31	37.02229	40.42229	938	200	0.323132
3.4	1.25	32	32	38.21656	41.61656	938	200	0.314687
3.4	1.25	33	33	39.41083	42.81083	938	200	0.306667
3.4	1.25	34	34	40.6051	44.0051	938	200	0.299043
3.4	1.25	35	35	41.79936	45.19936	938	200	0.291786
3.4	1.25	36	36	42.99363	46.39363	938	200	0.28487
3.4	1.25	37	37	44.1879	47.5879	938	200	0.278272
3.4	1.25	38	38	45.38217	48.78217	938	200	0.271971
3.4	1.25	39	39	46.57643	49.97643	938	200	0.265947
3.4	1.25	40	40	47.7707	51.1707	938	200	0.260182

4.31 ZIG-ZAG (b=1.65) (k_1=938,k_2=200):

Table 4.31 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.65	5	0	4.55077	7.95077	938	200	0.845127
3.4	1.65	6	0	5.460925	8.860925	938	200	0.816514
3.4	1.65	7	0	6.371079	9.771079	938	200	0.7834
3.4	1.65	8	0	7.281233	10.68123	938	200	0.749234
3.4	1.65	9	0	8.191387	11.59139	938	200	0.715718
3.4	1.65	10	0	9.101541	12.50154	938	200	0.683665
3.4	1.65	11	0	10.01169	13.41169	938	200	0.653425
3.4	1.65	12	0	10.92185	14.32185	938	200	0.625106
3.4	1.65	13	0	11.832	15.232	938	200	0.598687
3.4	1.65	14	0	12.74216	16.14216	938	200	0.574084
3.4	1.65	15	0	13.65231	17.05231	938	200	0.551182
3.4	1.65	16	0	14.56247	17.96247	938	200	0.529857
3.4	1.65	17	0	15.47262	18.87262	938	200	0.509982
3.4	1.65	18	0	16.38277	19.78277	938	200	0.491438
3.4	1.65	19	0	17.29293	20.69293	938	200	0.474111
3.4	1.65	20	0	18.20308	21.60308	938	200	0.457898
3.4	1.65	21	0	19.11324	22.51324	938	200	0.442704
3.4	1.65	22	0	20.02339	23.42339	938	200	0.428443
3.4	1.65	23	0	20.93354	24.33354	938	200	0.415038
3.4	1.65	24	0	21.8437	25.2437	938	200	0.402416
3.4	1.65	25	0	22.75385	26.15385	938	200	0.390516
3.4	1.65	26	0	23.66401	27.06401	938	200	0.37928
3.4	1.65	27	0	24.57416	27.97416	938	200	0.368655
3.4	1.65	28	0	25.48431	28.88431	938	200	0.358595
3.4	1.65	29	0	26.39447	29.79447	938	200	0.349058
3.4	1.65	30	0	27.30462	30.70462	938	200	0.340004
3.4	1.65	31	0	28.21478	31.61478	938	200	0.331399
3.4	1.65	32	0	29.12493	32.52493	938	200	0.323212
3.4	1.65	33	0	30.03508	33.43508	938	200	0.315413
3.4	1.65	34	0	30.94524	34.34524	938	200	0.307976
3.4	1.65	35	0	31.85539	35.25539	938	200	0.300876
3.4	1.65	36	0	32.76555	36.16555	938	200	0.294092
3.4	1.65	37	0	33.6757	37.0757	938	200	0.287603
3.4	1.65	38	0	34.58586	37.98586	938	200	0.281391
3.4	1.65	39	0	35.49601	38.89601	938	200	0.275439
3.4	1.65	40	0	36.40616	39.80616	938	200	0.26973

4.32 ARMCHAIR (b=1.65)(k_1=938,k_2=200):

Table 4.32 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.65	5	5	7.882166	11.28217	938	200	0.726969
3.4	1.65	6	6	9.458599	12.8586	938	200	0.671576
3.4	1.65	7	7	11.03503	14.43503	938	200	0.621718
3.4	1.65	8	8	12.61146	16.01146	938	200	0.577509
3.4	1.65	9	9	14.1879	17.5879	938	200	0.53845
3.4	1.65	10	10	15.76433	19.16433	938	200	0.503899
3.4	1.65	11	11	17.34076	20.74076	938	200	0.473232
3.4	1.65	12	12	18.9172	22.3172	938	200	0.445895
3.4	1.65	13	13	20.49363	23.89363	938	200	0.421415
3.4	1.65	14	14	22.07006	25.47006	938	200	0.399392
3.4	1.65	15	15	23.6465	27.0465	938	200	0.37949
3.4	1.65	16	16	25.22293	28.62293	938	200	0.361429
3.4	1.65	17	17	26.79936	30.19936	938	200	0.344972
3.4	1.65	18	18	28.3758	31.7758	938	200	0.329921
3.4	1.65	19	19	29.95223	33.35223	938	200	0.316108
3.4	1.65	20	20	31.52866	34.92866	938	200	0.303387
3.4	1.65	21	21	33.1051	36.5051	938	200	0.291637
3.4	1.65	22	22	34.68153	38.08153	938	200	0.280753
3.4	1.65	23	23	36.25796	39.65796	938	200	0.270644
3.4	1.65	24	24	37.83439	41.23439	938	200	0.26123
3.4	1.65	25	25	39.41083	42.81083	938	200	0.252443
3.4	1.65	26	26	40.98726	44.38726	938	200	0.244224
3.4	1.65	27	27	42.56369	45.96369	938	200	0.236518
3.4	1.65	28	28	44.14013	47.54013	938	200	0.229281
3.4	1.65	29	29	45.71656	49.11656	938	200	0.222471
3.4	1.65	30	30	47.29299	50.69299	938	200	0.216051
3.4	1.65	31	31	48.86943	52.26943	938	200	0.209989
3.4	1.65	32	32	50.44586	53.84586	938	200	0.204257
3.4	1.65	33	33	52.02229	55.42229	938	200	0.198827
3.4	1.65	34	34	53.59873	56.99873	938	200	0.193678
3.4	1.65	35	35	55.17516	58.57516	938	200	0.188787
3.4	1.65	36	36	56.75159	60.15159	938	200	0.184136
3.4	1.65	37	37	58.32803	61.72803	938	200	0.179708
3.4	1.65	38	38	59.90446	63.30446	938	200	0.175487
3.4	1.65	39	39	61.48089	64.88089	938	200	0.17146
3.4	1.65	40	40	63.05732	66.45732	938	200	0.167612

4.33 ZIG-ZAG (b=1.35) (k_1=960,k_2=180):

Table 4.33 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.35	5	0	3.723358	7.123358	960	180	0.978594
3.4	1.35	6	0	4.468029	7.868029	960	180	0.962546
3.4	1.35	7	0	5.212701	8.612701	960	180	0.937176
3.4	1.35	8	0	5.957372	9.357372	960	180	0.90737
3.4	1.35	9	0	6.702044	10.10204	960	180	0.875843
3.4	1.35	10	0	7.446715	10.84672	960	180	0.844123
3.4	1.35	11	0	8.191387	11.59139	960	180	0.813062
3.4	1.35	12	0	8.936058	12.33606	960	180	0.783124
3.4	1.35	13	0	9.68073	13.08073	960	180	0.754539
3.4	1.35	14	0	10.4254	13.8254	960	180	0.727402
3.4	1.35	15	0	11.17007	14.57007	960	180	0.70173
3.4	1.35	16	0	11.91474	15.31474	960	180	0.677489
3.4	1.35	17	0	12.65942	16.05942	960	180	0.654623
3.4	1.35	18	0	13.40409	16.80409	960	180	0.63306
3.4	1.35	19	0	14.14876	17.54876	960	180	0.612721
3.4	1.35	20	0	14.89343	18.29343	960	180	0.593529
3.4	1.35	21	0	15.6381	19.0381	960	180	0.575406
3.4	1.35	22	0	16.38277	19.78277	960	180	0.558278
3.4	1.35	23	0	17.12745	20.52745	960	180	0.542076
3.4	1.35	24	0	17.87212	21.27212	960	180	0.526735
3.4	1.35	25	0	18.61679	22.01679	960	180	0.512194
3.4	1.35	26	0	19.36146	22.76146	960	180	0.498397
3.4	1.35	27	0	20.10613	23.50613	960	180	0.485292
3.4	1.35	28	0	20.8508	24.2508	960	180	0.472833
3.4	1.35	29	0	21.59547	24.99547	960	180	0.460975
3.4	1.35	30	0	22.34015	25.74015	960	180	0.449678
3.4	1.35	31	0	23.08482	26.48482	960	180	0.438904
3.4	1.35	32	0	23.82949	27.22949	960	180	0.428621
3.4	1.35	33	0	24.57416	27.97416	960	180	0.418795
3.4	1.35	34	0	25.31883	28.71883	960	180	0.4094
3.4	1.35	35	0	26.0635	29.4635	960	180	0.400407
3.4	1.35	36	0	26.80817	30.20817	960	180	0.391792
3.4	1.35	37	0	27.55285	30.95285	960	180	0.383533
3.4	1.35	38	0	28.29752	31.69752	960	180	0.375608
3.4	1.35	39	0	29.04219	32.44219	960	180	0.367999
3.4	1.35	40	0	29.78686	33.18686	960	180	0.360686

4.34 ARMCHAIR (b=1.35)(k_1=960,k_2=180):

Table 4.34 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.35	5	5	6.449045	9.849045	960	180	0.886634
3.4	1.35	6	6	7.738854	11.13885	960	180	0.831827
3.4	1.35	7	7	9.028662	12.42866	960	180	0.779492
3.4	1.35	8	8	10.31847	13.71847	960	180	0.731208
3.4	1.35	9	9	11.60828	15.00828	960	180	0.687295
3.4	1.35	10	10	12.89809	16.29809	960	180	0.647574
3.4	1.35	11	11	14.1879	17.5879	960	180	0.611684
3.4	1.35	12	12	15.47771	18.87771	960	180	0.579223
3.4	1.35	13	13	16.76752	20.16752	960	180	0.549796
3.4	1.35	14	14	18.05732	21.45732	960	180	0.523046
3.4	1.35	15	15	19.34713	22.74713	960	180	0.498655
3.4	1.35	16	16	20.63694	24.03694	960	180	0.476348
3.4	1.35	17	17	21.92675	25.32675	960	180	0.455882
3.4	1.35	18	18	23.21656	26.61656	960	180	0.43705
3.4	1.35	19	19	24.50637	27.90637	960	180	0.419672
3.4	1.35	20	20	25.79618	29.19618	960	180	0.40359
3.4	1.35	21	21	27.08599	30.48599	960	180	0.38867
3.4	1.35	22	22	28.3758	31.7758	960	180	0.374794
3.4	1.35	23	23	29.66561	33.06561	960	180	0.361857
3.4	1.35	24	24	30.95541	34.35541	960	180	0.349771
3.4	1.35	25	25	32.24522	35.64522	960	180	0.338454
3.4	1.35	26	26	33.53503	36.93503	960	180	0.327838
3.4	1.35	27	27	34.82484	38.22484	960	180	0.317859
3.4	1.35	28	28	36.11465	39.51465	960	180	0.308464
3.4	1.35	29	29	37.40446	40.80446	960	180	0.299602
3.4	1.35	30	30	38.69427	42.09427	960	180	0.291231
3.4	1.35	31	31	39.98408	43.38408	960	180	0.283311
3.4	1.35	32	32	41.27389	44.67389	960	180	0.275807
3.4	1.35	33	33	42.56369	45.96369	960	180	0.268687
3.4	1.35	34	34	43.8535	47.2535	960	180	0.261923
3.4	1.35	35	35	45.14331	48.54331	960	180	0.255489
3.4	1.35	36	36	46.43312	49.83312	960	180	0.249361
3.4	1.35	37	37	47.72293	51.12293	960	180	0.243519
3.4	1.35	38	38	49.01274	52.41274	960	180	0.237943
3.4	1.35	39	39	50.30255	53.70255	960	180	0.232615
3.4	1.35	40	40	51.59236	54.99236	960	180	0.227519

4.35 ZIG-ZAG (b=1.5) (k_1=960,k_2=180):

Table 4.35 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.5	5	0	4.137064	7.537064	960	180	0.897423
3.4	1.5	6	0	4.964477	8.364477	960	180	0.87439
3.4	1.5	7	0	5.79189	9.19189	960	180	0.844734
3.4	1.5	8	0	6.619302	10.0193	960	180	0.812543
3.4	1.5	9	0	7.446715	10.84672	960	180	0.779969
3.4	1.5	10	0	8.274128	11.67413	960	180	0.74814
3.4	1.5	11	0	9.101541	12.50154	960	180	0.717624
3.4	1.5	12	0	9.928954	13.32895	960	180	0.688685
3.4	1.5	13	0	10.75637	14.15637	960	180	0.661411
3.4	1.5	14	0	11.58378	14.98378	960	180	0.635795
3.4	1.5	15	0	12.41119	15.81119	960	180	0.611778
3.4	1.5	16	0	13.2386	16.6386	960	180	0.589275
3.4	1.5	17	0	14.06602	17.46602	960	180	0.568189
3.4	1.5	18	0	14.89343	18.29343	960	180	0.548421
3.4	1.5	19	0	15.72084	19.12084	960	180	0.529872
3.4	1.5	20	0	16.54826	19.94826	960	180	0.51245
3.4	1.5	21	0	17.37567	20.77567	960	180	0.496067
3.4	1.5	22	0	18.20308	21.60308	960	180	0.480643
3.4	1.5	23	0	19.03049	22.43049	960	180	0.466103
3.4	1.5	24	0	19.85791	23.25791	960	180	0.452378
3.4	1.5	25	0	20.68532	24.08532	960	180	0.439407
3.4	1.5	26	0	21.51273	24.91273	960	180	0.427132
3.4	1.5	27	0	22.34015	25.74015	960	180	0.415502
3.4	1.5	28	0	23.16756	26.56756	960	180	0.40447
3.4	1.5	29	0	23.99497	27.39497	960	180	0.393992
3.4	1.5	30	0	24.82238	28.22238	960	180	0.38403
3.4	1.5	31	0	25.6498	29.0498	960	180	0.374548
3.4	1.5	32	0	26.47721	29.87721	960	180	0.365512
3.4	1.5	33	0	27.30462	30.70462	960	180	0.356893
3.4	1.5	34	0	28.13204	31.53204	960	180	0.348663
3.4	1.5	35	0	28.95945	32.35945	960	180	0.340798
3.4	1.5	36	0	29.78686	33.18686	960	180	0.333274
3.4	1.5	37	0	30.61427	34.01427	960	180	0.32607
3.4	1.5	38	0	31.44169	34.84169	960	180	0.319166
3.4	1.5	39	0	32.2691	35.6691	960	180	0.312544
3.4	1.5	40	0	33.09651	36.49651	960	180	0.306188

4.36 ARMCHAIR (b=1.5) (k_1=960,k_2=180):

Table 4.36 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.5	5	5	7.165605	10.56561	960	180	0.790994
3.4	1.5	6	6	8.598726	11.99873	960	180	0.735992
3.4	1.5	7	7	10.03185	13.43185	960	180	0.685202
3.4	1.5	8	8	11.46497	14.86497	960	180	0.639373
3.4	1.5	9	9	12.89809	16.29809	960	180	0.598358
3.4	1.5	10	10	14.33121	17.73121	960	180	0.561714
3.4	1.5	11	11	15.76433	19.16433	960	180	0.528929
3.4	1.5	12	12	17.19745	20.59745	960	180	0.499513
3.4	1.5	13	13	18.63057	22.03057	960	180	0.473025
3.4	1.5	14	14	20.06369	23.46369	960	180	0.449084
3.4	1.5	15	15	21.49682	24.89682	960	180	0.427362
3.4	1.5	16	16	22.92994	26.32994	960	180	0.40758
3.4	1.5	17	17	24.36306	27.76306	960	180	0.389499
3.4	1.5	18	18	25.79618	29.19618	960	180	0.372917
3.4	1.5	19	19	27.2293	30.6293	960	180	0.357661
3.4	1.5	20	20	28.66242	32.06242	960	180	0.343581
3.4	1.5	21	21	30.09554	33.49554	960	180	0.33055
3.4	1.5	22	22	31.52866	34.92866	960	180	0.318457
3.4	1.5	23	23	32.96178	36.36178	960	180	0.307206
3.4	1.5	24	24	34.3949	37.7949	960	180	0.296713
3.4	1.5	25	25	35.82803	39.22803	960	180	0.286906
3.4	1.5	26	26	37.26115	40.66115	960	180	0.277719
3.4	1.5	27	27	38.69427	42.09427	960	180	0.269098
3.4	1.5	28	28	40.12739	43.52739	960	180	0.260991
3.4	1.5	29	29	41.56051	44.96051	960	180	0.253354
3.4	1.5	30	30	42.99363	46.39363	960	180	0.246148
3.4	1.5	31	31	44.42675	47.82675	960	180	0.239338
3.4	1.5	32	32	45.85987	49.25987	960	180	0.232893
3.4	1.5	33	33	47.29299	50.69299	960	180	0.226783
3.4	1.5	34	34	48.72611	52.12611	960	180	0.220984
3.4	1.5	35	35	50.15924	53.55924	960	180	0.215472
3.4	1.5	36	36	51.59236	54.99236	960	180	0.210228
3.4	1.5	37	37	53.02548	56.42548	960	180	0.205231
3.4	1.5	38	38	54.4586	57.8586	960	180	0.200466
3.4	1.5	39	39	55.89172	59.29172	960	180	0.195915
3.4	1.5	40	40	57.32484	60.72484	960	180	0.191566

4.37 ZIG-ZAG (b=1.3) (k_1=960,k_2=180):

Table 4.37 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.3	5	0	3.585455	6.985455	960	180	1.005558
3.4	1.3	6	0	4.302547	7.702547	960	180	0.992451
3.4	1.3	7	0	5.019638	8.419638	960	180	0.969032
3.4	1.3	8	0	5.736729	9.136729	960	180	0.940449
3.4	1.3	9	0	6.45382	9.85382	960	180	0.90962
3.4	1.3	10	0	7.170911	10.57091	960	180	0.878217
3.4	1.3	11	0	7.888002	11.288	960	180	0.847199
3.4	1.3	12	0	8.605093	12.00509	960	180	0.817103
3.4	1.3	13	0	9.322184	12.72218	960	180	0.788219
3.4	1.3	14	0	10.03928	13.43928	960	180	0.760682
3.4	1.3	15	0	10.75637	14.15637	960	180	0.734538
3.4	1.3	16	0	11.47346	14.87346	960	180	0.709778
3.4	1.3	17	0	12.19055	15.59055	960	180	0.686361
3.4	1.3	18	0	12.90764	16.30764	960	180	0.664228
3.4	1.3	19	0	13.62473	17.02473	960	180	0.643309
3.4	1.3	20	0	14.34182	17.74182	960	180	0.623534
3.4	1.3	21	0	15.05891	18.45891	960	180	0.604831
3.4	1.3	22	0	15.776	19.176	960	180	0.587128
3.4	1.3	23	0	16.4931	19.8931	960	180	0.570361
3.4	1.3	24	0	17.21019	20.61019	960	180	0.554465
3.4	1.3	25	0	17.92728	21.32728	960	180	0.539381
3.4	1.3	26	0	18.64437	22.04437	960	180	0.525055
3.4	1.3	27	0	19.36146	22.76146	960	180	0.511435
3.4	1.3	28	0	20.07855	23.47855	960	180	0.498474
3.4	1.3	29	0	20.79564	24.19564	960	180	0.486128
3.4	1.3	30	0	21.51273	24.91273	960	180	0.474357
3.4	1.3	31	0	22.22982	25.62982	960	180	0.463124
3.4	1.3	32	0	22.94692	26.34692	960	180	0.452394
3.4	1.3	33	0	23.66401	27.06401	960	180	0.442137
3.4	1.3	34	0	24.3811	27.7811	960	180	0.432321
3.4	1.3	35	0	25.09819	28.49819	960	180	0.422922
3.4	1.3	36	0	25.81528	29.21528	960	180	0.413913
3.4	1.3	37	0	26.53237	29.93237	960	180	0.405272
3.4	1.3	38	0	27.24946	30.64946	960	180	0.396976
3.4	1.3	39	0	27.96655	31.36655	960	180	0.389007
3.4	1.3	40	0	28.68364	32.08364	960	180	0.381346

