Modeling and Simulation of Polymer Nano-Composite to Study Mechanical Properties

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Dedication

Dedicated to my family, friends, teachers and mentors.

Kamran

Behold! In the creation of the heavens and the earth; in the alternation of the Night and the Day; in the sailing of the ships through the Ocean for the profit of mankind; in the rain which Allah sends down from the skies, and the life which He gives therewith to an earth that is dead; in the beasts of all kinds that He scatters through the earth; in the change of the winds, and the clouds which they trail like their slaves between the sky and the earth; (here) indeed are signs for a people that are wise

Al - Baqara 2-164

Acknowledgement

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My sincere thanks to my wife for keeping up with me during the countless hours I spent in pursuit of this thesis and course work. I attribute my Masters degree to her encouragement and effort. Prayers of my parents will always be the ultimate source of encouragement to me. Gratitude to all.

Kamran Hashmi

Abstract

In the competitive environment of aircraft industries it becomes absolutely necessary to improve the efficiency and performance. Modern aircrafts like Boeing 787 and Airbus A350 comprise of around 50% of composite materials by weight. The performance advantages associated with reducing the weight of aircraft structural elements has been the major impetus for military aviation in composites development. Polymer Nano Composites (PNC) due to low cost, light weight, ease of production and designing of end product polymer material are extensively produced in most of the bulk industrial consumable production. However, the lack in strength and low modulus hinders its utility at high end engineering application due to fatigue and creep failure as compared to metal and ceramics. In order to enhance its properties reinforcement are introduced nano scale to increase is mechanical strength, heat and temperature resistance and decrease in permeability. Nano scale is so small that its visualization and manipulation of properties creates challenges at experimental perspective. Thereby, employing computational approach to develop a structure and examine further how properties varies with change of time and conditions that temperature, pressure, stress and concentration. Modeling and optimization of Polymer Nano Composites, that is, Graphene Nano Sheet with Polyvinyl Alcohol (GNS-PVA) , Graphene Nano Sheet with Polyvinyl Chloride (GNS-PVC) through Simulation Software (Material Studio). Series of simulation shows its Young’s Modulus has increased to considerable value. By virtue of exceptional properties demonstration Graphene based polymer nano composite are used where high performance and strength desired under extreme temperatures and pressures like aerospace. The increase in Young’s Modulus is evident as its raise from 67 % up to 124 % with in-cooperation GNS in PVA. Young’s Modulus value through simulation shows linear increase in Young’s Modulus is observed with increase of weight percentage of Graphene from 3.5 to 5 weight percent whereas after 5.1 to 6 weight percent the increases in not linear. The maximum achieved value is approximately 124 percent increase. With incorporation of Graphene Nano Sheet in Polyvinyl Chloride the maximum value observed after increase weight percent is 4.42 GPa which is almost 53 percent increase in Young’s Modulus

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List of Abbreviations

Graphene Nano Sheet - GNS

Polyvinyl Alcohol - PVA

Polyvinyl Chloride - PVC

Boron Nitride - BN

Boron Nitride Nano Sheet – BNNS

Molybdenum disulfide - MoS_2

Molecular Dynamic - MD

Carbon Nano Tube - CNT

Giga Pascal - GPa

Hexagonal Boron Nitride - h-BN

Quantum mechanics - QM
Monte Carlo - MC

Introduction

1.1 Motivation

Composite materials are widely used in the aircraft industry and have allowed engineers to overcome obstacles that had been there when using the materials individually. Composite materials can help to reduce costs and boost product integrity in the design and manufacturing of aerospace parts; Strength to weight ratio – composites can be extremely strong without being heavy, boosting the structural integrity of parts and overall aircraft fuel efficiency. Rapid advancement in manufacturing technique along with revolution in material technology has opened venture in field of advance composite material. Improve material strength with least compromise on weight enhancement is always a challenging task in designing parameter of aerospace industry. Thereby various metallic component in aircraft are being replaced with composites such as swapping of Metallic blades with Composite blades with 10 time more operating life in helicopters. This was my motivation to study the properties of composite materials.

1.2 Thesis Requirements

The work done in this thesis includes modeling and optimization of Polymer Nano Composites that is, Graphene Nano Sheet with Polyvinyl Alcohol (GNS-PVA), Graphene Nano Sheet with Polyvinyl Chloride (GNS-PVC) and Boron Nitride with Polyvinyl Chloride (BN-PVC) through Simulation Software (Material Studio). Series of simulation have been performed to calculate its Young Modulus. Furthermore, simulation results were analyzed to draw comparisons with results obtained from simulation vis-à-vis properties observed through experimental results.

Graphene has revolutionized the nanotechnology since its discovery. The in-cooperation of Graphene Nano Sheet (GNS) in a material resulted into an enhanced composite material with promising utility in various industries that is aerospace, mechanical structural, electronics etc. Lately, efforts are in hand to impart other material nano-fillers such as Boron Nitride (BN), Molybdenum disulfide (MoS_2) in all dimensionalities (one, two and three dimension) with polymer based matrix.

1.3 Background

In the competitive environment of aircraft industries it becomes absolutely necessary to improve the efficiency, performance of the aircrafts. For instance if we see Modern aircrafts like Boeing 787 and Airbus A350 comprise of around 50% of composite materials by weight, where pursuit of high speed and efficiency has enforced material requirement with high strength without increasing excessive weight. The use of composites in the aerospace industry has increased dramatically since the 1970s. Traditional materials for aircraft construction include aluminum, steel and titanium. The primary benefits that composite components can offer are reduced weight and assembly simplification. The performance advantages associated with reducing the weight of aircraft structural elements has been the major impetus for military aviation composites development. New aircraft utilize carbon, boron and aramid fibers combined with epoxy resins. Such materials have replaced fiberglass reinforcements.

1.4 Composites

Composites are engineered products made from two or more different materials. A composite product provides a designed solution that surpasses the performance of the starting materials. Most composites are made by taking one material (the matrix) and having it surrounds fibers or fragments of a stronger material (the reinforcement). Usually discontinuous phase is stronger in comparison with continuous phase and known as reinforcement or fiber. The continuous phase is termed as matrix. Enhanced stiffness and strength in the composite material is due in-cooperation of reinforcement. Matrix and fiber composition is shown below:-

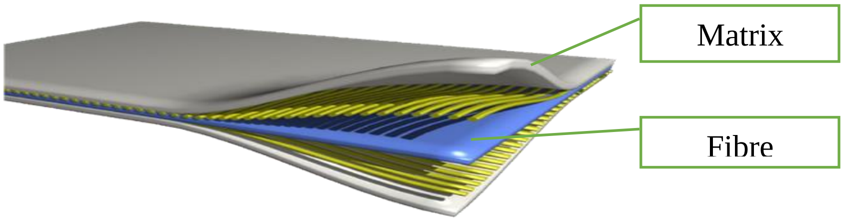


Figure 1-1 Fiber and Matrix Layered Structure

Fibers are bonded by the matrix, which transfer load on it and also provides protection from environment. Due to high aspect ratio of fiber (length to diameter) provisioning of load transfer is effective from matrix. Thereby, resulting composite material of much greater strength, stiffness and toughness than the fibers and matrix acting alone [1].

1.5 Nano Composites

Nano composite are designed with one content must be at least of nano-scale [1 nanometer (nm) = 10^{-9} meter (m)]. Nano-composite has drastically overcome the limitation of elemental composition control confronted during application of micro-composite and monolithic material. They exhibit unique design possibility and desired properties. The properties can be altered at nano-scale where interaction at phase interphase can be largely improved to enhance its overall material properties. In preparation of nano-composite surface area and volume ratio is crucial to manipulate its properties [1, 2].

1.5.1 Classification of Nano-composites (CMNC)

Nano-composite materials are classified on the basis of matrix utilized to form it [2]:-

a. Ceramic Matrix Nanocomposites materials (CMNC)
b. Metal Matrix Nanocomposites materials (MMNC)
c. Polymer Matrix Nanocomposites materials (PMNC)

1.5.1.1 Ceramic Matrix Nanocomposites (CMNC)

Ceramic are brittle material with high thermal and wear resistance properties. However, due to low toughness its utility as remained a stumbling block for their wider usage in industry. This short coming can be addressed through in-corporation of reinforcement in ceramic matrix. The nano-filler creates bridging medium to deflect crack propagation and hinders further opening of crack. Thus, increase the fracture toughness. Moreover, nano-filler experiences phase transition due to volume extension induced by the stress field of before propagation of crack.