4.38 ARMCHAIR (b=1.3) (k_1=960,k_2=180):

Table 4.38 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.3	5	5	6.210191	9.610191	960	180	0.920223
3.4	1.3	6	6	7.452229	10.85223	960	180	0.865966
3.4	1.3	7	7	8.694268	12.09427	960	180	0.813441
3.4	1.3	8	8	9.936306	13.33631	960	180	0.764551
3.4	1.3	9	9	11.17834	14.57834	960	180	0.719803
3.4	1.3	10	10	12.42038	15.82038	960	180	0.679131
3.4	1.3	11	11	13.66242	17.06242	960	180	0.642242
3.4	1.3	12	12	14.90446	18.30446	960	180	0.608772
3.4	1.3	13	13	16.1465	19.5465	960	180	0.578353
3.4	1.3	14	14	17.38854	20.78854	960	180	0.55064
3.4	1.3	15	15	18.63057	22.03057	960	180	0.525324
3.4	1.3	16	16	19.87261	23.27261	960	180	0.502131
3.4	1.3	17	17	21.11465	24.51465	960	180	0.480823
3.4	1.3	18	18	22.35669	25.75669	960	180	0.46119
3.4	1.3	19	19	23.59873	26.99873	960	180	0.443052
3.4	1.3	20	20	24.84076	28.24076	960	180	0.42625
3.4	1.3	21	21	26.0828	29.4828	960	180	0.410647
3.4	1.3	22	22	27.32484	30.72484	960	180	0.396124
3.4	1.3	23	23	28.56688	31.96688	960	180	0.382573
3.4	1.3	24	24	29.80892	33.20892	960	180	0.369904
3.4	1.3	25	25	31.05096	34.45096	960	180	0.358034
3.4	1.3	26	26	32.29299	35.69299	960	180	0.346892
3.4	1.3	27	27	33.53503	36.93503	960	180	0.336414
3.4	1.3	28	28	34.77707	38.17707	960	180	0.326543
3.4	1.3	29	29	36.01911	39.41911	960	180	0.317228
3.4	1.3	30	30	37.26115	40.66115	960	180	0.308425
3.4	1.3	31	31	38.50318	41.90318	960	180	0.300092
3.4	1.3	32	32	39.74522	43.14522	960	180	0.292194
3.4	1.3	33	33	40.98726	44.38726	960	180	0.284698
3.4	1.3	34	34	42.2293	45.6293	960	180	0.277574
3.4	1.3	35	35	43.47134	46.87134	960	180	0.270795
3.4	1.3	36	36	44.71338	48.11338	960	180	0.264337
3.4	1.3	37	37	45.95541	49.35541	960	180	0.258178
3.4	1.3	38	38	47.19745	50.59745	960	180	0.252298
3.4	1.3	39	39	48.43949	51.83949	960	180	0.246678
3.4	1.3	40	40	49.68153	53.08153	960	180	0.241302

4.39 ARMCHAIR (b=1.55) (k_1=960,k_2=180):

Table 4.39 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.55	5	0	4.274966	7.674966	960	180	0.870706
3.4	1.55	6	0	5.129959	8.529959	960	180	0.845886
3.4	1.55	7	0	5.984953	9.384953	960	180	0.815245
3.4	1.55	8	0	6.839946	10.23995	960	180	0.782617
3.4	1.55	9	0	7.694939	11.09494	960	180	0.749976
3.4	1.55	10	0	8.549932	11.94993	960	180	0.718329
3.4	1.55	11	0	9.404926	12.80493	960	180	0.688166
3.4	1.55	12	0	10.25992	13.65992	960	180	0.659689
3.4	1.55	13	0	11.11491	14.51491	960	180	0.632949
3.4	1.55	14	0	11.96991	15.36991	960	180	0.607911
3.4	1.55	15	0	12.8249	16.2249	960	180	0.584496
3.4	1.55	16	0	13.67989	17.07989	960	180	0.562606
3.4	1.55	17	0	14.53488	17.93488	960	180	0.542133
3.4	1.55	18	0	15.38988	18.78988	960	180	0.522973
3.4	1.55	19	0	16.24487	19.64487	960	180	0.505021
3.4	1.55	20	0	17.09986	20.49986	960	180	0.488183
3.4	1.55	21	0	17.95486	21.35486	960	180	0.472368
3.4	1.55	22	0	18.80985	22.20985	960	180	0.457495
3.4	1.55	23	0	19.66484	23.06484	960	180	0.443487
3.4	1.55	24	0	20.51984	23.91984	960	180	0.430278
3.4	1.55	25	0	21.37483	24.77483	960	180	0.417805
3.4	1.55	26	0	22.22982	25.62982	960	180	0.40601
3.4	1.55	27	0	23.08482	26.48482	960	180	0.394843
3.4	1.55	28	0	23.93981	27.33981	960	180	0.384257
3.4	1.55	29	0	24.7948	28.1948	960	180	0.374209
3.4	1.55	30	0	25.6498	29.0498	960	180	0.364661
3.4	1.55	31	0	26.50479	29.90479	960	180	0.355578
3.4	1.55	32	0	27.35978	30.75978	960	180	0.346927
3.4	1.55	33	0	28.21478	31.61478	960	180	0.338679
3.4	1.55	34	0	29.06977	32.46977	960	180	0.330807
3.4	1.55	35	0	29.92476	33.32476	960	180	0.323287
3.4	1.55	36	0	30.77976	34.17976	960	180	0.316096
3.4	1.55	37	0	31.63475	35.03475	960	180	0.309213
3.4	1.55	38	0	32.48974	35.88974	960	180	0.30262
3.4	1.55	39	0	33.34474	36.74474	960	180	0.296298
3.4	1.55	40	0	34.19973	37.59973	960	180	0.290232

4.40 ARMCHAIR (b=1.55) (k_1=960,k_2=180):

Table 4.40 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.55	5	5	7.404459	10.80446	960	180	0.76099
3.4	1.55	6	6	8.88535	12.28535	960	180	0.706303
3.4	1.55	7	7	10.36624	13.76624	960	180	0.65627
3.4	1.55	8	8	11.84713	15.24713	960	180	0.611405
3.4	1.55	9	9	13.32803	16.72803	960	180	0.571437
3.4	1.55	10	10	14.80892	18.20892	960	180	0.535855
3.4	1.55	11	11	16.28981	19.68981	960	180	0.504109
3.4	1.55	12	12	17.7707	21.1707	960	180	0.475692
3.4	1.55	13	13	19.25159	22.65159	960	180	0.450154
3.4	1.55	14	14	20.73248	24.13248	960	180	0.427109
3.4	1.55	15	15	22.21338	25.61338	960	180	0.406231
3.4	1.55	16	16	23.69427	27.09427	960	180	0.38724
3.4	1.55	17	17	25.17516	28.57516	960	180	0.369902
3.4	1.55	18	18	26.65605	30.05605	960	180	0.354017
3.4	1.55	19	19	28.13694	31.53694	960	180	0.339414
3.4	1.55	20	20	29.61783	33.01783	960	180	0.325948
3.4	1.55	21	21	31.09873	34.49873	960	180	0.313493
3.4	1.55	22	22	32.57962	35.97962	960	180	0.301943
3.4	1.55	23	23	34.06051	37.46051	960	180	0.291203
3.4	1.55	24	24	35.5414	38.9414	960	180	0.281192
3.4	1.55	25	25	37.02229	40.42229	960	180	0.27184
3.4	1.55	26	26	38.50318	41.90318	960	180	0.263084
3.4	1.55	27	27	39.98408	43.38408	960	180	0.25487
3.4	1.55	28	28	41.46497	44.86497	960	180	0.247149
3.4	1.55	29	29	42.94586	46.34586	960	180	0.239878
3.4	1.55	30	30	44.42675	47.82675	960	180	0.233021
3.4	1.55	31	31	45.90764	49.30764	960	180	0.226542
3.4	1.55	32	32	47.38854	50.78854	960	180	0.220411
3.4	1.55	33	33	48.86943	52.26943	960	180	0.214602
3.4	1.55	34	34	50.35032	53.75032	960	180	0.209089
3.4	1.55	35	35	51.83121	55.23121	960	180	0.203852
3.4	1.55	36	36	53.3121	56.7121	960	180	0.198869
3.4	1.55	37	37	54.79299	58.19299	960	180	0.194122
3.4	1.55	38	38	56.27389	59.67389	960	180	0.189596
3.4	1.55	39	39	57.75478	61.15478	960	180	0.185276
3.4	1.55	40	40	59.23567	62.63567	960	180	0.181147

4.41 ZIG-ZAG (b=1.25) (k_1=960,k_2=180):

Table 4.41 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.25	5	0	3.447553	6.847553	960	180	1.032202
3.4	1.25	6	0	4.137064	7.537064	960	180	1.02238
3.4	1.25	7	0	4.826575	8.226575	960	180	1.001211
3.4	1.25	8	0	5.516085	8.916085	960	180	0.974108
3.4	1.25	9	0	6.205596	9.605596	960	180	0.94419
3.4	1.25	10	0	6.895107	10.29511	960	180	0.91328
3.4	1.25	11	0	7.584617	10.98462	960	180	0.882447
3.4	1.25	12	0	8.274128	11.67413	960	180	0.852311
3.4	1.25	13	0	8.963639	12.36364	960	180	0.823221
3.4	1.25	14	0	9.653149	13.05315	960	180	0.795359
3.4	1.25	15	0	10.34266	13.74266	960	180	0.768803
3.4	1.25	16	0	11.03217	14.43217	960	180	0.743571
3.4	1.25	17	0	11.72168	15.12168	960	180	0.719639
3.4	1.25	18	0	12.41119	15.81119	960	180	0.696962
3.4	1.25	19	0	13.1007	16.5007	960	180	0.675483
3.4	1.25	20	0	13.79021	17.19021	960	180	0.655139
3.4	1.25	21	0	14.47972	17.87972	960	180	0.635863
3.4	1.25	22	0	15.16923	18.56923	960	180	0.61759
3.4	1.25	23	0	15.85875	19.25875	960	180	0.600257
3.4	1.25	24	0	16.54826	19.94826	960	180	0.583804
3.4	1.25	25	0	17.23777	20.63777	960	180	0.568173
3.4	1.25	26	0	17.92728	21.32728	960	180	0.55331
3.4	1.25	27	0	18.61679	22.01679	960	180	0.539165
3.4	1.25	28	0	19.3063	22.7063	960	180	0.525692
3.4	1.25	29	0	19.99581	23.39581	960	180	0.512847
3.4	1.25	30	0	20.68532	24.08532	960	180	0.50059
3.4	1.25	31	0	21.37483	24.77483	960	180	0.488884
3.4	1.25	32	0	22.06434	25.46434	960	180	0.477695
3.4	1.25	33	0	22.75385	26.15385	960	180	0.466991
3.4	1.25	34	0	23.44336	26.84336	960	180	0.456742
3.4	1.25	35	0	24.13287	27.53287	960	180	0.446921
3.4	1.25	36	0	24.82238	28.22238	960	180	0.437503
3.4	1.25	37	0	25.51189	28.91189	960	180	0.428464
3.4	1.25	38	0	26.20141	29.60141	960	180	0.419783
3.4	1.25	39	0	26.89092	30.29092	960	180	0.411439
3.4	1.25	40	0	27.58043	30.98043	960	180	0.403414

4.42 ARMCHAIR (b=1.25)(k_1=960,k_2=180):

Table 4.42 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.25	5	5	5.971338	9.371338	960	180	0.954538
3.4	1.25	6	6	7.165605	10.56561	960	180	0.901133
3.4	1.25	7	7	8.359873	11.75987	960	180	0.848631
3.4	1.25	8	8	9.55414	12.95414	960	180	0.79928
3.4	1.25	9	9	10.74841	14.14841	960	180	0.753796
3.4	1.25	10	10	11.94268	15.34268	960	180	0.712236
3.4	1.25	11	11	13.13694	16.53694	960	180	0.674386
3.4	1.25	12	12	14.33121	17.73121	960	180	0.639928
3.4	1.25	13	13	15.52548	18.92548	960	180	0.608522
3.4	1.25	14	14	16.71975	20.11975	960	180	0.579842
3.4	1.25	15	15	17.91401	21.31401	960	180	0.553589
3.4	1.25	16	16	19.10828	22.50828	960	180	0.529495
3.4	1.25	17	17	20.30255	23.70255	960	180	0.507324
3.4	1.25	18	18	21.49682	24.89682	960	180	0.486868
3.4	1.25	19	19	22.69108	26.09108	960	180	0.467946
3.4	1.25	20	20	23.88535	27.28535	960	180	0.450399
3.4	1.25	21	21	25.07962	28.47962	960	180	0.434087
3.4	1.25	22	22	26.27389	29.67389	960	180	0.41889
3.4	1.25	23	23	27.46815	30.86815	960	180	0.4047
3.4	1.25	24	24	28.66242	32.06242	960	180	0.391422
3.4	1.25	25	25	29.85669	33.25669	960	180	0.378973
3.4	1.25	26	26	31.05096	34.45096	960	180	0.36728
3.4	1.25	27	27	32.24522	35.64522	960	180	0.356277
3.4	1.25	28	28	33.43949	36.83949	960	180	0.345905
3.4	1.25	29	29	34.63376	38.03376	960	180	0.336113
3.4	1.25	30	30	35.82803	39.22803	960	180	0.326855
3.4	1.25	31	31	37.02229	40.42229	960	180	0.318087
3.4	1.25	32	32	38.21656	41.61656	960	180	0.309773
3.4	1.25	33	33	39.41083	42.81083	960	180	0.301879
3.4	1.25	34	34	40.6051	44.0051	960	180	0.294374
3.4	1.25	35	35	41.79936	45.19936	960	180	0.28723
3.4	1.25	36	36	42.99363	46.39363	960	180	0.280422
3.4	1.25	37	37	44.1879	47.5879	960	180	0.273927
3.4	1.25	38	38	45.38217	48.78217	960	180	0.267724
3.4	1.25	39	39	46.57643	49.97643	960	180	0.261794
3.4	1.25	40	40	47.7707	51.1707	960	180	0.25612

4.43 ZIG-ZAG (b=1.65) (k_1=960,k_2=180):

Table 4.43 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.65	5	0	4.55077	7.95077	960	180	0.818364
3.4	1.65	6	0	5.460925	8.860925	960	180	0.790657
3.4	1.65	7	0	6.371079	9.771079	960	180	0.758591
3.4	1.65	8	0	7.281233	10.68123	960	180	0.725508
3.4	1.65	9	0	8.191387	11.59139	960	180	0.693053
3.4	1.65	10	0	9.101541	12.50154	960	180	0.662015
3.4	1.65	11	0	10.01169	13.41169	960	180	0.632733
3.4	1.65	12	0	10.92185	14.32185	960	180	0.60531
3.4	1.65	13	0	11.832	15.232	960	180	0.579728
3.4	1.65	14	0	12.74216	16.14216	960	180	0.555904
3.4	1.65	15	0	13.65231	17.05231	960	180	0.533728
3.4	1.65	16	0	14.56247	17.96247	960	180	0.513078
3.4	1.65	17	0	15.47262	18.87262	960	180	0.493832
3.4	1.65	18	0	16.38277	19.78277	960	180	0.475875
3.4	1.65	19	0	17.29293	20.69293	960	180	0.459097
3.4	1.65	20	0	18.20308	21.60308	960	180	0.443398
3.4	1.65	21	0	19.11324	22.51324	960	180	0.428685
3.4	1.65	22	0	20.02339	23.42339	960	180	0.414876
3.4	1.65	23	0	20.93354	24.33354	960	180	0.401894
3.4	1.65	24	0	21.8437	25.2437	960	180	0.389673
3.4	1.65	25	0	22.75385	26.15385	960	180	0.37815
3.4	1.65	26	0	23.66401	27.06401	960	180	0.367269
3.4	1.65	27	0	24.57416	27.97416	960	180	0.356981
3.4	1.65	28	0	25.48431	28.88431	960	180	0.347239
3.4	1.65	29	0	26.39447	29.79447	960	180	0.338004
3.4	1.65	30	0	27.30462	30.70462	960	180	0.329237
3.4	1.65	31	0	28.21478	31.61478	960	180	0.320905
3.4	1.65	32	0	29.12493	32.52493	960	180	0.312977
3.4	1.65	33	0	30.03508	33.43508	960	180	0.305425
3.4	1.65	34	0	30.94524	34.34524	960	180	0.298223
3.4	1.65	35	0	31.85539	35.25539	960	180	0.291348
3.4	1.65	36	0	32.76555	36.16555	960	180	0.284779
3.4	1.65	37	0	33.6757	37.0757	960	180	0.278495
3.4	1.65	38	0	34.58586	37.98586	960	180	0.27248
3.4	1.65	39	0	35.49601	38.89601	960	180	0.266716
3.4	1.65	40	0	36.40616	39.80616	960	180	0.261189