Thereby, contributing strengthening and reinforcement even in nano-level [2]. Few Ceramic based Nano composite are tabulated below [2]:-

Table 1-1: Ceramic Based Nano Composites

Nano-Composites	**Applications**
Silicon Di Oxide / Cobalt	Application of optical fibers
Aluminum Oxide / Silicon Carbide	Structural materials application
Silicon Nitride / Silicon Carbide	Structural materials application

1.5.1.2 Metal Matrix Nano-composites (MMNC)

Metals due to its toughness and ductility are always a preference for high end engineering application for aerospace, automobile, space industry etc. The properties manipulation to enhance modulus and strength metal are reinforced with fibre. This nano-scale manipulation resulted improvement of various mechanical properties without affecting drastically on weight parameters. This will increase MMNC potential usage in aerospace and high temperature applications [2]. Few Metal based Nano composite are tabulated below [2]:-

Table 1-2: Metal Based Nano Composites

Nano composites	**Applications**
Aluminum / Aluminum Nitride	Usage in microelectronic industry
Copper-Niobium	Fabrication of structure for high temperature applications

1.5.1.3 Polymer Matrix Nano-composites (PMNC)

Due to low cost, light weight, ease of production and designing of end product polymer material are extensively produced in most of the bulk industrial consumable production. However, the lack in strength and low modulus hinders its utility at high end engineering application due to fatigue and creep failure as compared to metal and ceramics. In order to enhance its properties reinforcement are introduced nano-scale to increase is mechanical strength, heat and temperature resistance and decrease in permeability. This will enhance its properties without its weight increment [2]. Few polymer based Nano composite are tabulated below [2]:-

Table 1-3: Polymer Based Nano Composites

Nano-composites	**Applications**
Poly(amide-imide) / Titanium oxide	Gas separation applications.
Thermoplastic olefin/clay	Containerized Packaging for beverage.
Polyimide/clay	Parts for automobile

Nano scale composite has giving new venture for scientists and engineers to explore. However, at the same time it’s a challenging job to deal with material at such small level that is Nano-scale. The improvement in Nano composite has addressed various limitations that are faced by conventional component. At current its usage has been manifold in various industries, while continuous efforts are in hand for this to address emerging for various applications.

Literature Review

2.1 Introduction

When reviewing a composite material, it is mandatory to understand properties of each component individually. This gives a fair understanding of the resulting composite's physical and chemical properties. A noteworthy work exists on Graphene and Boron Nitride based Polymer Nano composite. Some relevant work was reviewed to develop understanding of said Nano composite's atomic structure, properties and composition. This understanding led to formulate the scope of this thesis and basis for simulation. Different methodologies used by researchers for modeling, optimization and simulation of Nano composites was analyzed and most appropriate method was adopted for this research.

2.2 Configuration of Polymer Nano-composite

Polymer nano composites are material with at least one component is of nano-scale. One dimensional nanowire [6, 7] or two dimensional layered material [9, 10, 11] filling exhibit improved electrical, mechanical and thermal properties. Thereby offers an opportunity to explore various concentration and component manipulation to enhance function and behaviors of primary material. Nano level manipulation at very low volume fraction influenced drastic changes in properties. This is because of small inter-particle distance, interaction at interphase and change in morphology. This allows polymer nano-composite to reached desired properties with retention of macroscopic homogeneity and low density of polymer [9]. It inherent low density allows usage of all three dimension of nano filler like silica particle as one dimension and Carbon Nano Tube (CNT) and whiskers in two and three dimension respectively [11].

2.3 Graphene and Graphene Nano Sheet Structure

Graphene is a hexagonal arrangement of sp2 hybridized carbon atoms in form of single layer sheet. Since its discovery it has attracted exceptional attention in nanotechnology usage due to its unique properties [3].

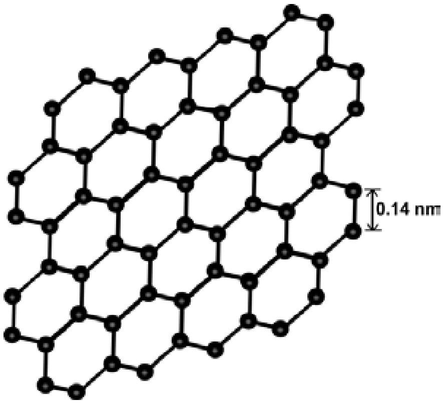


Figure 2-1 Honeycomb lattice structure with carbon-carbon bond distance [3]

In order to address market need for various state of the art composite materials, constant attempts are undertaken to synthesize Graphene at large scale. In recent years, dispersion of Graphene at nano level in a polymer matrix has opened innovative area of research for material scientist and engineers [3]. Polymer wide application in various industries like aerospace, automobile, construction, food package industry etc. has been hindered due to its inherent low strength property and gas permeability is now being addressed with creating of various Graphene based polymer nano composite [3].