4.44 ARMCHAIR (b=1.65)(k_1=960,k_2=180):

Table 4.44 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.65	5	5	7.882166	11.28217	960	180	0.703948
3.4	1.65	6	6	9.458599	12.8586	960	180	0.650309
3.4	1.65	7	7	11.03503	14.43503	960	180	0.60203
3.4	1.65	8	8	12.61146	16.01146	960	180	0.559221
3.4	1.65	9	9	14.1879	17.5879	960	180	0.521399
3.4	1.65	10	10	15.76433	19.16433	960	180	0.487942
3.4	1.65	11	11	17.34076	20.74076	960	180	0.458246
3.4	1.65	12	12	18.9172	22.3172	960	180	0.431775
3.4	1.65	13	13	20.49363	23.89363	960	180	0.40807
3.4	1.65	14	14	22.07006	25.47006	960	180	0.386744
3.4	1.65	15	15	23.6465	27.0465	960	180	0.367472
3.4	1.65	16	16	25.22293	28.62293	960	180	0.349983
3.4	1.65	17	17	26.79936	30.19936	960	180	0.334048
3.4	1.65	18	18	28.3758	31.7758	960	180	0.319474
3.4	1.65	19	19	29.95223	33.35223	960	180	0.306097
3.4	1.65	20	20	31.52866	34.92866	960	180	0.29378
3.4	1.65	21	21	33.1051	36.5051	960	180	0.282402
3.4	1.65	22	22	34.68153	38.08153	960	180	0.271863
3.4	1.65	23	23	36.25796	39.65796	960	180	0.262073
3.4	1.65	24	24	37.83439	41.23439	960	180	0.252957
3.4	1.65	25	25	39.41083	42.81083	960	180	0.244449
3.4	1.65	26	26	40.98726	44.38726	960	180	0.23649
3.4	1.65	27	27	42.56369	45.96369	960	180	0.229028
3.4	1.65	28	28	44.14013	47.54013	960	180	0.22202
3.4	1.65	29	29	45.71656	49.11656	960	180	0.215426
3.4	1.65	30	30	47.29299	50.69299	960	180	0.209209
3.4	1.65	31	31	48.86943	52.26943	960	180	0.203339
3.4	1.65	32	32	50.44586	53.84586	960	180	0.197788
3.4	1.65	33	33	52.02229	55.42229	960	180	0.192531
3.4	1.65	34	34	53.59873	56.99873	960	180	0.187544
3.4	1.65	35	35	55.17516	58.57516	960	180	0.182809
3.4	1.65	36	36	56.75159	60.15159	960	180	0.178305
3.4	1.65	37	37	58.32803	61.72803	960	180	0.174017
3.4	1.65	38	38	59.90446	63.30446	960	180	0.16993
3.4	1.65	39	39	61.48089	64.88089	960	180	0.16603
3.4	1.65	40	40	63.05732	66.45732	960	180	0.162304

4.45 ZIG-ZAG (b=1.35) (k_1=1068,k_2=200):

Table 4.45 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.35	5	0	3.723358	7.123358	1068	200	1.088209
3.4	1.35	6	0	4.468029	7.868029	1068	200	1.070363
3.4	1.35	7	0	5.212701	8.612701	1068	200	1.042152
3.4	1.35	8	0	5.957372	9.357372	1068	200	1.009006
3.4	1.35	9	0	6.702044	10.10204	1068	200	0.973948
3.4	1.35	10	0	7.446715	10.84672	1068	200	0.938675
3.4	1.35	11	0	8.191387	11.59139	1068	200	0.904136
3.4	1.35	12	0	8.936058	12.33606	1068	200	0.870844
3.4	1.35	13	0	9.68073	13.08073	1068	200	0.839056
3.4	1.35	14	0	10.4254	13.8254	1068	200	0.80888
3.4	1.35	15	0	11.17007	14.57007	1068	200	0.780332
3.4	1.35	16	0	11.91474	15.31474	1068	200	0.753377
3.4	1.35	17	0	12.65942	16.05942	1068	200	0.727949
3.4	1.35	18	0	13.40409	16.80409	1068	200	0.70397
3.4	1.35	19	0	14.14876	17.54876	1068	200	0.681354
3.4	1.35	20	0	14.89343	18.29343	1068	200	0.660011
3.4	1.35	21	0	15.6381	19.0381	1068	200	0.639858
3.4	1.35	22	0	16.38277	19.78277	1068	200	0.620812
3.4	1.35	23	0	17.12745	20.52745	1068	200	0.602795
3.4	1.35	24	0	17.87212	21.27212	1068	200	0.585736
3.4	1.35	25	0	18.61679	22.01679	1068	200	0.569566
3.4	1.35	26	0	19.36146	22.76146	1068	200	0.554223
3.4	1.35	27	0	20.10613	23.50613	1068	200	0.539651
3.4	1.35	28	0	20.8508	24.2508	1068	200	0.525796
3.4	1.35	29	0	21.59547	24.99547	1068	200	0.51261
3.4	1.35	30	0	22.34015	25.74015	1068	200	0.500047
3.4	1.35	31	0	23.08482	26.48482	1068	200	0.488067
3.4	1.35	32	0	23.82949	27.22949	1068	200	0.476632
3.4	1.35	33	0	24.57416	27.97416	1068	200	0.465706
3.4	1.35	34	0	25.31883	28.71883	1068	200	0.455258
3.4	1.35	35	0	26.0635	29.4635	1068	200	0.445257
3.4	1.35	36	0	26.80817	30.20817	1068	200	0.435678
3.4	1.35	37	0	27.55285	30.95285	1068	200	0.426493
3.4	1.35	38	0	28.29752	31.69752	1068	200	0.417681
3.4	1.35	39	0	29.04219	32.44219	1068	200	0.409219
3.4	1.35	40	0	29.78686	33.18686	1068	200	0.401088

4.46 ARMCHAIR (b=1.35)(k_1=1068,k_2=200):

Table 4.46 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.35	5	5	6.449045	9.849045	1068	200	0.985948
3.4	1.35	6	6	7.738854	11.13885	1068	200	0.925002
3.4	1.35	7	7	9.028662	12.42866	1068	200	0.866805
3.4	1.35	8	8	10.31847	13.71847	1068	200	0.813113
3.4	1.35	9	9	11.60828	15.00828	1068	200	0.764281
3.4	1.35	10	10	12.89809	16.29809	1068	200	0.72011
3.4	1.35	11	11	14.1879	17.5879	1068	200	0.680201
3.4	1.35	12	12	15.47771	18.87771	1068	200	0.644103
3.4	1.35	13	13	16.76752	20.16752	1068	200	0.61138
3.4	1.35	14	14	18.05732	21.45732	1068	200	0.581633
3.4	1.35	15	15	19.34713	22.74713	1068	200	0.554511
3.4	1.35	16	16	20.63694	24.03694	1068	200	0.529705
3.4	1.35	17	17	21.92675	25.32675	1068	200	0.506947
3.4	1.35	18	18	23.21656	26.61656	1068	200	0.486005
3.4	1.35	19	19	24.50637	27.90637	1068	200	0.46668
3.4	1.35	20	20	25.79618	29.19618	1068	200	0.448797
3.4	1.35	21	21	27.08599	30.48599	1068	200	0.432206
3.4	1.35	22	22	28.3758	31.7758	1068	200	0.416775
3.4	1.35	23	23	29.66561	33.06561	1068	200	0.40239
3.4	1.35	24	24	30.95541	34.35541	1068	200	0.38895
3.4	1.35	25	25	32.24522	35.64522	1068	200	0.376365
3.4	1.35	26	26	33.53503	36.93503	1068	200	0.36456
3.4	1.35	27	27	34.82484	38.22484	1068	200	0.353464
3.4	1.35	28	28	36.11465	39.51465	1068	200	0.343016
3.4	1.35	29	29	37.40446	40.80446	1068	200	0.333162
3.4	1.35	30	30	38.69427	42.09427	1068	200	0.323853
3.4	1.35	31	31	39.98408	43.38408	1068	200	0.315046
3.4	1.35	32	32	41.27389	44.67389	1068	200	0.306701
3.4	1.35	33	33	42.56369	45.96369	1068	200	0.298783
3.4	1.35	34	34	43.8535	47.2535	1068	200	0.291262
3.4	1.35	35	35	45.14331	48.54331	1068	200	0.284107
3.4	1.35	36	36	46.43312	49.83312	1068	200	0.277293
3.4	1.35	37	37	47.72293	51.12293	1068	200	0.270796
3.4	1.35	38	38	49.01274	52.41274	1068	200	0.264595
3.4	1.35	39	39	50.30255	53.70255	1068	200	0.258671
3.4	1.35	40	40	51.59236	54.99236	1068	200	0.253004

4.47 ZIG-ZAG (b=1.5) (k_1=1068,k_2=200):

Table 4.47 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.5	5	0	4.137064	7.537064	1068	200	0.997884
3.4	1.5	6	0	4.964477	8.364477	1068	200	0.972273
3.4	1.5	7	0	5.79189	9.19189	1068	200	0.939297
3.4	1.5	8	0	6.619302	10.0193	1068	200	0.903503
3.4	1.5	9	0	7.446715	10.84672	1068	200	0.867282
3.4	1.5	10	0	8.274128	11.67413	1068	200	0.831889
3.4	1.5	11	0	9.101541	12.50154	1068	200	0.797958
3.4	1.5	12	0	9.928954	13.32895	1068	200	0.765779
3.4	1.5	13	0	10.75637	14.15637	1068	200	0.735452
3.4	1.5	14	0	11.58378	14.98378	1068	200	0.706968
3.4	1.5	15	0	12.41119	15.81119	1068	200	0.680262
3.4	1.5	16	0	13.2386	16.6386	1068	200	0.65524
3.4	1.5	17	0	14.06602	17.46602	1068	200	0.631794
3.4	1.5	18	0	14.89343	18.29343	1068	200	0.609813
3.4	1.5	19	0	15.72084	19.12084	1068	200	0.589188
3.4	1.5	20	0	16.54826	19.94826	1068	200	0.569816
3.4	1.5	21	0	17.37567	20.77567	1068	200	0.551599
3.4	1.5	22	0	18.20308	21.60308	1068	200	0.534448
3.4	1.5	23	0	19.03049	22.43049	1068	200	0.51828
3.4	1.5	24	0	19.85791	23.25791	1068	200	0.503019
3.4	1.5	25	0	20.68532	24.08532	1068	200	0.488596
3.4	1.5	26	0	21.51273	24.91273	1068	200	0.474947
3.4	1.5	27	0	22.34015	25.74015	1068	200	0.462015
3.4	1.5	28	0	23.16756	26.56756	1068	200	0.449748
3.4	1.5	29	0	23.99497	27.39497	1068	200	0.438097
3.4	1.5	30	0	24.82238	28.22238	1068	200	0.42702
3.4	1.5	31	0	25.6498	29.0498	1068	200	0.416476
3.4	1.5	32	0	26.47721	29.87721	1068	200	0.406429
3.4	1.5	33	0	27.30462	30.70462	1068	200	0.396845
3.4	1.5	34	0	28.13204	31.53204	1068	200	0.387694
3.4	1.5	35	0	28.95945	32.35945	1068	200	0.378949
3.4	1.5	36	0	29.78686	33.18686	1068	200	0.370582
3.4	1.5	37	0	30.61427	34.01427	1068	200	0.362572
3.4	1.5	38	0	31.44169	34.84169	1068	200	0.354895
3.4	1.5	39	0	32.2691	35.6691	1068	200	0.347532
3.4	1.5	40	0	33.09651	36.49651	1068	200	0.340464

4.48 ARMCHAIR (b=1.5)(k_1=1068,k_2=200):

Table 4.48 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.5	5	5	7.165605	10.56561	1068	200	0.879541
3.4	1.5	6	6	8.598726	11.99873	1068	200	0.818382
3.4	1.5	7	7	10.03185	13.43185	1068	200	0.761906
3.4	1.5	8	8	11.46497	14.86497	1068	200	0.710947
3.4	1.5	9	9	12.89809	16.29809	1068	200	0.665341
3.4	1.5	10	10	14.33121	17.73121	1068	200	0.624595
3.4	1.5	11	11	15.76433	19.16433	1068	200	0.58814
3.4	1.5	12	12	17.19745	20.59745	1068	200	0.55543
3.4	1.5	13	13	18.63057	22.03057	1068	200	0.525977
3.4	1.5	14	14	20.06369	23.46369	1068	200	0.499356
3.4	1.5	15	15	21.49682	24.89682	1068	200	0.475202
3.4	1.5	16	16	22.92994	26.32994	1068	200	0.453206
3.4	1.5	17	17	24.36306	27.76306	1068	200	0.433101
3.4	1.5	18	18	25.79618	29.19618	1068	200	0.414663
3.4	1.5	19	19	27.2293	30.6293	1068	200	0.397699
3.4	1.5	20	20	28.66242	32.06242	1068	200	0.382043
3.4	1.5	21	21	30.09554	33.49554	1068	200	0.367553
3.4	1.5	22	22	31.52866	34.92866	1068	200	0.354106
3.4	1.5	23	23	32.96178	36.36178	1068	200	0.341596
3.4	1.5	24	24	34.3949	37.7949	1068	200	0.329928
3.4	1.5	25	25	35.82803	39.22803	1068	200	0.319023
3.4	1.5	26	26	37.26115	40.66115	1068	200	0.308808
3.4	1.5	27	27	38.69427	42.09427	1068	200	0.299222
3.4	1.5	28	28	40.12739	43.52739	1068	200	0.290207
3.4	1.5	29	29	41.56051	44.96051	1068	200	0.281715
3.4	1.5	30	30	42.99363	46.39363	1068	200	0.273703
3.4	1.5	31	31	44.42675	47.82675	1068	200	0.266131
3.4	1.5	32	32	45.85987	49.25987	1068	200	0.258963
3.4	1.5	33	33	47.29299	50.69299	1068	200	0.25217
3.4	1.5	34	34	48.72611	52.12611	1068	200	0.245722
3.4	1.5	35	35	50.15924	53.55924	1068	200	0.239593
3.4	1.5	36	36	51.59236	54.99236	1068	200	0.233761
3.4	1.5	37	37	53.02548	56.42548	1068	200	0.228206
3.4	1.5	38	38	54.4586	57.8586	1068	200	0.222907
3.4	1.5	39	39	55.89172	59.29172	1068	200	0.217847
3.4	1.5	40	40	57.32484	60.72484	1068	200	0.213011

4.49 ZIG-ZAG (b=1.3) (k_1=1068,k_2=200):

Table 4.49 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.3	5	0	3.585455	6.985455	1068	200	1.118217
3.4	1.3	6	0	4.302547	7.702547	1068	200	1.103642
3.4	1.3	7	0	5.019638	8.419638	1068	200	1.077598
3.4	1.3	8	0	5.736729	9.136729	1068	200	1.045813
3.4	1.3	9	0	6.45382	9.85382	1068	200	1.01153
3.4	1.3	10	0	7.170911	10.57091	1068	200	0.976609
3.4	1.3	11	0	7.888002	11.288	1068	200	0.942115
3.4	1.3	12	0	8.605093	12.00509	1068	200	0.908648
3.4	1.3	13	0	9.322184	12.72218	1068	200	0.876528
3.4	1.3	14	0	10.03928	13.43928	1068	200	0.845906
3.4	1.3	15	0	10.75637	14.15637	1068	200	0.816833
3.4	1.3	16	0	11.47346	14.87346	1068	200	0.789299
3.4	1.3	17	0	12.19055	15.59055	1068	200	0.763259
3.4	1.3	18	0	12.90764	16.30764	1068	200	0.738645
3.4	1.3	19	0	13.62473	17.02473	1068	200	0.715383
3.4	1.3	20	0	14.34182	17.74182	1068	200	0.693393
3.4	1.3	21	0	15.05891	18.45891	1068	200	0.672593
3.4	1.3	22	0	15.776	19.176	1068	200	0.652908
3.4	1.3	23	0	16.4931	19.8931	1068	200	0.634262
3.4	1.3	24	0	17.21019	20.61019	1068	200	0.616585
3.4	1.3	25	0	17.92728	21.32728	1068	200	0.599811
3.4	1.3	26	0	18.64437	22.04437	1068	200	0.58388
3.4	1.3	27	0	19.36146	22.76146	1068	200	0.568734
3.4	1.3	28	0	20.07855	23.47855	1068	200	0.554321
3.4	1.3	29	0	20.79564	24.19564	1068	200	0.540592
3.4	1.3	30	0	21.51273	24.91273	1068	200	0.527502
3.4	1.3	31	0	22.22982	25.62982	1068	200	0.51501
3.4	1.3	32	0	22.94692	26.34692	1068	200	0.503079
3.4	1.3	33	0	23.66401	27.06401	1068	200	0.491672
3.4	1.3	34	0	24.3811	27.7811	1068	200	0.480757
3.4	1.3	35	0	25.09819	28.49819	1068	200	0.470304
3.4	1.3	36	0	25.81528	29.21528	1068	200	0.460286
3.4	1.3	37	0	26.53237	29.93237	1068	200	0.450677
3.4	1.3	38	0	27.24946	30.64946	1068	200	0.441452
3.4	1.3	39	0	27.96655	31.36655	1068	200	0.43259
3.4	1.3	40	0	28.68364	32.08364	1068	200	0.424071

4.50 ARMCHAIR (b=1.3)(k_1=1068,k_2=200):

Table 4.50 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.3	5	5	6.210191	9.610191	1068	200	1.023322
3.4	1.3	6	6	7.452229	10.85223	1068	200	0.962985
3.4	1.3	7	7	8.694268	12.09427	1068	200	0.904576
3.4	1.3	8	8	9.936306	13.33631	1068	200	0.850208
3.4	1.3	9	9	11.17834	14.57834	1068	200	0.800447
3.4	1.3	10	10	12.42038	15.82038	1068	200	0.755218
3.4	1.3	11	11	13.66242	17.06242	1068	200	0.714196
3.4	1.3	12	12	14.90446	18.30446	1068	200	0.676977
3.4	1.3	13	13	16.1465	19.5465	1068	200	0.643149
3.4	1.3	14	14	17.38854	20.78854	1068	200	0.612331
3.4	1.3	15	15	18.63057	22.03057	1068	200	0.584179
3.4	1.3	16	16	19.87261	23.27261	1068	200	0.558388
3.4	1.3	17	17	21.11465	24.51465	1068	200	0.534692
3.4	1.3	18	18	22.35669	25.75669	1068	200	0.51286
3.4	1.3	19	19	23.59873	26.99873	1068	200	0.492689
3.4	1.3	20	20	24.84076	28.24076	1068	200	0.474005
3.4	1.3	21	21	26.0828	29.4828	1068	200	0.456655
3.4	1.3	22	22	27.32484	30.72484	1068	200	0.440504
3.4	1.3	23	23	28.56688	31.96688	1068	200	0.425435
3.4	1.3	24	24	29.80892	33.20892	1068	200	0.411347
3.4	1.3	25	25	31.05096	34.45096	1068	200	0.398147
3.4	1.3	26	26	32.29299	35.69299	1068	200	0.385757
3.4	1.3	27	27	33.53503	36.93503	1068	200	0.374105
3.4	1.3	28	28	34.77707	38.17707	1068	200	0.363127
3.4	1.3	29	29	36.01911	39.41911	1068	200	0.352769
3.4	1.3	30	30	37.26115	40.66115	1068	200	0.34298
3.4	1.3	31	31	38.50318	41.90318	1068	200	0.333714
3.4	1.3	32	32	39.74522	43.14522	1068	200	0.324931
3.4	1.3	33	33	40.98726	44.38726	1068	200	0.316595
3.4	1.3	34	34	42.2293	45.6293	1068	200	0.308672
3.4	1.3	35	35	43.47134	46.87134	1068	200	0.301134
3.4	1.3	36	36	44.71338	48.11338	1068	200	0.293952
3.4	1.3	37	37	45.95541	49.35541	1068	200	0.287103
3.4	1.3	38	38	47.19745	50.59745	1068	200	0.280564
3.4	1.3	39	39	48.43949	51.83949	1068	200	0.274315
3.4	1.3	40	40	49.68153	53.08153	1068	200	0.268336

4.51 ZIG-ZAG (b=1.55)(k_1=1068,k_2=200):

Table 4.51 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.55	5	0	4.274966	7.674966	1068	200	0.968157
3.4	1.55	6	0	5.129959	8.529959	1068	200	0.940559
3.4	1.55	7	0	5.984953	9.384953	1068	200	0.906489
3.4	1.55	8	0	6.839946	10.23995	1068	200	0.870209
3.4	1.55	9	0	7.694939	11.09494	1068	200	0.833914
3.4	1.55	10	0	8.549932	11.94993	1068	200	0.798726
3.4	1.55	11	0	9.404926	12.80493	1068	200	0.765187
3.4	1.55	12	0	10.25992	13.65992	1068	200	0.733523
3.4	1.55	13	0	11.11491	14.51491	1068	200	0.70379
3.4	1.55	14	0	11.96991	15.36991	1068	200	0.67595
3.4	1.55	15	0	12.8249	16.2249	1068	200	0.649914
3.4	1.55	16	0	13.67989	17.07989	1068	200	0.625574
3.4	1.55	17	0	14.53488	17.93488	1068	200	0.60281
3.4	1.55	18	0	15.38988	18.78988	1068	200	0.581505
3.4	1.55	19	0	16.24487	19.64487	1068	200	0.561544
3.4	1.55	20	0	17.09986	20.49986	1068	200	0.542821
3.4	1.55	21	0	17.95486	21.35486	1068	200	0.525236
3.4	1.55	22	0	18.80985	22.20985	1068	200	0.508698
3.4	1.55	23	0	19.66484	23.06484	1068	200	0.493123
3.4	1.55	24	0	20.51984	23.91984	1068	200	0.478436
3.4	1.55	25	0	21.37483	24.77483	1068	200	0.464566
3.4	1.55	26	0	22.22982	25.62982	1068	200	0.451451
3.4	1.55	27	0	23.08482	26.48482	1068	200	0.439034
3.4	1.55	28	0	23.93981	27.33981	1068	200	0.427264
3.4	1.55	29	0	24.7948	28.1948	1068	200	0.416091
3.4	1.55	30	0	25.6498	29.0498	1068	200	0.405475
3.4	1.55	31	0	26.50479	29.90479	1068	200	0.395375
3.4	1.55	32	0	27.35978	30.75978	1068	200	0.385756
3.4	1.55	33	0	28.21478	31.61478	1068	200	0.376585
3.4	1.55	34	0	29.06977	32.46977	1068	200	0.367832
3.4	1.55	35	0	29.92476	33.32476	1068	200	0.35947
3.4	1.55	36	0	30.77976	34.17976	1068	200	0.351474
3.4	1.55	37	0	31.63475	35.03475	1068	200	0.343821
3.4	1.55	38	0	32.48974	35.88974	1068	200	0.33649
3.4	1.55	39	0	33.34474	36.74474	1068	200	0.32946
3.4	1.55	40	0	34.19973	37.59973	1068	200	0.322715

4.52 ARMCHAIR (b=1.55)(k_1=1068,k_2=200):

Table 4.52 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.55	5	5	7.404459	10.80446	1068	200	0.846162
3.4	1.55	6	6	8.88535	12.28535	1068	200	0.785354
3.4	1.55	7	7	10.36624	13.76624	1068	200	0.729721
3.4	1.55	8	8	11.84713	15.24713	1068	200	0.679834
3.4	1.55	9	9	13.32803	16.72803	1068	200	0.635393
3.4	1.55	10	10	14.80892	18.20892	1068	200	0.595828
3.4	1.55	11	11	16.28981	19.68981	1068	200	0.56053
3.4	1.55	12	12	17.7707	21.1707	1068	200	0.528933
3.4	1.55	13	13	19.25159	22.65159	1068	200	0.500536
3.4	1.55	14	14	20.73248	24.13248	1068	200	0.474912
3.4	1.55	15	15	22.21338	25.61338	1068	200	0.451697
3.4	1.55	16	16	23.69427	27.09427	1068	200	0.430581
3.4	1.55	17	17	25.17516	28.57516	1068	200	0.411302
3.4	1.55	18	18	26.65605	30.05605	1068	200	0.393639
3.4	1.55	19	19	28.13694	31.53694	1068	200	0.377402
3.4	1.55	20	20	29.61783	33.01783	1068	200	0.362428
3.4	1.55	21	21	31.09873	34.49873	1068	200	0.34858
3.4	1.55	22	22	32.57962	35.97962	1068	200	0.335737
3.4	1.55	23	23	34.06051	37.46051	1068	200	0.323795
3.4	1.55	24	24	35.5414	38.9414	1068	200	0.312664
3.4	1.55	25	25	37.02229	40.42229	1068	200	0.302265
3.4	1.55	26	26	38.50318	41.90318	1068	200	0.292529
3.4	1.55	27	27	39.98408	43.38408	1068	200	0.283395
3.4	1.55	28	28	41.46497	44.86497	1068	200	0.27481
3.4	1.55	29	29	42.94586	46.34586	1068	200	0.266726
3.4	1.55	30	30	44.42675	47.82675	1068	200	0.259101
3.4	1.55	31	31	45.90764	49.30764	1068	200	0.251897
3.4	1.55	32	32	47.38854	50.78854	1068	200	0.24508
3.4	1.55	33	33	48.86943	52.26943	1068	200	0.238621
3.4	1.55	34	34	50.35032	53.75032	1068	200	0.232491
3.4	1.55	35	35	51.83121	55.23121	1068	200	0.226667
3.4	1.55	36	36	53.3121	56.7121	1068	200	0.221126
3.4	1.55	37	37	54.79299	58.19299	1068	200	0.215849
3.4	1.55	38	38	56.27389	59.67389	1068	200	0.210816
3.4	1.55	39	39	57.75478	61.15478	1068	200	0.206012
3.4	1.55	40	40	59.23567	62.63567	1068	200	0.201422

4.53 ZIG-ZAG (b=1.25) (k_1=1068,k_2=200):

Table 4.53 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (900 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.25	5	0	3.447553	6.847553	1068	200	1.147871
3.4	1.25	6	0	4.137064	7.537064	1068	200	1.136948
3.4	1.25	7	0	4.826575	8.226575	1068	200	1.113407
3.4	1.25	8	0	5.516085	8.916085	1068	200	1.083267
3.4	1.25	9	0	6.205596	9.605596	1068	200	1.049996
3.4	1.25	10	0	6.895107	10.29511	1068	200	1.015622
3.4	1.25	11	0	7.584617	10.98462	1068	200	0.981334
3.4	1.25	12	0	8.274128	11.67413	1068	200	0.947821
3.4	1.25	13	0	8.963639	12.36364	1068	200	0.915471
3.4	1.25	14	0	9.653149	13.05315	1068	200	0.884487
3.4	1.25	15	0	10.34266	13.74266	1068	200	0.854956
3.4	1.25	16	0	11.03217	14.43217	1068	200	0.826895
3.4	1.25	17	0	11.72168	15.12168	1068	200	0.800281
3.4	1.25	18	0	12.41119	15.81119	1068	200	0.775063
3.4	1.25	19	0	13.1007	16.5007	1068	200	0.751178
3.4	1.25	20	0	13.79021	17.19021	1068	200	0.728553
3.4	1.25	21	0	14.47972	17.87972	1068	200	0.707118
3.4	1.25	22	0	15.16923	18.56923	1068	200	0.686797
3.4	1.25	23	0	15.85875	19.25875	1068	200	0.667522
3.4	1.25	24	0	16.54826	19.94826	1068	200	0.649225
3.4	1.25	25	0	17.23777	20.63777	1068	200	0.631842
3.4	1.25	26	0	17.92728	21.32728	1068	200	0.615313
3.4	1.25	27	0	18.61679	22.01679	1068	200	0.599584
3.4	1.25	28	0	19.3063	22.7063	1068	200	0.584601
3.4	1.25	29	0	19.99581	23.39581	1068	200	0.570316
3.4	1.25	30	0	20.68532	24.08532	1068	200	0.556686
3.4	1.25	31	0	21.37483	24.77483	1068	200	0.543669
3.4	1.25	32	0	22.06434	25.46434	1068	200	0.531226
3.4	1.25	33	0	22.75385	26.15385	1068	200	0.519322
3.4	1.25	34	0	23.44336	26.84336	1068	200	0.507924
3.4	1.25	35	0	24.13287	27.53287	1068	200	0.497003
3.4	1.25	36	0	24.82238	28.22238	1068	200	0.486529
3.4	1.25	37	0	25.51189	28.91189	1068	200	0.476478
3.4	1.25	38	0	26.20141	29.60141	1068	200	0.466824
3.4	1.25	39	0	26.89092	30.29092	1068	200	0.457545
3.4	1.25	40	0	27.58043	30.98043	1068	200	0.448621

4.54 ARMCHAIR (b=1.25)(k_1=1068,k_2=200):

Table 4.54 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.25	5	5	5.971338	9.371338	1068	200	1.061503
3.4	1.25	6	6	7.165605	10.56561	1068	200	1.002114
3.4	1.25	7	7	8.359873	11.75987	1068	200	0.943729
3.4	1.25	8	8	9.55414	12.95414	1068	200	0.888848
3.4	1.25	9	9	10.74841	14.14841	1068	200	0.838266
3.4	1.25	10	10	11.94268	15.34268	1068	200	0.79205
3.4	1.25	11	11	13.13694	16.53694	1068	200	0.749958
3.4	1.25	12	12	14.33121	17.73121	1068	200	0.711638
3.4	1.25	13	13	15.52548	18.92548	1068	200	0.676713
3.4	1.25	14	14	16.71975	20.11975	1068	200	0.644819
3.4	1.25	15	15	17.91401	21.31401	1068	200	0.615624
3.4	1.25	16	16	19.10828	22.50828	1068	200	0.58883
3.4	1.25	17	17	20.30255	23.70255	1068	200	0.564174
3.4	1.25	18	18	21.49682	24.89682	1068	200	0.541426
3.4	1.25	19	19	22.69108	26.09108	1068	200	0.520384
3.4	1.25	20	20	23.88535	27.28535	1068	200	0.500871
3.4	1.25	21	21	25.07962	28.47962	1068	200	0.482731
3.4	1.25	22	22	26.27389	29.67389	1068	200	0.465831
3.4	1.25	23	23	27.46815	30.86815	1068	200	0.45005
3.4	1.25	24	24	28.66242	32.06242	1068	200	0.435284
3.4	1.25	25	25	29.85669	33.25669	1068	200	0.421441
3.4	1.25	26	26	31.05096	34.45096	1068	200	0.408437
3.4	1.25	27	27	32.24522	35.64522	1068	200	0.396201
3.4	1.25	28	28	33.43949	36.83949	1068	200	0.384667
3.4	1.25	29	29	34.63376	38.03376	1068	200	0.373778
3.4	1.25	30	30	35.82803	39.22803	1068	200	0.363482
3.4	1.25	31	31	37.02229	40.42229	1068	200	0.353732
3.4	1.25	32	32	38.21656	41.61656	1068	200	0.344486
3.4	1.25	33	33	39.41083	42.81083	1068	200	0.335708
3.4	1.25	34	34	40.6051	44.0051	1068	200	0.327361
3.4	1.25	35	35	41.79936	45.19936	1068	200	0.319417
3.4	1.25	36	36	42.99363	46.39363	1068	200	0.311846
3.4	1.25	37	37	44.1879	47.5879	1068	200	0.304623
3.4	1.25	38	38	45.38217	48.78217	1068	200	0.297725
3.4	1.25	39	39	46.57643	49.97643	1068	200	0.291131
3.4	1.25	40	40	47.7707	51.1707	1068	200	0.284821

4.55 ZIG-ZAG (b=1.65)(k_1=1068,k_2=200):

Table 4.55 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.65	5	0	4.55077	7.95077	1068	200	0.909922
3.4	1.65	6	0	5.460925	8.860925	1068	200	0.879115
3.4	1.65	7	0	6.371079	9.771079	1068	200	0.843462
3.4	1.65	8	0	7.281233	10.68123	1068	200	0.806677
3.4	1.65	9	0	8.191387	11.59139	1068	200	0.770592
3.4	1.65	10	0	9.101541	12.50154	1068	200	0.736081
3.4	1.65	11	0	10.01169	13.41169	1068	200	0.703522
3.4	1.65	12	0	10.92185	14.32185	1068	200	0.673032
3.4	1.65	13	0	11.832	15.232	1068	200	0.644588
3.4	1.65	14	0	12.74216	16.14216	1068	200	0.618098
3.4	1.65	15	0	13.65231	17.05231	1068	200	0.593441
3.4	1.65	16	0	14.56247	17.96247	1068	200	0.57048
3.4	1.65	17	0	15.47262	18.87262	1068	200	0.549082
3.4	1.65	18	0	16.38277	19.78277	1068	200	0.529116
3.4	1.65	19	0	17.29293	20.69293	1068	200	0.510461
3.4	1.65	20	0	18.20308	21.60308	1068	200	0.493005
3.4	1.65	21	0	19.11324	22.51324	1068	200	0.476646
3.4	1.65	22	0	20.02339	23.42339	1068	200	0.461292
3.4	1.65	23	0	20.93354	24.33354	1068	200	0.446858
3.4	1.65	24	0	21.8437	25.2437	1068	200	0.433269
3.4	1.65	25	0	22.75385	26.15385	1068	200	0.420457
3.4	1.65	26	0	23.66401	27.06401	1068	200	0.408359
3.4	1.65	27	0	24.57416	27.97416	1068	200	0.396919
3.4	1.65	28	0	25.48431	28.88431	1068	200	0.386088
3.4	1.65	29	0	26.39447	29.79447	1068	200	0.37582
3.4	1.65	30	0	27.30462	30.70462	1068	200	0.366072
3.4	1.65	31	0	28.21478	31.61478	1068	200	0.356808
3.4	1.65	32	0	29.12493	32.52493	1068	200	0.347992
3.4	1.65	33	0	30.03508	33.43508	1068	200	0.339595
3.4	1.65	34	0	30.94524	34.34524	1068	200	0.331588
3.4	1.65	35	0	31.85539	35.25539	1068	200	0.323944
3.4	1.65	36	0	32.76555	36.16555	1068	200	0.316639
3.4	1.65	37	0	33.6757	37.0757	1068	200	0.309653
3.4	1.65	38	0	34.58586	37.98586	1068	200	0.302965
3.4	1.65	39	0	35.49601	38.89601	1068	200	0.296556
3.4	1.65	40	0	36.40616	39.80616	1068	200	0.29041

4.56 ARMCHAIR (b=1.65)(k_1=1068,k_2=200):

Table 4.56 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$

At extremities of bond length at (2300 k)

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
3.4	1.65	5	5	7.882166	11.28217	1068	200	0.782705
3.4	1.65	6	6	9.458599	12.8586	1068	200	0.723065
3.4	1.65	7	7	11.03503	14.43503	1068	200	0.669385
3.4	1.65	8	8	12.61146	16.01146	1068	200	0.621786
3.4	1.65	9	9	14.1879	17.5879	1068	200	0.579733
3.4	1.65	10	10	15.76433	19.16433	1068	200	0.542533
3.4	1.65	11	11	17.34076	20.74076	1068	200	0.509514
3.4	1.65	12	12	18.9172	22.3172	1068	200	0.480082
3.4	1.65	13	13	20.49363	23.89363	1068	200	0.453725
3.4	1.65	14	14	22.07006	25.47006	1068	200	0.430013
3.4	1.65	15	15	23.6465	27.0465	1068	200	0.408585
3.4	1.65	16	16	25.22293	28.62293	1068	200	0.389139
3.4	1.65	17	17	26.79936	30.19936	1068	200	0.371421
3.4	1.65	18	18	28.3758	31.7758	1068	200	0.355216
3.4	1.65	19	19	29.95223	33.35223	1068	200	0.340343
3.4	1.65	20	20	31.52866	34.92866	1068	200	0.326647
3.4	1.65	21	21	33.1051	36.5051	1068	200	0.313997
3.4	1.65	22	22	34.68153	38.08153	1068	200	0.302278
3.4	1.65	23	23	36.25796	39.65796	1068	200	0.291394
3.4	1.65	24	24	37.83439	41.23439	1068	200	0.281258
3.4	1.65	25	25	39.41083	42.81083	1068	200	0.271798
3.4	1.65	26	26	40.98726	44.38726	1068	200	0.262948
3.4	1.65	27	27	42.56369	45.96369	1068	200	0.254652
3.4	1.65	28	28	44.14013	47.54013	1068	200	0.24686
3.4	1.65	29	29	45.71656	49.11656	1068	200	0.239527
3.4	1.65	30	30	47.29299	50.69299	1068	200	0.232615
3.4	1.65	31	31	48.86943	52.26943	1068	200	0.226089
3.4	1.65	32	32	50.44586	53.84586	1068	200	0.219917
3.4	1.65	33	33	52.02229	55.42229	1068	200	0.214071
3.4	1.65	34	34	53.59873	56.99873	1068	200	0.208527
3.4	1.65	35	35	55.17516	58.57516	1068	200	0.203261
3.4	1.65	36	36	56.75159	60.15159	1068	200	0.198254
3.4	1.65	37	37	58.32803	61.72803	1068	200	0.193486
3.4	1.65	38	38	59.90446	63.30446	1068	200	0.188942
3.4	1.65	39	39	61.48089	64.88089	1068	200	0.184605

4.57 ZIG-ZAG (b=1.42)(k_1=938,k_2=200):

Table 4.57 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$ and thickness =0.66 Å

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
0.66	1.42	5	0	3.91642	4.5764	938	200	2.46007
0.66	1.42	6	0	4.6997	5.3597	938	200	2.15228
0.66	1.42	7	0	5.48299	6.143	938	200	1.91147
0.66	1.42	8	0	6.26627	6.9263	938	200	1.71838
0.66	1.42	9	0	7.04956	7.7096	938	200	1.56032
0.66	1.42	10	0	7.83284	8.4928	938	200	1.42864
0.66	1.42	11	0	8.61613	9.2761	938	200	1.31731
0.66	1.42	12	0	9.39941	10.059	938	200	1.22199
0.66	1.42	13	0	10.1827	10.843	938	200	1.13946
0.66	1.42	14	0	10.966	11.626	938	200	1.06733
0.66	1.42	15	0	11.7493	12.409	938	200	1.00376
0.66	1.42	16	0	12.5325	13.193	938	200	0.94731
0.66	1.42	17	0	13.3158	13.976	938	200	0.89686
0.66	1.42	18	0	14.0991	14.759	938	200	0.85149
0.66	1.42	19	0	14.8824	15.542	938	200	0.81049
0.66	1.42	20	0	15.6657	16.326	938	200	0.77324
0.66	1.42	21	0	16.449	17.109	938	200	0.73927
0.66	1.42	22	0	17.2323	17.892	938	200	0.70815
0.66	1.42	23	0	18.0155	18.676	938	200	0.67953
0.66	1.42	24	0	18.7988	19.459	938	200	0.65314
0.66	1.42	25	0	19.5821	20.242	938	200	0.62872
0.66	1.42	26	0	20.3654	21.025	938	200	0.60606
0.66	1.42	27	0	21.1487	21.809	938	200	0.58497
0.66	1.42	28	0	21.932	22.592	938	200	0.5653
0.66	1.42	29	0	22.7152	23.375	938	200	0.54691
0.66	1.42	30	0	23.4985	24.159	938	200	0.52968
0.66	1.42	31	0	24.2818	24.942	938	200	0.51349
0.66	1.42	32	0	25.0651	25.725	938	200	0.49827
0.66	1.42	33	0	25.8484	26.508	938	200	0.48392
0.66	1.42	34	0	26.6317	27.292	938	200	0.47038
0.66	1.42	35	0	27.4149	28.075	938	200	0.45757
0.66	1.42	36	0	28.1982	28.858	938	200	0.44544
0.66	1.42	37	0	28.9815	29.642	938	200	0.43394
0.66	1.42	38	0	29.7648	30.425	938	200	0.42302
0.66	1.42	39	0	30.5481	31.208	938	200	0.41263
0.66	1.42	40	0	31.3314	31.991	938	200	0.40274