2.4 Graphene based nano-composites and their properties

Diverse usage of Graphene based nano-composite has been observed. In case of Silicon Nitride-Graphene, Silicon Carbide-Graphene, Zirconium diboride–Graphene; few layers of Graphene has enhanced thermal conductivity, refractory and anti-friction properties [13].

Zirconium diboride–Graphene based nano-composite sheets are used on space vehicle to stand against extreme temperatures observed during re-entry. These ultrahigh temperature ceramic composites are consistently used at space shuttles nose caps and ballistic military equipment and shown promising results to restrict severe thermal impact loading [3, 12].

Titanium nitride - Graphene based nano-composites are used for construction of membrane to restrict permeability of hydrogen gas. The membrane obtained was reviewed for hydrogen gas permeability at various pressure (0.1 and 0.3 Mega Pascal) and temperature (473, 573 and 673 Kelvin). It has displayed better hydrogen permeability observed then Palladium-Silver membrane used previously [3].

Young’s modulus of Graphene Nano Sheet and Poly Vinyl Alcohol based nano-composite rises; linearly with increase of Graphene Nano Sheet fraction up to a certain level. It has been reported that Young Modulus value increase up to 1.3 Gega Pascal (GPa) with increase of nano filler concentration from initial value of 0.74 Gega Pascal of neat Polyvinyl Alcohol. Furthermore, approximately ~20 % increase in strength is observed in neat Polyvinyl Alcohol even at lesser loading of only 0.001 Volume fractions Graphene Nano Sheet [5].

Moreover, with uniaxial drawing of composite and reinforcement that is alignment of polymer chain substantial 4 time increase strength is observed in composite properties. The value increases from 38 MegaPascal (MPa) to 60 MPa [5].

Introduction of Graphene Nano Sheet up to 0.5 weight percent in epoxy resin; increase of Modulus from 2 GPa to 3.1 GPa at room temperature. [26]

Incorporation of 2 weight percent in Graphene in Poly Vinyl Chloride (PVC) increase Young Modulus to 71 percent as compared to neat PVC [42].

58 percent increase in Young's modulus was obtained with a 2 weight percentage loading of Graphene in Pure Polyvinyl Chloride films [42].

2.5 Application of Graphene based Nano-composites

Graphene dispersion in the host matrix improves the properties of entire composite system through strengthening and increasing interfacial bond between host and matrix. This bonding overall dictates the cumulative properties of nano-composite [3]. Various Graphene based composites are used in medical, electronics, aerospace, automobile industry. The Graphene based nano composite generally exploits its high strength properties [3].

By virtue of exceptional properties demonstration Graphene based polymer nano composite are used where high performance and strength is desired under extreme temperatures and pressures like aerospace. However, defect free and large scale production remains an issue. After going through various research papers it can be concluded that due to exceptional properties "Graphene" remains a promising candidate for nano-filler.

2.6 Boron Nitride Structure

Boron nitride (BN) is a compound of boron and nitrogen with inherent properties to withstand high temperatures. It is chemically resistant and possess considerable refractory properties. It exists in various crystalline structures similar to carbon. Its hexagonal structural configuration is stable and corresponds to Graphene structure. Its cubic structure is called c-BN and it corresponds to diamond structure. It is softer but its thermal and chemical stability is concurrent to diamond. This significantly opens ways for BN as nano-filler in nano-material. BN can be shaped in similar structure as carbon nanotubes or sheets, but its properties differ as of carbon [14]. Various structures are shown below:-

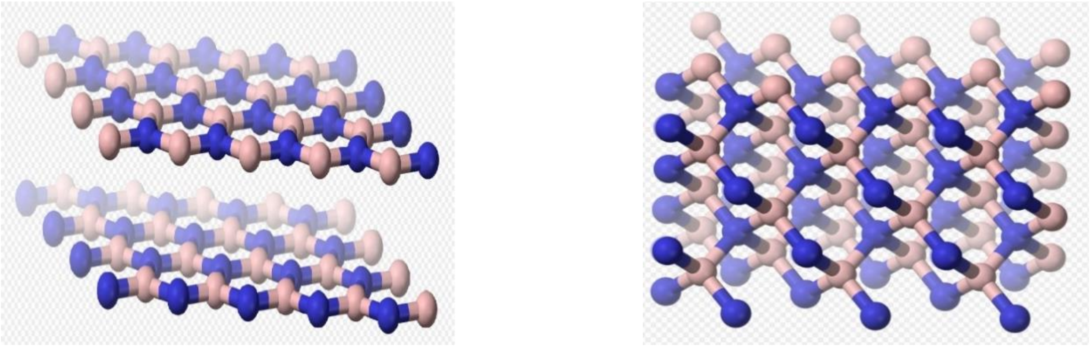


Figure 2-2: Structural configuration of Boron Nitride

Hexagonal Boron Nitride (h-BN) is the most stable crystalline form of Boron Nitride (BN), where boron and nitride is having strong covalent between them; whereas weak van der Waals forces exists between the layers. It is the commonly used morphology of BN [35].

2.7 Boron Nitride base Nano-composite and its properties

Hexagonal Boron Nitride Nano Sheets (BNNSs) are developed as nano-filler for reinforcing various polymers. These are electrically insulating and enhance mechanical and barrier properties in polymers without changing electrical properties. Due to hexagonal structure mechanical properties are considered to be comparable with Graphene. In a recent research, BNNSs has been mixed with Polyvinyl chloride (PVC). Young Modulus of neat PVC increases from initial value of 1.45 Gega Pascal (GPa) to enhance value of 2 GPa after in-cooperation of BNNSs [17].

2.8 Applications of Boron Nitride based Nano-composites

2D nano-materials have tremendous potential in fabrication of next generation electronic device. Hexagonal boron nitride (h-BN) monolayer can be considered as example which is equivalent as a honeycomb lattice structure of Graphene [15]. Due to its chemical inertness along with temperature resistance to oxidation and high thermal conductivity, its utility in micro and nano electronic devices has increased manifold as insulator [15] and considered to be a nano-fillers in high strength and thermal conductive nano-material.

In recent past carbon-based and inorganic nano fillers gained attention both in academia and industries. These are extensively used in energy storage devices and complex integrated electronic systems. The inorganic nano-fillers like boron nitride can substantially alter the properties of the composite materials. It is used in variety of application such as pencil leads, paints, dental cements, cosmetics. It is even used space applications [36].

Boron nitride is used as parts of high-temperature equipment such as bearing. Hexagonal Boron Nitride (h-BN) is included in plastics, rubbers and ceramics for introducing self-lubricating properties [36, 37].

2.9 Polymer Material usage in Aerospace Industry

Various Polymers based products qualified specified requirements for flame, heat and impact resistance; they are available un-limited surface textures / colours providing unmatched brilliance and scratch resistance [40].

2.9.1 Polyvinyl Chloride (PVC)

Traditional material Aluminum, Titanium and advance material are versatile but it weight penalty; which is contrary to reduce weight for better fuel efficiency and increase loading capacity [40, 41]. Thereby, various fuselage cabin fitting is made from a thermoplastic which caters the complex design and light weight issues. During assembling of Boeing 767, looking for weight reduction cabin interior was initially focused. The hinge bracket of overhead cabin was made of Aluminum; which is heavy and cost additional machining which increase the cost. It was replaced with PVC structure with can withstand the mishandling overhead bin received while luggage loading; moreover, it can molded in white colour [41].

2.9.2 Polyvinyl Alcohol (PVA)

PVA Tape and threads are used at many places in aircraft such as interior cabin and Plexi - glass windshield. This material is used woven / repair of wind shield structure and then on the outside with a coating layer treatment. It is waterproof coating until the coating is not damaged [40, 41].

2.10 Computational Methods

In order to enhance the distinct mechanical properties, researchers are evaluating material structures at 0.1-300 Nano-meter length (Nano-scale) [18]. Nano scale is so small that its visualization and manipulation of properties creates challenges at experimental perspective. Thereby, employing computational approach to develop a structure and examine further how properties varies with change of time and conditions that temperature, pressure, stress and concentration [18].

2.10.1 Methodology for Computation

Various computational methods are developed to simulate a real system. Now the question arises how to figure out which model is suitable for our system [18, 19]. The compatible model should suitability study physics and chemistry of molecular interactions within the system [18, 19]. Computational methodology has several benefits [18]:-

a. Modeling of complex molecular system with reduce budget and time which is required to prepare physical material samples.

b. Provisioning of information on the atomic and molecular behaviors at atomic and sub-atomic level through simulation. This is difficult to obtain from experimental approach.

c. Allows one to understand the material properties and behavior more accurately.