4.58 ARMCHAIR (b=1.42)(k_1=938,k_2=200):

Table 4.58 Summary of Young's modulus variation in accordance with $k_1 = 938$ & $k_2 = 200$ and thickness =0.66 Å

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
0.66	1.42	5	5	6.78344	7.4434	938	200	1.61069
0.66	1.42	6	6	8.14013	8.8001	938	200	1.38281
0.66	1.42	7	7	9.49682	10.157	938	200	1.21108
0.66	1.42	8	8	10.8535	11.514	938	200	1.07712
0.66	1.42	9	9	12.2102	12.87	938	200	0.96976
0.66	1.42	10	10	13.5669	14.227	938	200	0.8818
0.66	1.42	11	11	14.9236	15.584	938	200	0.80844
0.66	1.42	12	12	16.2803	16.94	938	200	0.74633
0.66	1.42	13	13	17.6369	18.297	938	200	0.69307
0.66	1.42	14	14	18.9936	19.654	938	200	0.64689
0.66	1.42	15	15	20.3503	21.01	938	200	0.60648
0.66	1.42	16	16	21.707	22.367	938	200	0.57081
0.66	1.42	17	17	23.0637	23.724	938	200	0.53911
0.66	1.42	18	18	24.4204	25.08	938	200	0.51073
0.66	1.42	19	19	25.7771	26.437	938	200	0.4852
0.66	1.42	20	20	27.1338	27.794	938	200	0.46209
0.66	1.42	21	21	28.4904	29.15	938	200	0.44108
0.66	1.42	22	22	29.8471	30.507	938	200	0.4219
0.66	1.42	23	23	31.2038	31.864	938	200	0.40432
0.66	1.42	24	24	32.5605	33.221	938	200	0.38814
0.66	1.42	25	25	33.9172	34.577	938	200	0.37321
0.66	1.42	26	26	35.2739	35.934	938	200	0.35938
0.66	1.42	27	27	36.6306	37.291	938	200	0.34654
0.66	1.42	28	28	37.9873	38.647	938	200	0.33459
0.66	1.42	29	29	39.3439	40.004	938	200	0.32343
0.66	1.42	30	30	40.7006	41.361	938	200	0.31299
0.66	1.42	31	31	42.0573	42.717	938	200	0.30321
0.66	1.42	32	32	43.414	44.074	938	200	0.29402
0.66	1.42	33	33	44.7707	45.431	938	200	0.28537
0.66	1.42	34	34	46.1274	46.787	938	200	0.27721
0.66	1.42	35	35	47.4841	48.144	938	200	0.26951
0.66	1.42	36	36	48.8408	49.501	938	200	0.26222
0.66	1.42	37	37	50.1975	50.857	938	200	0.25532
0.66	1.42	38	38	51.5541	52.214	938	200	0.24877
0.66	1.42	39	39	52.9108	53.571	938	200	0.24255
0.66	1.42	40	40	54.2675	54.928	938	200	0.23663

4.59 ZIG-ZAG (b=1.42)(k_1=960,k_2=180):

Table 4.59 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$ and thickness =0.66 Å

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
0.66	1.42	5	0	3.916421	4.576421	960	180	2.404184
0.66	1.42	6	0	4.699705	5.359705	960	180	2.103386
0.66	1.42	7	0	5.482989	6.142989	960	180	1.868048
0.66	1.42	8	0	6.266273	6.926273	960	180	1.679347
0.66	1.42	9	0	7.049557	7.709557	960	180	1.524871
0.66	1.42	10	0	7.832841	8.492841	960	180	1.396187
0.66	1.42	11	0	8.616125	9.276125	960	180	1.287387
0.66	1.42	12	0	9.399409	10.05941	960	180	1.194224
0.66	1.42	13	0	10.18269	10.84269	960	180	1.113573
0.66	1.42	14	0	10.96598	11.62598	960	180	1.043082
0.66	1.42	15	0	11.74926	12.40926	960	180	0.980955
0.66	1.42	16	0	12.53255	13.19255	960	180	0.92579
0.66	1.42	17	0	13.31583	13.97583	960	180	0.876483
0.66	1.42	18	0	14.09911	14.75911	960	180	0.83215
0.66	1.42	19	0	14.8824	15.5424	960	180	0.792076
0.66	1.42	20	0	15.66568	16.32568	960	180	0.755678
0.66	1.42	21	0	16.44897	17.10897	960	180	0.722472
0.66	1.42	22	0	17.23225	17.89225	960	180	0.692058
0.66	1.42	23	0	18.01553	18.67553	960	180	0.664097
0.66	1.42	24	0	18.79882	19.45882	960	180	0.638304
0.66	1.42	25	0	19.5821	20.2421	960	180	0.614438
0.66	1.42	26	0	20.36539	21.02539	960	180	0.592291
0.66	1.42	27	0	21.14867	21.80867	960	180	0.571683
0.66	1.42	28	0	21.93196	22.59196	960	180	0.552459
0.66	1.42	29	0	22.71524	23.37524	960	180	0.534485
0.66	1.42	30	0	23.49852	24.15852	960	180	0.517643
0.66	1.42	31	0	24.28181	24.94181	960	180	0.501829
0.66	1.42	32	0	25.06509	25.72509	960	180	0.486951
0.66	1.42	33	0	25.84838	26.50838	960	180	0.47293
0.66	1.42	34	0	26.63166	27.29166	960	180	0.459694
0.66	1.42	35	0	27.41494	28.07494	960	180	0.447177
0.66	1.42	36	0	28.19823	28.85823	960	180	0.435324
0.66	1.42	37	0	28.98151	29.64151	960	180	0.424083
0.66	1.42	38	0	29.7648	30.4248	960	180	0.413407
0.66	1.42	39	0	30.54808	31.20808	960	180	0.403255
0.66	1.42	40	0	31.33136	31.99136	960	180	0.39359

4.60 ARMCHAIR (b=1.42)(k_1=960,k_2=180):

Table 4.60 Summary of Young's modulus variation in accordance with $k_1 = 960$ & $k_2 = 180$ and thickness =0.66 Å

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
0.66	1.42	5	5	6.783439	7.443439	960	180	1.574102
0.66	1.42	6	6	8.140127	8.800127	960	180	1.351399
0.66	1.42	7	7	9.496815	10.15682	960	180	1.183568
0.66	1.42	8	8	10.8535	11.5135	960	180	1.052653
0.66	1.42	9	9	12.21019	12.87019	960	180	0.947726
0.66	1.42	10	10	13.56688	14.22688	960	180	0.861769
0.66	1.42	11	11	14.92357	15.58357	960	180	0.790076
0.66	1.42	12	12	16.28025	16.94025	960	180	0.729376
0.66	1.42	13	13	17.63694	18.29694	960	180	0.677324
0.66	1.42	14	14	18.99363	19.65363	960	180	0.632197
0.66	1.42	15	15	20.35032	21.01032	960	180	0.592702
0.66	1.42	16	16	21.70701	22.36701	960	180	0.557846
0.66	1.42	17	17	23.06369	23.72369	960	180	0.526859
0.66	1.42	18	18	24.42038	25.08038	960	180	0.499131
0.66	1.42	19	19	25.77707	26.43707	960	180	0.474173
0.66	1.42	20	20	27.13376	27.79376	960	180	0.451591
0.66	1.42	21	21	28.49045	29.15045	960	180	0.431061
0.66	1.42	22	22	29.84713	30.50713	960	180	0.412316
0.66	1.42	23	23	31.20382	31.86382	960	180	0.395132
0.66	1.42	24	24	32.56051	33.22051	960	180	0.379323
0.66	1.42	25	25	33.9172	34.5772	960	180	0.364729
0.66	1.42	26	26	35.27389	35.93389	960	180	0.351217
0.66	1.42	27	27	36.63057	37.29057	960	180	0.338669
0.66	1.42	28	28	37.98726	38.64726	960	180	0.326987
0.66	1.42	29	29	39.34395	40.00395	960	180	0.316084
0.66	1.42	30	30	40.70064	41.36064	960	180	0.305884
0.66	1.42	31	31	42.05732	42.71732	960	180	0.296322
0.66	1.42	32	32	43.41401	44.07401	960	180	0.287339
0.66	1.42	33	33	44.7707	45.4307	960	180	0.278885
0.66	1.42	34	34	46.12739	46.78739	960	180	0.270914
0.66	1.42	35	35	47.48408	48.14408	960	180	0.263386
0.66	1.42	36	36	48.84076	49.50076	960	180	0.256265
0.66	1.42	37	37	50.19745	50.85745	960	180	0.249518
0.66	1.42	38	38	51.55414	52.21414	960	180	0.243118
0.66	1.42	39	39	52.91083	53.57083	960	180	0.237038
0.66	1.42	40	40	54.26752	54.92752	960	180	0.231255

4.61 ZIG-ZAG (b=1.42)(k_1=1068,k_2=200):

Table 4.61 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$ and thickness =0.66 Å

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
0.66	1.42	5	0	3.916421	4.576421	1068	200	2.673405
0.66	1.42	6	0	4.699705	5.359705	1068	200	2.338924
0.66	1.42	7	0	5.482989	6.142989	1068	200	2.077233
0.66	1.42	8	0	6.266273	6.926273	1068	200	1.8674
0.66	1.42	9	0	7.049557	7.709557	1068	200	1.695627
0.66	1.42	10	0	7.832841	8.492841	1068	200	1.552532
0.66	1.42	11	0	8.616125	9.276125	1068	200	1.431548
0.66	1.42	12	0	9.399409	10.05941	1068	200	1.327953
0.66	1.42	13	0	10.18269	10.84269	1068	200	1.238271
0.66	1.42	14	0	10.96598	11.62598	1068	200	1.159887
0.66	1.42	15	0	11.74926	12.40926	1068	200	1.090802
0.66	1.42	16	0	12.53255	13.19255	1068	200	1.02946
0.66	1.42	17	0	13.31583	13.97583	1068	200	0.974631
0.66	1.42	18	0	14.09911	14.75911	1068	200	0.925334
0.66	1.42	19	0	14.8824	15.5424	1068	200	0.880773
0.66	1.42	20	0	15.66568	16.32568	1068	200	0.840299
0.66	1.42	21	0	16.44897	17.10897	1068	200	0.803375
0.66	1.42	22	0	17.23225	17.89225	1068	200	0.769554
0.66	1.42	23	0	18.01553	18.67553	1068	200	0.738462
0.66	1.42	24	0	18.79882	19.45882	1068	200	0.709782
0.66	1.42	25	0	19.5821	20.2421	1068	200	0.683243
0.66	1.42	26	0	20.36539	21.02539	1068	200	0.658615
0.66	1.42	27	0	21.14867	21.80867	1068	200	0.6357
0.66	1.42	28	0	21.93196	22.59196	1068	200	0.614323
0.66	1.42	29	0	22.71524	23.37524	1068	200	0.594337
0.66	1.42	30	0	23.49852	24.15852	1068	200	0.575608
0.66	1.42	31	0	24.28181	24.94181	1068	200	0.558023
0.66	1.42	32	0	25.06509	25.72509	1068	200	0.54148
0.66	1.42	33	0	25.84838	26.50838	1068	200	0.525889
0.66	1.42	34	0	26.63166	27.29166	1068	200	0.51117
0.66	1.42	35	0	27.41494	28.07494	1068	200	0.497252
0.66	1.42	36	0	28.19823	28.85823	1068	200	0.484072
0.66	1.42	37	0	28.98151	29.64151	1068	200	0.471572
0.66	1.42	38	0	29.7648	30.4248	1068	200	0.4597
0.66	1.42	39	0	30.54808	31.20808	1068	200	0.448412
0.66	1.42	40	0	31.33136	31.99136	1068	200	0.437664

4.62 ARMCHAIR (b=1.42)(k_1=1068,k_2=200):

Table 4.62 Summary of Young's modulus variation in accordance with $k_1 = 1068$ & $k_2 = 200$ and thickness =0.66 Å

t(Å)	b(Å)	m	n	D_1	D_2	k_1	k_2	E(TPa)
0.66	1.42	5	5	6.783439	7.443439	1068	200	1.75037
0.66	1.42	6	6	8.140127	8.800127	1068	200	1.502729
0.66	1.42	7	7	9.496815	10.15682	1068	200	1.316104
0.66	1.42	8	8	10.8535	11.5135	1068	200	1.170529
0.66	1.42	9	9	12.21019	12.87019	1068	200	1.053852
0.66	1.42	10	10	13.56688	14.22688	1068	200	0.95827
0.66	1.42	11	11	14.92357	15.58357	1068	200	0.878549
0.66	1.42	12	12	16.28025	16.94025	1068	200	0.811052
0.66	1.42	13	13	17.63694	18.29694	1068	200	0.753171
0.66	1.42	14	14	18.99363	19.65363	1068	200	0.702991
0.66	1.42	15	15	20.35032	21.01032	1068	200	0.659073
0.66	1.42	16	16	21.70701	22.36701	1068	200	0.620314
0.66	1.42	17	17	23.06369	23.72369	1068	200	0.585857
0.66	1.42	18	18	24.42038	25.08038	1068	200	0.555024
0.66	1.42	19	19	25.77707	26.43707	1068	200	0.527271
0.66	1.42	20	20	27.13376	27.79376	1068	200	0.502161
0.66	1.42	21	21	28.49045	29.15045	1068	200	0.479332
0.66	1.42	22	22	29.84713	30.50713	1068	200	0.458487
0.66	1.42	23	23	31.20382	31.86382	1068	200	0.439379
0.66	1.42	24	24	32.56051	33.22051	1068	200	0.421799
0.66	1.42	25	25	33.9172	34.5772	1068	200	0.405572
0.66	1.42	26	26	35.27389	35.93389	1068	200	0.390546
0.66	1.42	27	27	36.63057	37.29057	1068	200	0.376594
0.66	1.42	28	28	37.98726	38.64726	1068	200	0.363603
0.66	1.42	29	29	39.34395	40.00395	1068	200	0.351479
0.66	1.42	30	30	40.70064	41.36064	1068	200	0.340137
0.66	1.42	31	31	42.05732	42.71732	1068	200	0.329504
0.66	1.42	32	32	43.41401	44.07401	1068	200	0.319516
0.66	1.42	33	33	44.7707	45.4307	1068	200	0.310115
0.66	1.42	34	34	46.12739	46.78739	1068	200	0.301251
0.66	1.42	35	35	47.48408	48.14408	1068	200	0.29288
0.66	1.42	36	36	48.84076	49.50076	1068	200	0.284961
0.66	1.42	37	37	50.19745	50.85745	1068	200	0.27746
0.66	1.42	38	38	51.55414	52.21414	1068	200	0.270343
0.66	1.42	39	39	52.91083	53.57083	1068	200	0.263582
0.66	1.42	40	40	54.26752	54.92752	1068	200	0.25715

CHAPTER 5

RESULTS AND DISCUSSIONS

According to our theory, different values of young's modulus are predicted with varying different parameters affecting the young's modulus of single walled carbon nanotubes. The influence of diameter and chirality on the elastic moduli (Young's modulus) of SWCNTs is investigated. It has been found that elastic modulus of a zigzag nanotube is the same with that of an armchair nanotube at the same diameter. And it has been found that there is independence of chirality in single walled carbon nanotubes. The axial modulus of the SWCNT is a function of nanotube diameter. The simulated results show an approximately inverse dependency on the nanotube diameter. The axial modulus decreases rapidly with increase in nanotube diameter. SWCNT's diameters are usually in the range of (3.4–67 Å). Based on the presented theory, it has been predicted that the young's modulus for zig-zag type single walled carbon nanotube lies in the range of (1.0460–0.6346 TPa) and for armchair type single walled carbon nanotube, it lies in the range (.9352–.5247 TPa). All the above results are derived by considering the tube effective tube thickness of 3.4 Å, which is usually assumed to be the thickness of graphitic layer spacing. In our case, different values of young's modulus are calculated and our results conclude that there is large variation in young's modulus values for lower diameter and small variation of young's modulus for larger diameter.

According to different researchers, the calculated elastic modulus (E) of the graphene sheet is equal to 0.8 TPa. And in accordance to our theory , it has been predicted that the optimum values young's modulus for zig-zag type SWCNT lies in the range of (1.0460–0.6346 TPa) and for armchair type SWCNT, it lies in the range (.9352–.5247 TPa). The graphs have been plotted which gives us the brief idea that how the young's modulus have been improved drastically. The predicted values of the elastic modulus depend strongly on the assumption of the tube thickness of SWNTs. It is seen that the values of modulus are quite sensitive to the nanotubes with small diameter.