However, one shortcoming of molecular simulations is that its results are never totally reliable and required validation through experimental data.

2.11 Selection of Computational Methodology

According to scale and type material configuration, number of computational methodologies has been developed based on various theoretical frameworks.

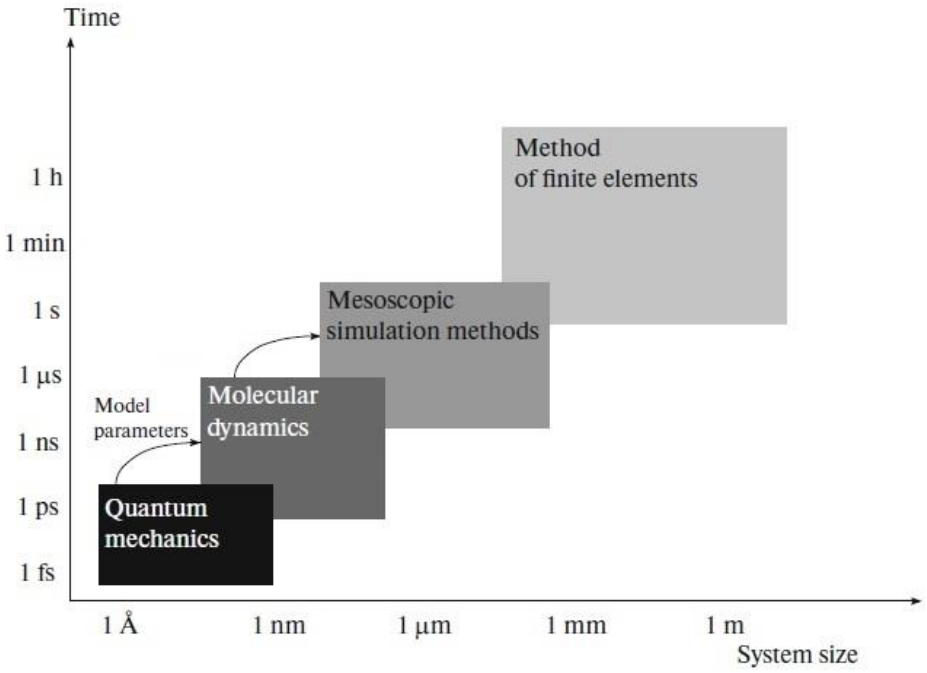


Figure 2-3: Structural Scale for Various Simulations

For explaining above cited statement (Figure. 2-3) clarify how Quantum mechanics (QM), Molecular dynamics (MD) and Monte Carlo (MC) are based on various theoretical framework and properties predicted by each method.