Comparison of different parameters taken into consideration:-

Table:5.1 Young's Modulus values for different types of zig-zag carbon nanotube(E in TPa)

b(Å)	k_1	k_2	(5,0)	(10,0)	(15,0)	(20,0)	(25,0)	(30,0)	(35,0)	(40,0)
1.42	634	126	0.6346	0.5385	0.4441	0.3738	0.3216	0.2817	0.2504	0.2253
1.42	1140	126	0.8862	0.7519	0.6201	0.5220	0.4491	0.3934	0.3497	0.3146
1.42	938	126	0.8006	0.6793	0.5602	0.4716	0.4057	0.3554	0.3159	0.2842
1.42	804	140	0.7658	0.6498	0.5359	0.4511	0.3881	0.3399	0.3022	0.2719
1.42	1068	200	1.0460	0.8875	0.7319	0.6161	0.5300	0.4643	0.4128	0.3713
1.42	1132	126	0.8831	0.7493	0.6179	0.5202	0.4475	0.3920	0.3485	0.3135
1.42	938	200	0.9625	0.8167	0.6735	0.5670	0.4877	0.4273	0.3798	0.3417
1.34	960	180	0.9840	0.8509	0.7082	0.5994	0.5175	0.4545	0.4048	0.3647
1.42	700	100	0.6141	0.5211	0.4297	0.3617	0.3112	0.2726	0.2423	0.2180
1.522	632	126	0.5975	0.4958	0.4045	0.3384	0.2899	0.2533	0.2246	0.2018

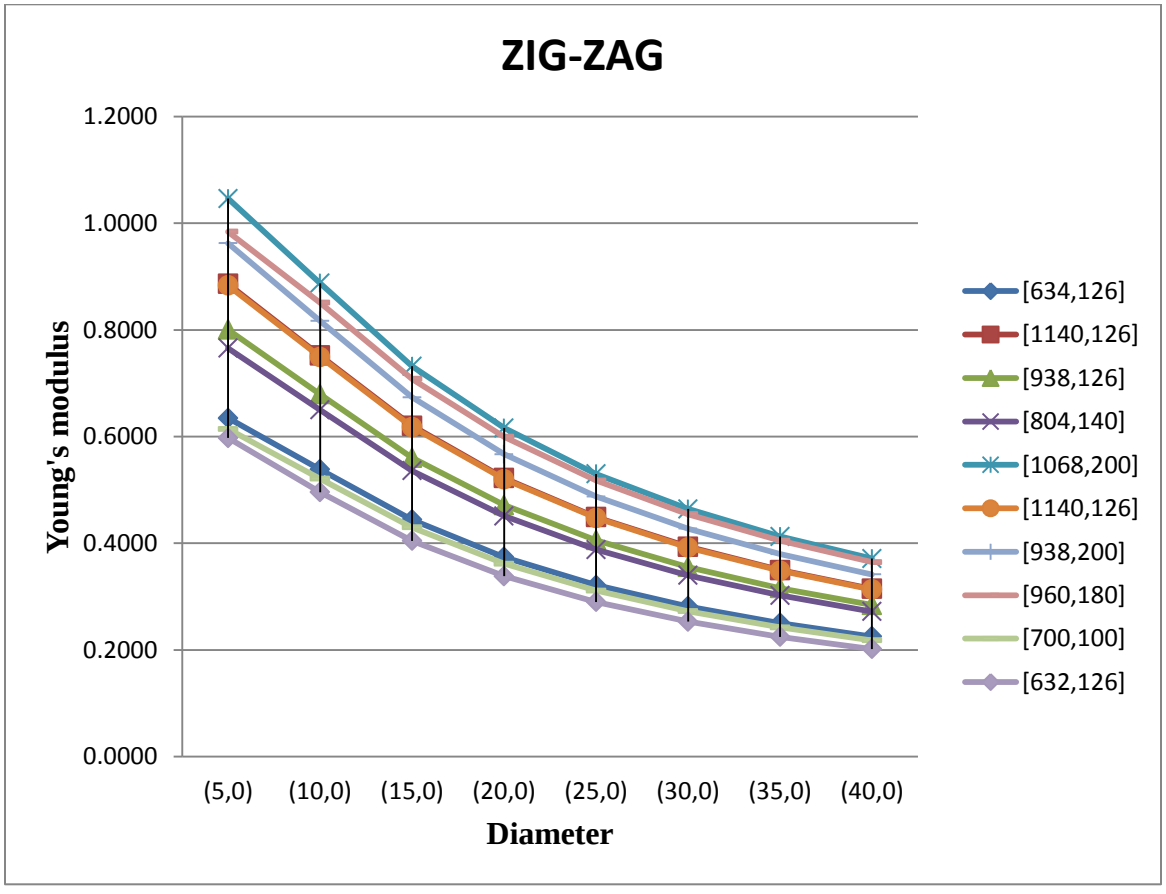

Fig.16 (young's modulus variation with diameter for zig-zag)

Table:5.2 Young's modulus values for different types of armchair carbon nanotube(E in TPa)

b(Å)	k_1	k_2	(5,5)	(10,10)	(15,15)	(20,20)	(25,25)	(30,30)	(35,35)	(40,40)
1.42	634	126	0.5674	0.4088	0.3129	0.2525	0.2113	0.1815	0.1591	0.1415
1.42	1140	126	0.7923	0.5708	0.4370	0.3525	0.2950	0.2535	0.2221	0.1977
1.42	938	126	0.7158	0.5157	0.3948	0.3185	0.2665	0.2290	0.2007	0.1786
1.42	804	140	0.6847	0.4933	0.3776	0.3046	0.2549	0.2190	0.1920	0.1708
1.42	1068	200	0.9352	0.6738	0.5158	0.4161	0.3482	0.2992	0.2622	0.2333
1.42	1132	126	0.7895	0.5688	0.4355	0.3513	0.2940	0.2526	0.2214	0.1970
1.42	938	200	0.8605	0.6200	0.4746	0.3829	0.3204	0.2753	0.2413	0.2147
1.34	960	180	0.8933	0.6538	0.5039	0.4080	0.3423	0.2946	0.2585	0.2302
1.42	700	100	0.5491	0.3956	0.3028	0.2443	0.2044	0.1757	0.1539	0.1370
1.522	632	126	0.5247	0.3712	0.2820	0.2265	0.1890	0.1621	0.1419	0.1261

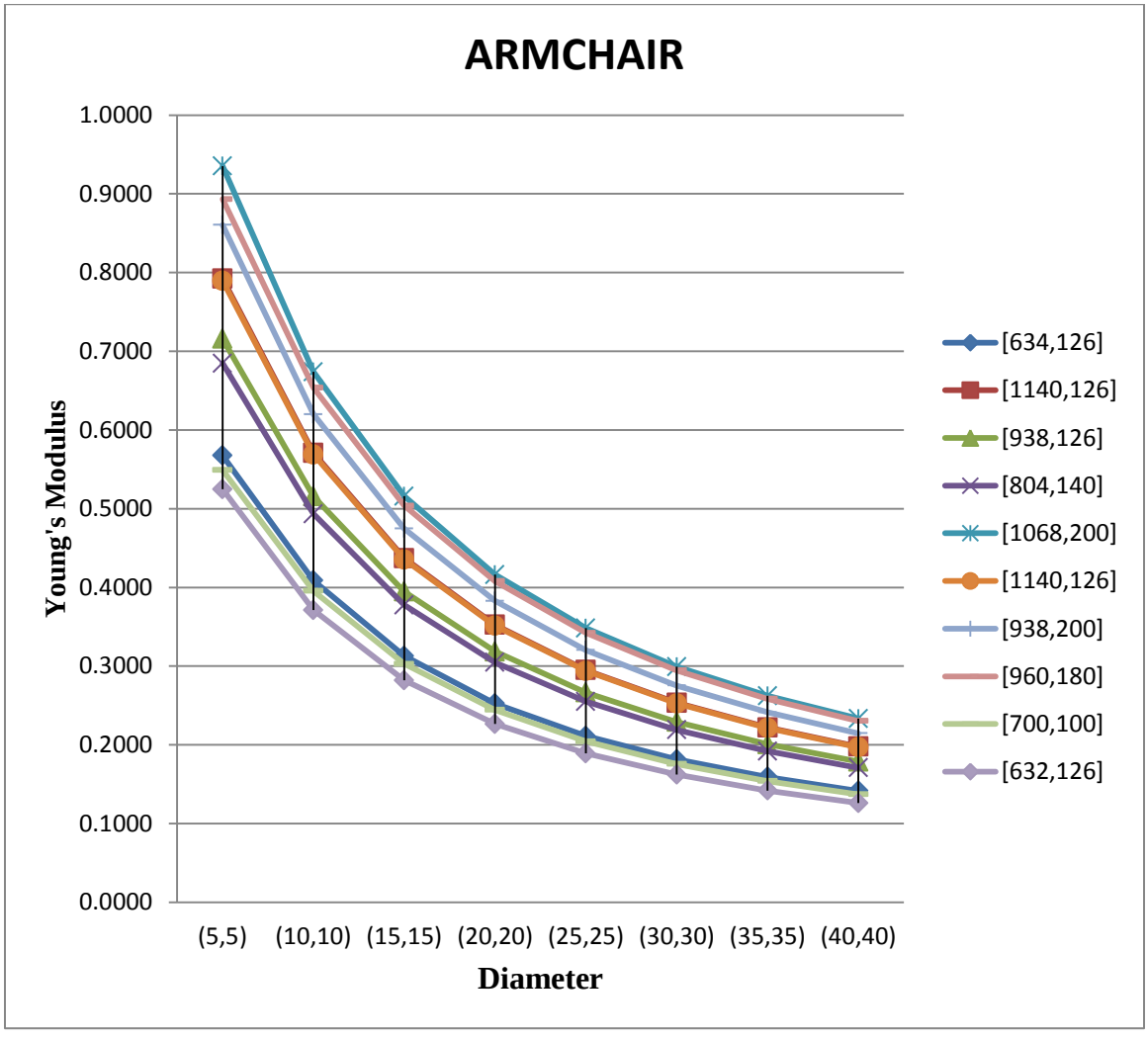

Fig.17 (young's modulus variation with diameter for armchair)

Comparison of different parameters with increasing temperature at the extremities of bond length taken into consideration:-

Table:5.3 Young's modulus values for different types of zig-zag carbon nanotube at different temp.

				young's modulus for zig-zag nanotube(E)							
T(K)	b (Å)	k_1	k_2	(5,0)	(10,0)	(15,0)	(20,0)	(25,0)	(30,0)	(35,0)	(40,0)
300	1.35	938	200	0.9984	0.8612	0.7159	0.6055	0.5226	0.4588	0.4085	0.3680
	1.35	960	180	0.9786	0.8441	0.7017	0.5935	0.5122	0.4497	0.4004	0.3607
	1.35	1068	200	1.0882	0.9387	0.7803	0.6600	0.5696	0.5000	0.4453	0.4011
	1.5	938	200	0.9213	0.7681	0.6281	0.5261	0.4511	0.3943	0.3499	0.3143
	1.5	960	180	0.8974	0.7481	0.6118	0.5125	0.4394	0.3840	0.3408	0.3062
	1.5	1068	200	0.9979	0.8319	0.6803	0.5698	0.4886	0.4270	0.3789	0.3405
900	1.3	938	200	1.0237	0.8941	0.7478	0.6348	0.5491	0.4829	0.4306	0.3882
	1.3	960	180	1.0056	0.8782	0.7345	0.6235	0.5394	0.4744	0.4229	0.3813
	1.3	1068	200	1.1182	0.9766	0.8168	0.6934	0.5998	0.5275	0.4703	0.4241
	1.55	938	200	0.8957	0.7389	0.6013	0.5022	0.4298	0.3751	0.3326	0.2986
	1.55	960	180	0.8707	0.7183	0.5845	0.4882	0.4178	0.3647	0.3233	0.2902
	1.55	1068	200	0.9682	0.7987	0.6499	0.5428	0.4646	0.4055	0.3595	0.3227
2300	1.25	938	200	1.0486	0.9278	0.7810	0.6655	0.5772	0.5085	0.4540	0.4098
	1.25	960	180	1.0322	0.9133	0.7688	0.6551	0.5682	0.5006	0.4469	0.4034
	1.25	1068	200	1.1479	1.0156	0.8550	0.7286	0.6318	0.5567	0.4970	0.4486
	1.65	938	200	0.8451	0.6837	0.5512	0.4579	0.3905	0.3400	0.3009	0.2697
	1.65	960	180	0.8184	0.6620	0.5337	0.4434	0.3781	0.3292	0.2913	0.2612
	1.65	1068	200	0.9099	0.7361	0.5934	0.4930	0.4205	0.3661	0.3239	0.2904

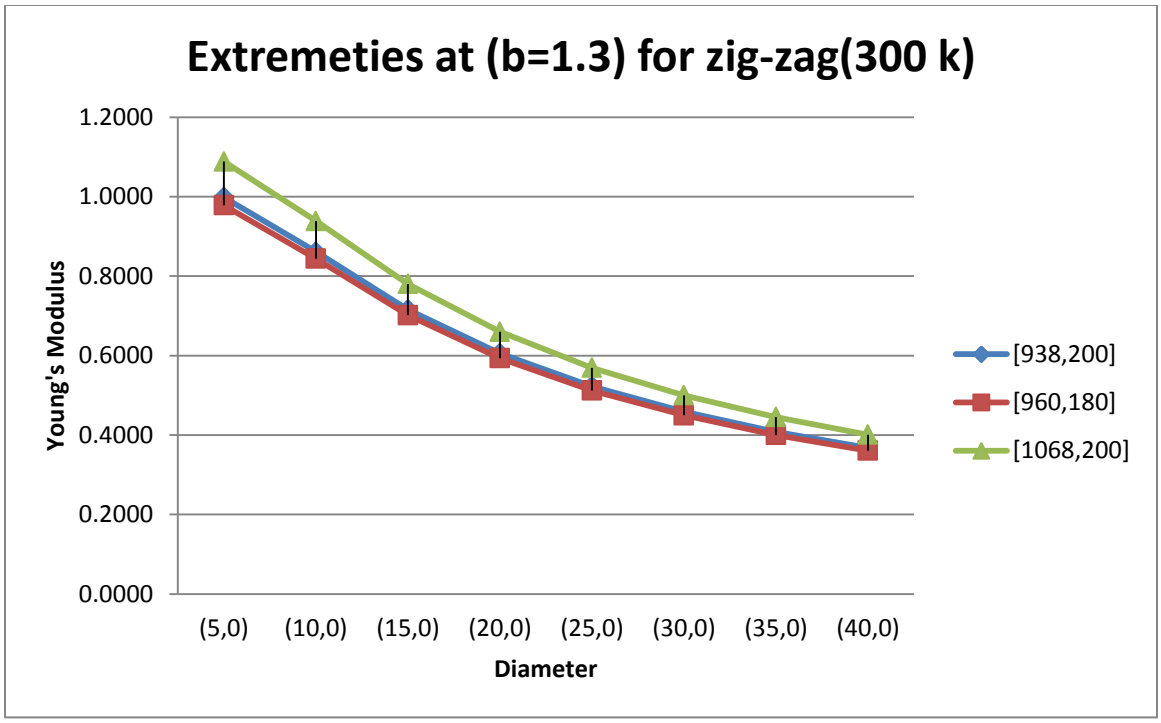

Fig.18 (young's modulus variation at extremities of bond length (1.35) at (300 k) for zig-zag)

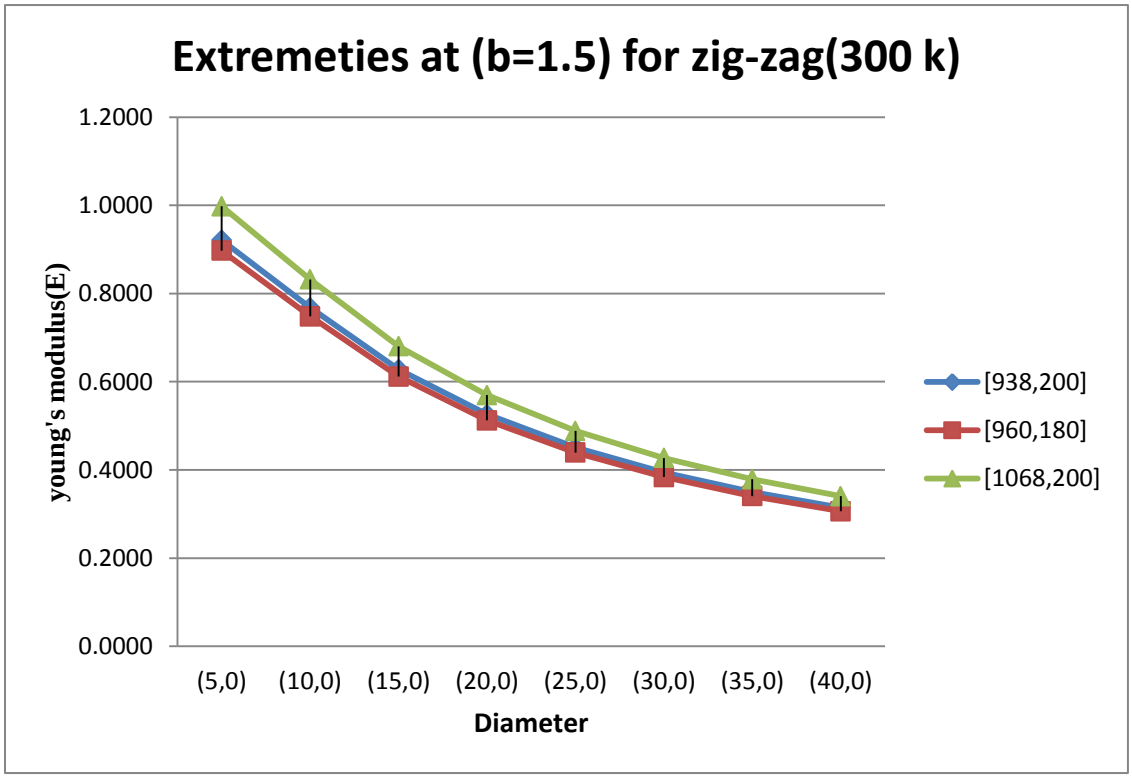

Fig.19 (young's modulus variation at extremities of bond length (1.5) at (300 k) for zig-zag)

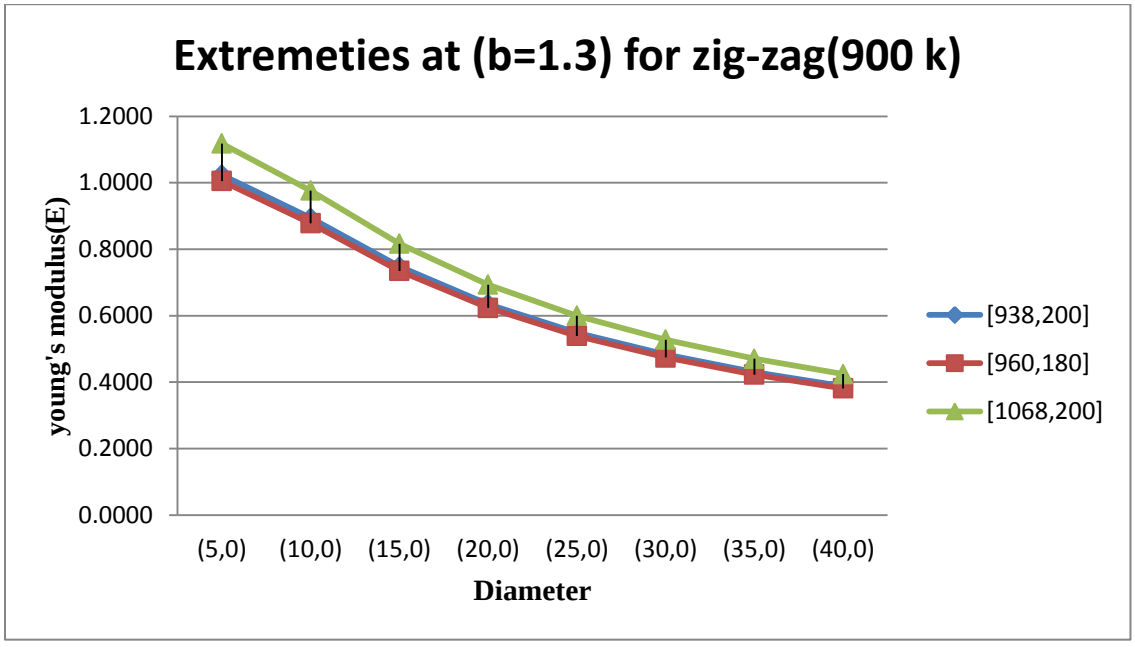

Fig.20 (young's modulus variation at extremities of bond length (1.3) at (900 k) for zig-zag)