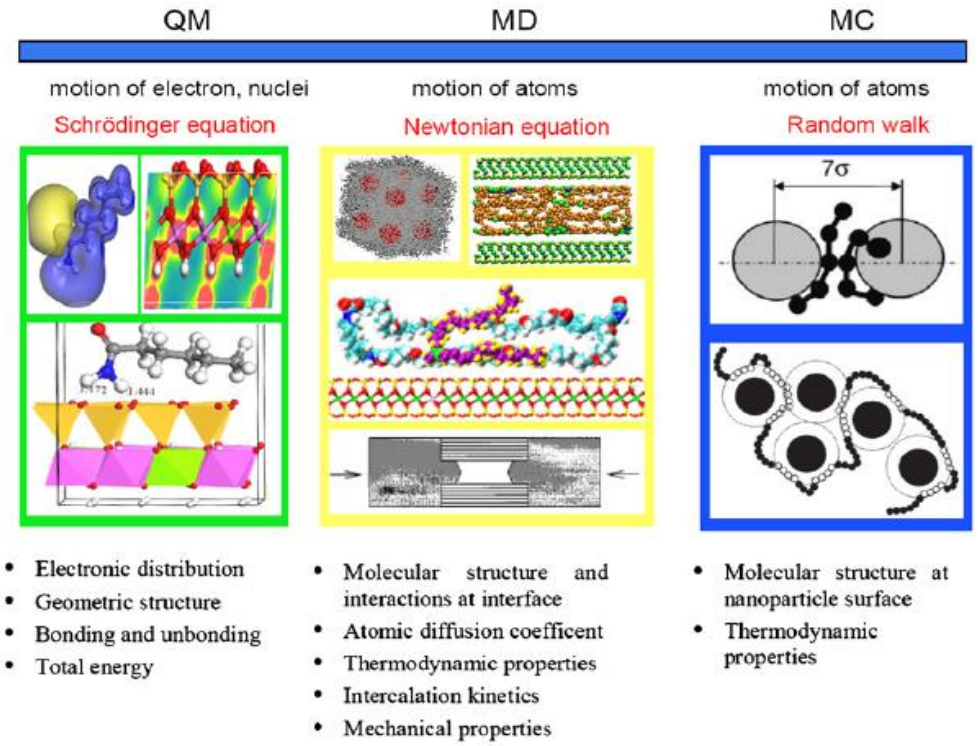


Figure 2-4: Simulation theoretical framework

Quantum mechanics (QM) theoretical frame work is based on motion of electron whereas; Molecular dynamics (MD) and Monte Carlo (MC) theoretical frame work is based on motion of atoms [19].

Polymer based nano-material simulation is mainly focused toward atoms and molecular interactions of structure along with its thermodynamics [19]. Therefore, simulation method adopted is based on Molecular Dynamics. MD simulations can predict thermo-mechanical properties of Polymer based Nano-composite like Elastic modulus, Tensile strength and Co-efficient of Thermal Expansion [20].

Computational approaches through Molecular Dynamic (MD) Simulation have been adopted to accurately examine the properties of nano-materials with respect to change in time and response to various physical conditions that is, temperature, pressure, stress or strain, and concentration.

2.12 Significance of Simulation

Interpretations through experimental techniques were previously used to depict material behavior. Models were developed by obtaining measurements during experimental process. This is essential to develop theoretical frame work. Subsequently theories can be utilized to predict new material properties before conducting physical experimental work. Consequently with advancement in computational field, accurate simulation can be carried out on the basis of already available theoretical frame work to describe structure properties before conducting experimental work.

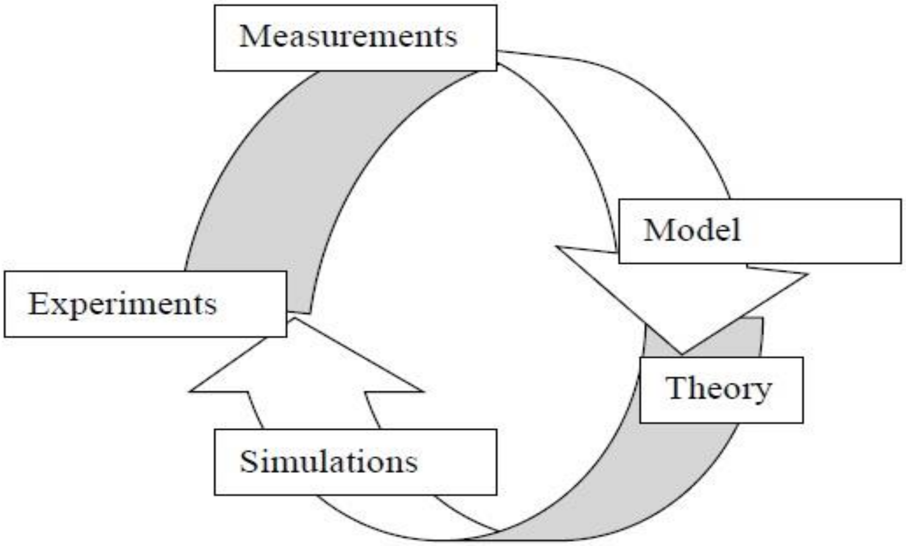


Figure 2-5: Significance of Simulation

Simulation encompasses computational approach to model molecular systems at various conditions. These methods are extensively used in several fields starting from chemistry, biological analysis, drug design and materials science to study molecular systems ranging from nano-scale to meso-scale system. Atomistic level explanation of the molecular systems can be deduced through simulation work.

As already discussed, our focus will be on Molecular Dynamics (MD) and its utility software corresponds to Polymer nano-composite. Polymers and their composites are categorized in macromolecules as it contains a large number of atoms. Therefore, potential based methods are computationally compatible for such molecular systems [21, 22].