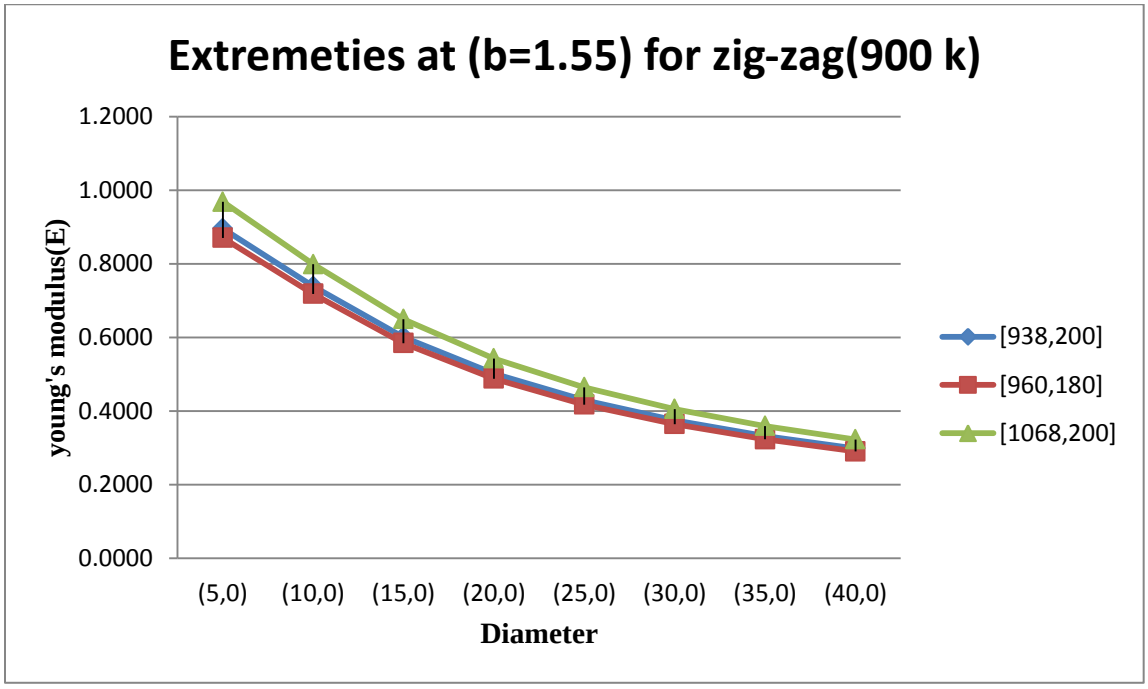

Fig.21 (young's modulus variation at extremities of bond length (1.55) at (900 k) for zig-zag)

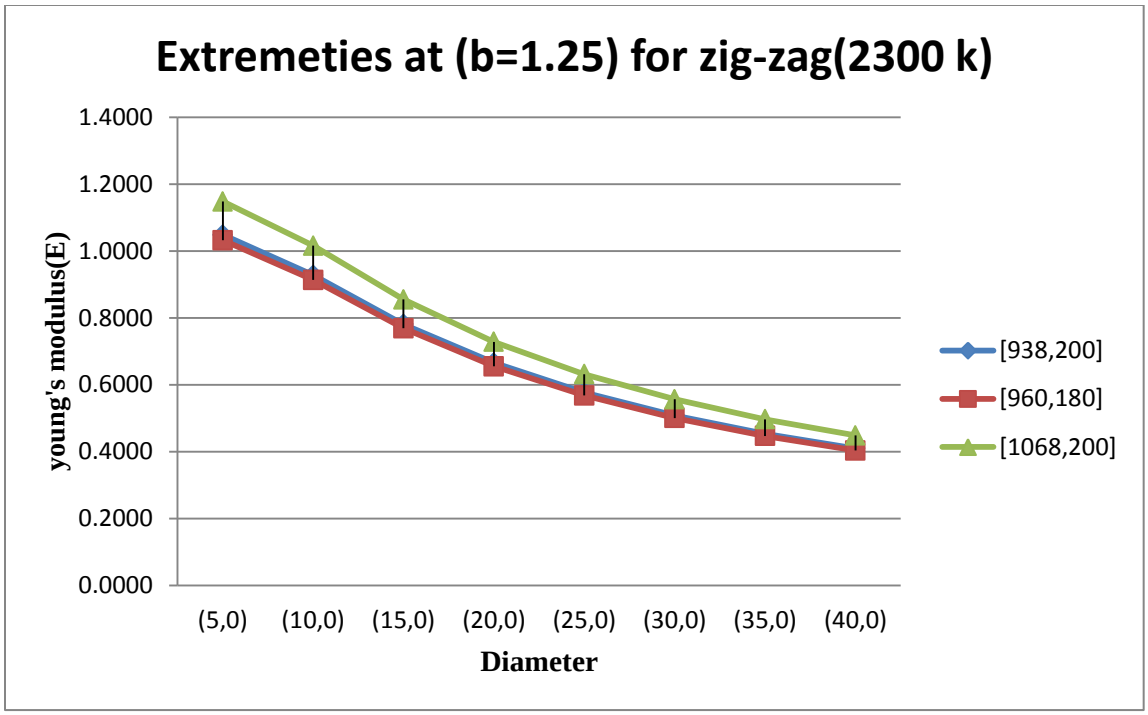

Fig.22 (young's modulus variation at extremities of bond length (1.25) at (2300 k) for zig-zag)

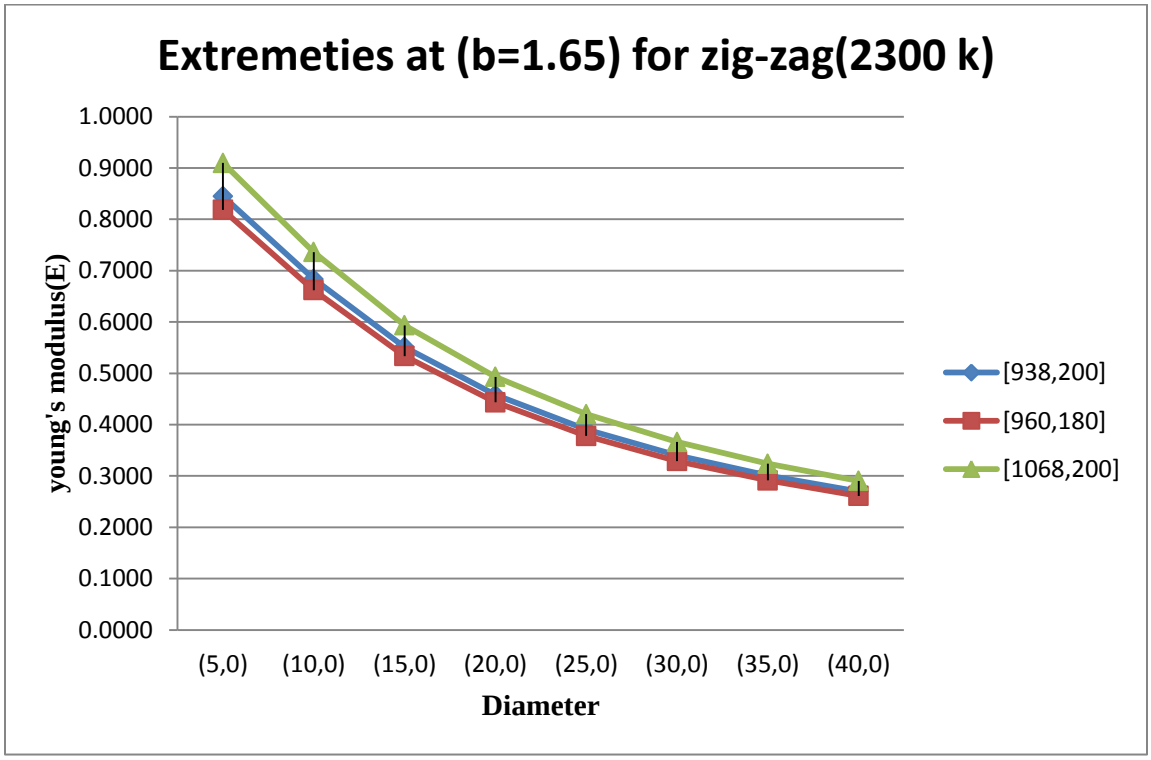

Fig.23 (young's modulus variation at extremities of bond length (1.65) at (2300 k) for zig-zag)

Also the effect of increasing temperature is also investigated on the extreme points of nanotube bond length in accordance with the optimum values of force constants. And the above results (table 5.3, table 5.4) states that the values lies in the range of (1.1479–.8184 TPa) for zig-zag nanotubes. And also, for armchair nanotubes the values lies in the range of (1.0615–.7015 TPa).

Table:5.4 Young's modulus values for different types of armchair carbon nanotube at different temp.

T (K)	b(Å)	k_1	k_2	(5,5)	(10,10)	(15,15)	(20,20)	(25,25)	(30,30)	(35,35)	(40,40)
300	1.35	938	200	0.9046	0.6607	0.5087	0.4118	0.3453	0.2971	0.2607	0.2321
	1.35	960	180	0.8866	0.6476	0.4987	0.4036	0.3385	0.2912	0.2555	0.2275
	1.35	1068	200	0.9859	0.7201	0.5545	0.4488	0.3764	0.3239	0.2841	0.2530
	1.5	938	200	0.8120	0.5767	0.4387	0.3527	0.2945	0.2527	0.2212	0.1967
	1.5	960	180	0.7910	0.5617	0.4274	0.3436	0.2869	0.2461	0.2155	0.1916
	1.5	1068	200	0.8795	0.6246	0.4752	0.3820	0.3190	0.2737	0.2396	0.2130
900	1.3	938	200	0.9368	0.6914	0.5348	0.4339	0.3645	0.3140	0.2757	0.2457
	1.3	960	180	0.9202	0.6791	0.5253	0.4263	0.3580	0.3084	0.2708	0.2413
	1.3	1068	200	1.0233	0.7552	0.5842	0.4740	0.3981	0.3430	0.3011	0.2683
	1.55	938	200	0.7828	0.5512	0.4179	0.3353	0.2796	0.2397	0.2097	0.1863
	1.55	960	180	0.7610	0.5359	0.4062	0.3259	0.2718	0.2330	0.2039	0.1811
	1.55	1068	200	0.8462	0.5958	0.4517	0.3624	0.3023	0.2591	0.2267	0.2014
2300	1.25	938	200	0.9697	0.7235	0.5624	0.4575	0.3850	0.3320	0.2918	0.2602
	1.25	960	180	0.9545	0.7122	0.5536	0.4504	0.3790	0.3269	0.2872	0.2561
	1.25	1068	200	1.0615	0.7920	0.6156	0.5009	0.4214	0.3635	0.3194	0.2848
	1.65	938	200	0.7270	0.5039	0.3795	0.3034	0.2524	0.2161	0.1888	0.1676
	1.65	960	180	0.7039	0.4879	0.3675	0.2938	0.2444	0.2092	0.1828	0.1623
	1.65	1068	200	0.7827	0.5425	0.4086	0.3266	0.2718	0.2326	0.2033	0.1805

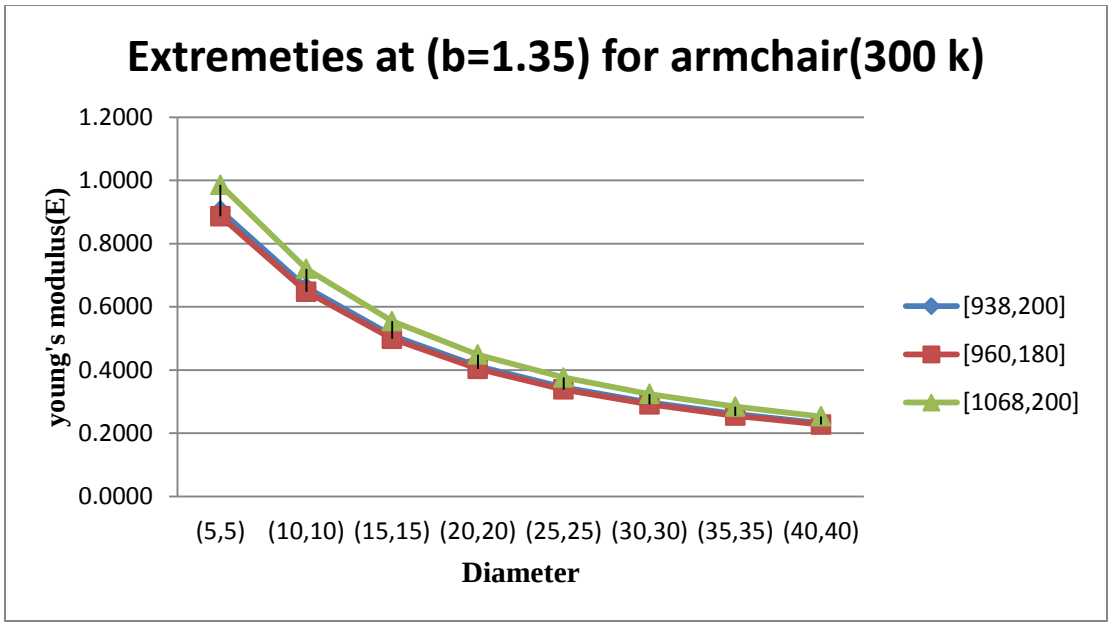

Fig.24 (young's modulus variation at extremities of bond length (1.35) at (300 k) for armchair)

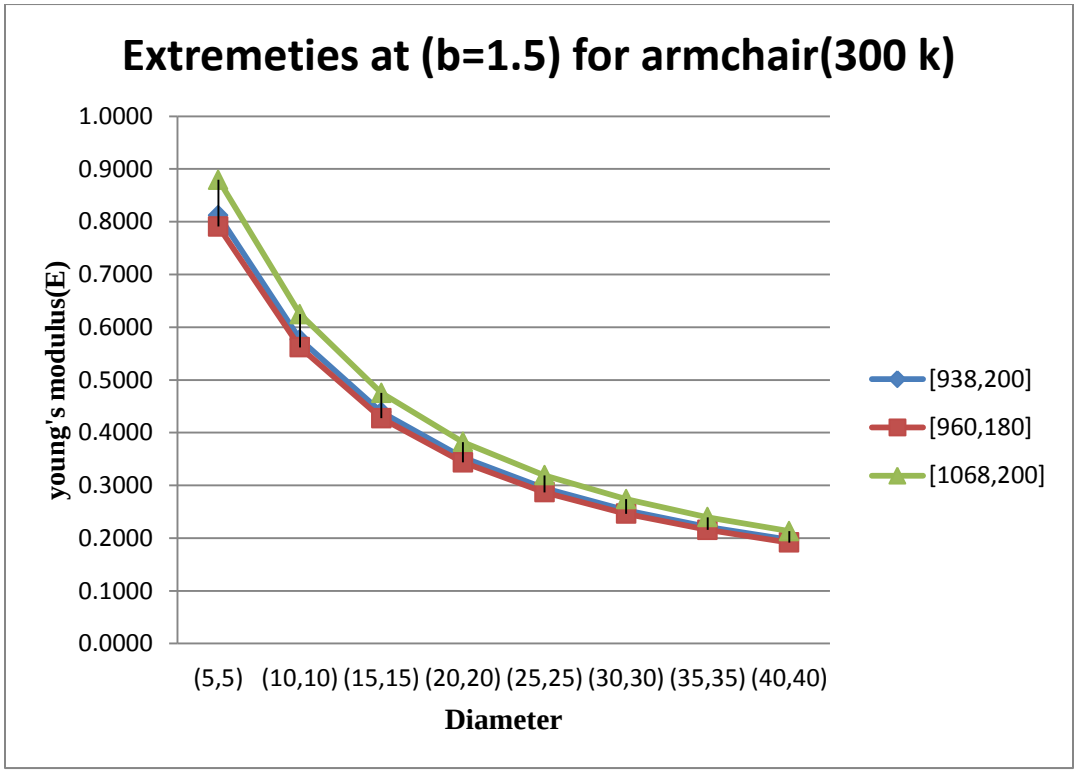

Fig.25 (young's modulus variation at extremities of bond length (1.5) at (300 k) for armchair)

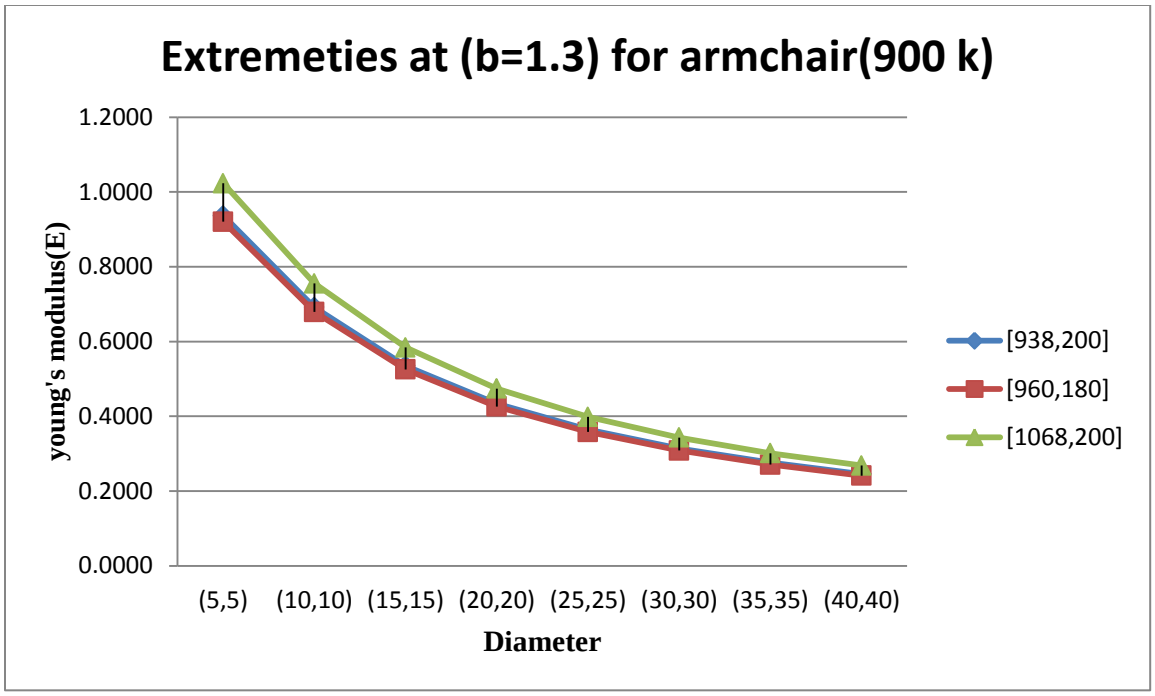

Fig.26 (young's modulus variation at extremities of bond length (1.3) at (900 k) for armchair)

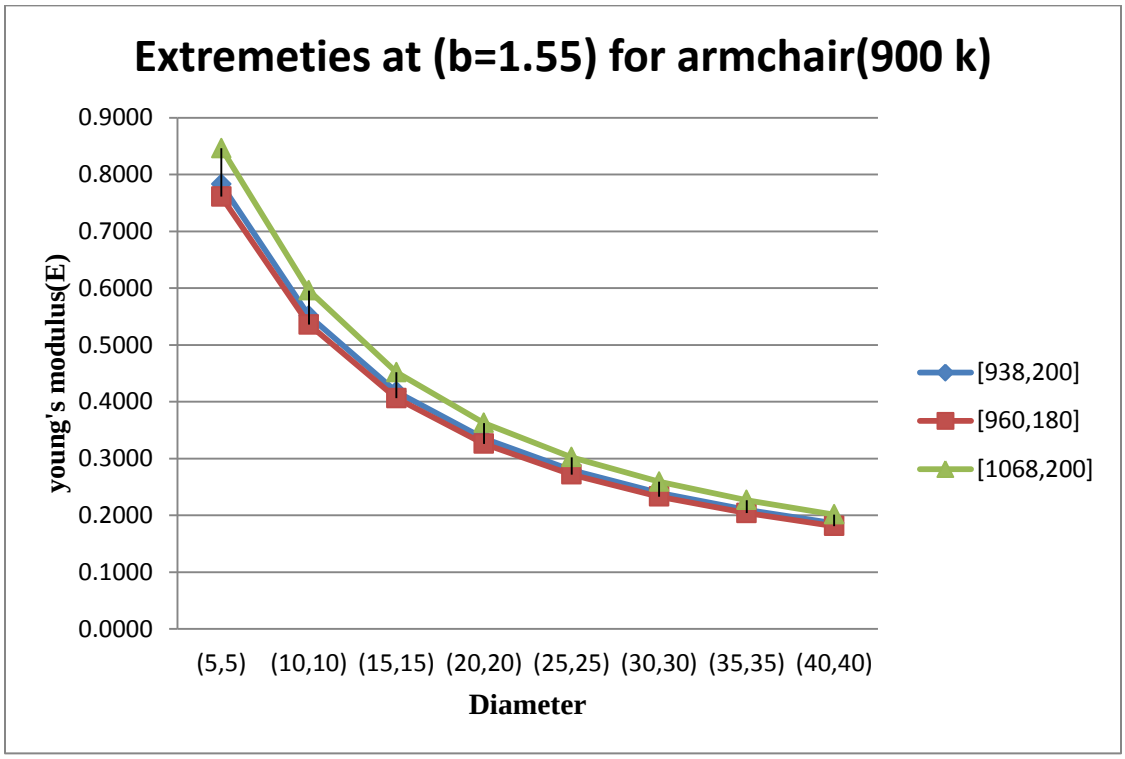

Fig.27 (young's modulus variation at extremities of bond length (1.55) at (900 k) for armchair)

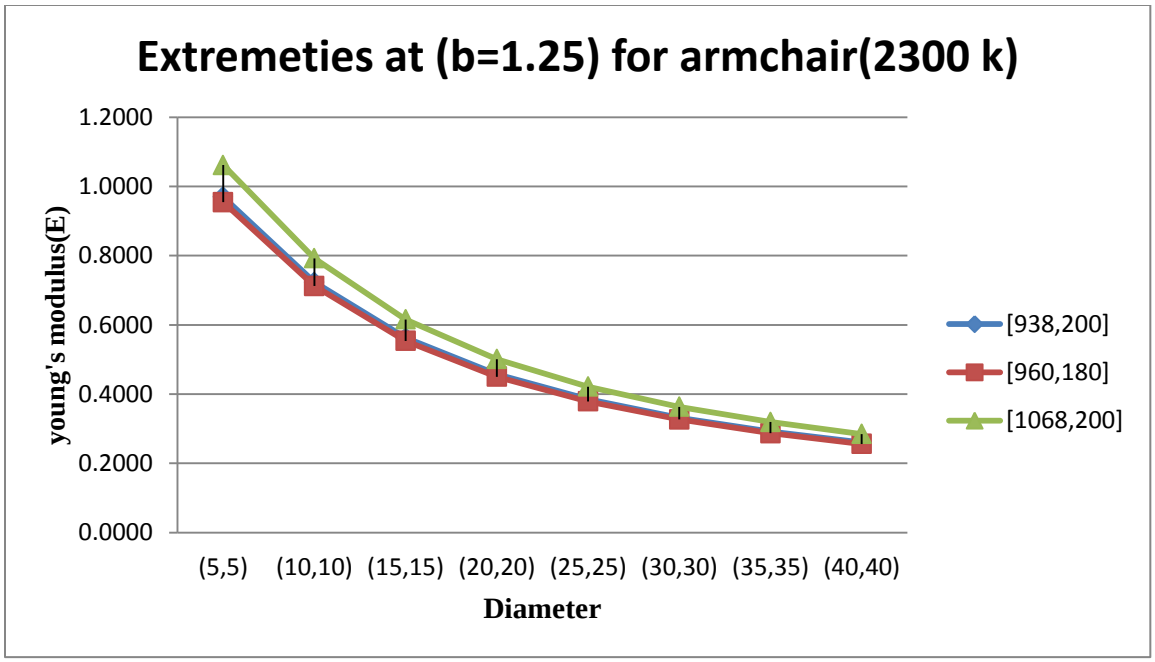

Fig.28 (young's modulus variation at extremities of bond length (1.25) at (2300 k) for armchair)

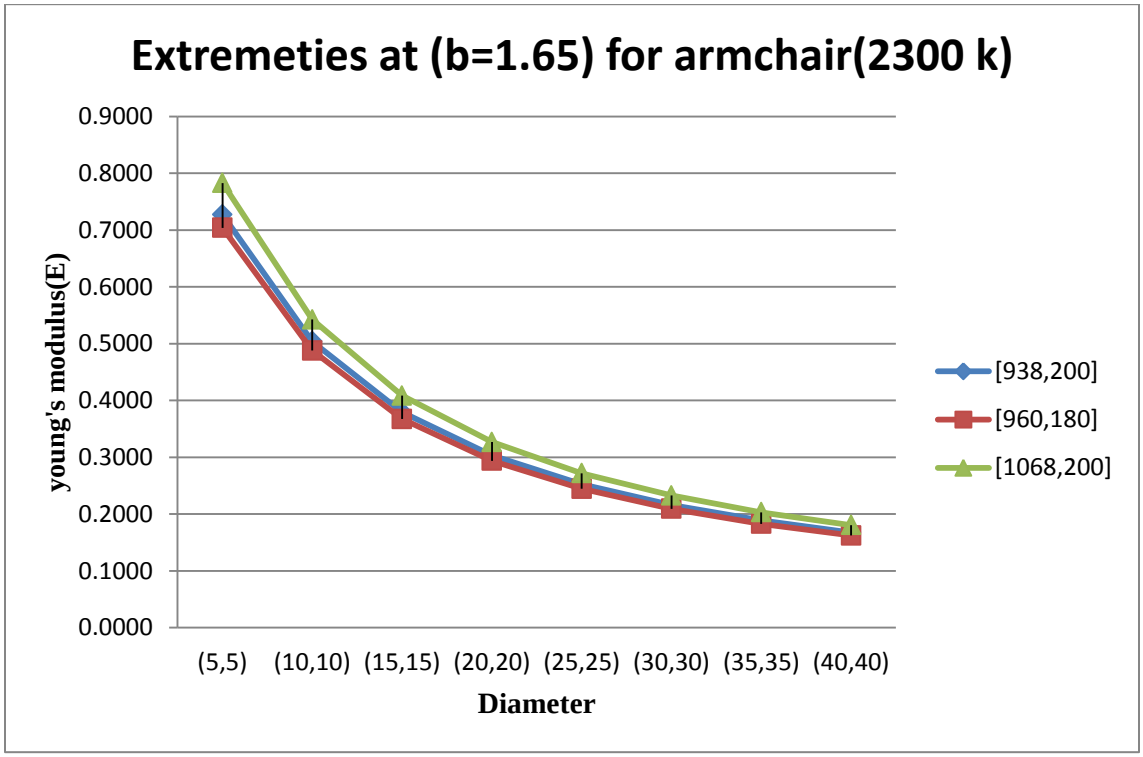

Fig.29 (young's modulus variation at extremities of bond length (1.65) at (2300 k) for armchair)

VARIATION OF YOUNG'S MODULUS AT (THICKNESS = 0.66 Å) CONSIDERING THE OPTIMUM VALUES OF FORCE CONSTANTS

Table 5.5 Young's Modulus values with optimum values of force constants for zig-zag (t = 0.66 Å)

b(Å)	t(Å)	k_1	k_2	(5,0)	(10,0)	(15,0)	(20,0)	(25,0)	(30,0)	(35,0)	(40,0)
1.42	0.66	938	200	2.4601	1.4286	1.0038	0.7732	0.6287	0.5297	0.4576	0.4027
1.42	0.66	960	180	2.4042	1.3962	0.9810	0.7557	0.6144	0.5176	0.4472	0.3936
1.42	0.66	1068	200	2.6734	1.5525	1.0908	0.8403	0.6832	0.5756	0.4973	0.4377

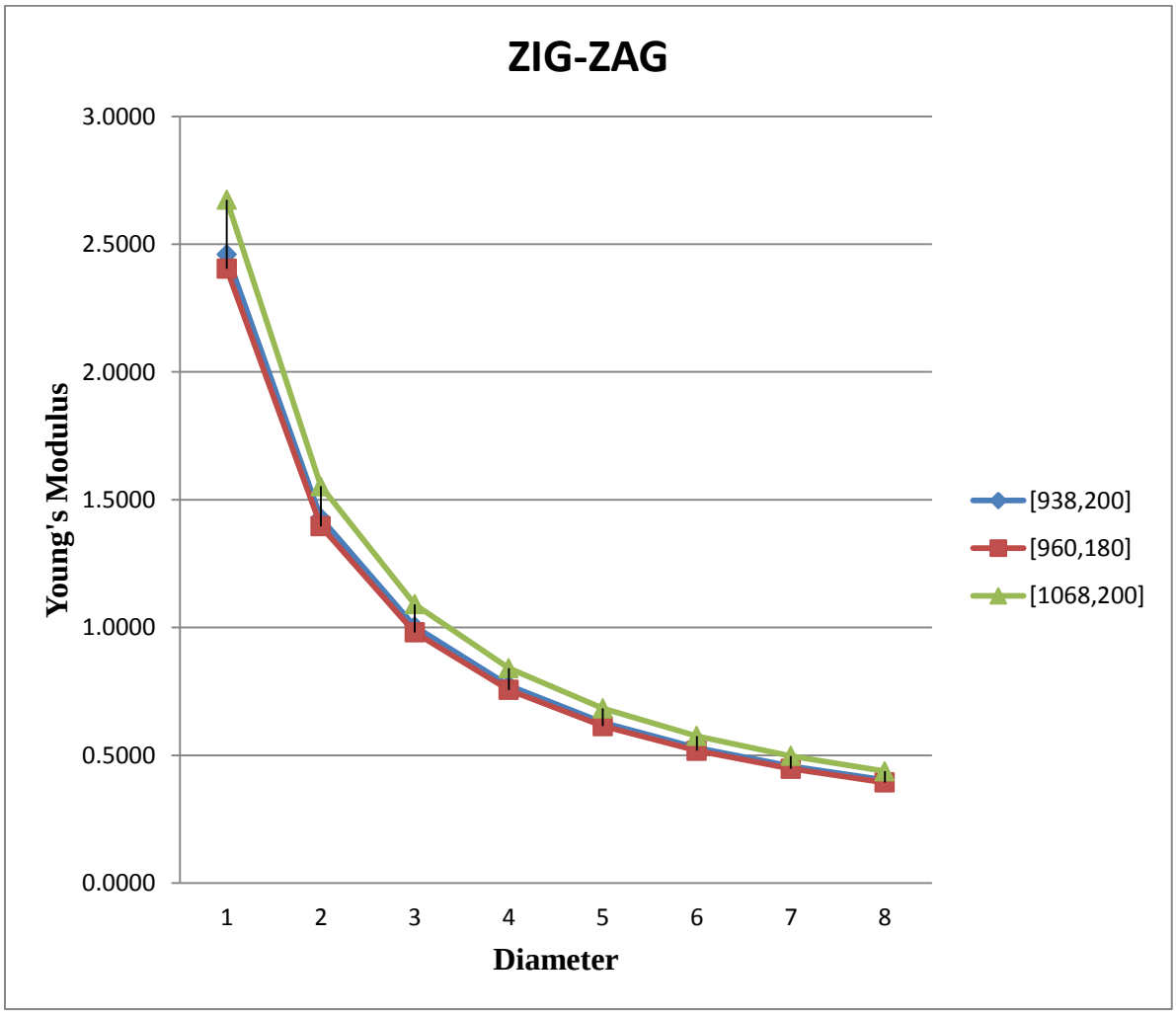

Fig.30 (young's modulus variation at thickness =0.66 Å for zig-zag)

Table 5.6 Young's Modulus values with optimum values of force constants for armchair (t = 0.66 Å)

b(Å)	t(Å)	k_1	k_2	(5,5)	(10,10)	(15,15)	(20,20)	(25,25)	(30,30)	(35,35)	(40,40)
1.42	0.66	938	200	1.6107	0.8818	0.6065	0.4621	0.3732	0.3130	0.2695	0.2366
1.42	0.66	960	180	1.5741	0.8618	0.5927	0.4516	0.3647	0.3059	0.2634	0.2313
1.42	0.66	1068	200	1.7504	0.9583	0.6591	0.5022	0.4056	0.3401	0.2929	0.2572

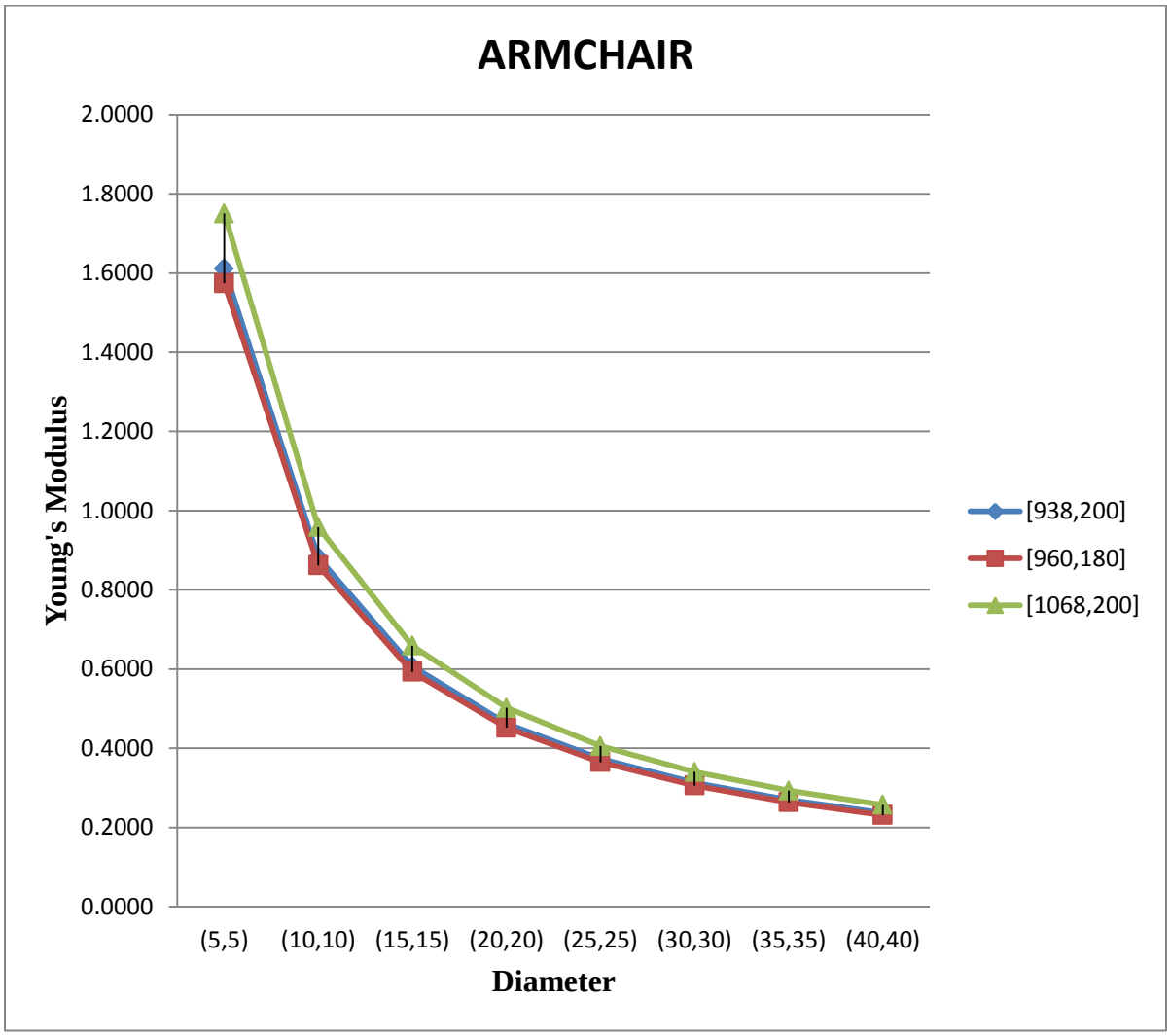

Fig.31 (young's modulus variation at thickness =0.66 Å for armchair)

CHAPTER 6

CONCLUSION AND FUTURE SCOPE

According to different researches the calculated young's modulus (E) of the graphene sheet is equal to 0.8 TPa. But based on the presented theory, it has been predicted that the optimum values for the young's modulus for zig-zag type single walled carbon nanotubes lies in the range of (1.0460–0.6346 TPa) and for armchair type single walled carbon nanotubes, the optimum values lies in the range (.9352–.5247 TPa). These optimum values of young's modulus are obtained in accordance to the better selection of force constants. Our findings shows that the improved values of young's modulus is obtained with force constants (k_1,k_2) taken as (938, 200), (960, 180) and (1068, 200). Also by varying the thickness of the SWCNT as 0.66 Å, the values for the young's modulus determined are in the range of (2.6734–.4027 TPa) for zig-zag. And for armchair, it lies in the range of (1.7504–.2366 TPa) respectively.

It is seen that the predicted values obtained from the nano scale continuum model agrees well with results from the molecular dynamics simulation. The elastic property predicted, agrees reasonably with the existing experimental and theoretical results. The simplified formulation is able to serve as a good approximation for SWCNT.

FUTURE POSSIBILITIES

1. The effect of low temperature (below zero) may also change the mechanical properties of SWCNT.
2. The same boundary conditions of high temp can be applied on MWCNT and its behavior on mechanical properties can be studied.
3. If the tube is considered of atom structures then its thickness lies near to zero and it affects the value of young's modulus through many folds.
4. In future, the other elastic properties can be investigated by using the present analysis.

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