2.13 Molecular Dynamics (MD) Simulation

Molecular Dynamic simulation is a tool for analysis of various material phenomena like mechanical, electrical and optical properties. It computes time dependent behavior through point masses and point charge of a molecular system in classic regime. Basic idea is to track motion of all atoms in a molecular arrangement by resolving Newton's equation of motions. A trajectory through integration is created which defines velocities, acceleration and position of each particle with respect to time. The achieved trajectories are linked to attain macroscopic thermodynamic quantities by means of statistical mechanics principles [33, 34].

The thermo-mechanical properties of polymeric materials and their nano-composites can be accurately quantified with MD simulation. MD simulations with reference to relative position and orientation of the nano-filler in the polymer matrix predict behavior of nano-composite system [34].

2.14 Molecular Dynamic Simulation Framework

Molecular Dynamics employs laws of classical Newtonian mechanics to calculate optimal geometry of a molecule as a function of potential energy. It is a function of the nuclei positions and calculated from relative positions of the atoms with respect to conformation of molecular system. In general, forces with respect to atomic positions are determined through gradients of potential energy functions. Choice of a particular force field depends on a system. For example, polymers computational energy at every time step requires specific force field. Graphic representation of the system sizes and simulation times for various simulation methods is depicted in fig below. For simulation comprising nano-scale, Molecular Dynamic simulation is mostly used by researcher. Computational simulation methods are most promising methods to reduce the cost of development of materials with specific properties [33].

2.14.1 Force Field

Force field is suitable for calculating structures and dynamics of molecules. It uses force constants and geometric parameters that depend on particular combination of atoms involved in because of bonding interaction (bend, angular, torsional) and Non-bonding interaction (electro static, Van der Waal). As, all bond distances are taken from atomic radii, therefore, one force constant is considered for bonds and angles [33, 34].

2.15 Limitation of Molecular Dynamics

Computational power inevitably limits the MD simulation. As we know that typical time scale for motion at atomic level is in order of pico-second (10^{-12} seconds), so in order to calculate move at several instance, time steps for calculation purpose is considered in femto scale (10^{-15} seconds). Therefore, millions of iteration will be generated to track a single atom for just micro second (10^{-6} seconds) [34]. Moreover, number of calculation with increase if number of atoms increase in the molecular system. Under these limitation and availability of lesser computational power, we should satisfy ourselves with small system [34].

Computer simulations act as a bridge between microscopic length and time scales and macroscopic world of the laboratory: It provides a guess at the interactions between molecules, and obtain 'exact' predictions of bulk properties. The predictions are 'exact' in the sense that it can be made as accurate, subject to the limitations imposed by our computer budge.

Due to limitations on the size of MD computational cell, boundary conditions has to be defined with specific temperature and pressure control along with adequate description of atomic interactions.

2.16 Software - Material Studio

In order to conduct simulation work within scope of thesis, selection of useful and available software i.e Material Studio was carried out. Materials Studio is software used for modeling and simulation of materials to examine various properties pertaining to mechanical, electric, optical etc. It is developed and distributed by BIOVIA, known for specializing in software for quantum mechanics, computational chemistry, bioinformatics, molecular dynamics simulation etc. This software is extensively used by universities, research centers and companies for advanced research on various materials, such as polymers, metals, and ceramics etc. Various Modules (tools) is used during the simulation process that is for construction of atomic and molecular structures. Subsequently, composite and its optimized structure for calculation of desired properties [38].

2.16.1 Material Studio – DFTB (Density Functional Base Binding)

It is an implementation of the Density Functional Theory based to study electronic properties of materials. It allows constructing variety of atomic and molecular structure to investigate its energy and optimized structural properties. With the help of electronic and repulsive energy contribution atomic parameters of modeled system are evaluated. It has capability to simulate systems containing hundreds of atoms [38].

With help of quantum mechanics it enables to optimize and study properties of materials. Calculations of properties like optimize structure, and Fermi surfaces can be predicted. It uses “Slater-Koster files” parameters to predict the interactions between the elements [38].

2.16.2 Material Studio – Amorphous Cell

It is a comprehensive model building tool for creating a wide range of polymeric materials. Its uses various Force field for building of wide range of systems including polymers as well as nanostructures. Building accurate models of polymers is a key to predicting the properties of these materials. Materials Studio Amorphous Cell has been designed to build realistic models of chain molecules enabling fast prediction of properties such as density, mechanical properties, and diffusivity [38].

2.16.3 Material Studio – Forcite Cell

Forcite is an advanced classical molecular mechanics tool that allows fast energy calculations and reliable geometry optimization of molecules systems. It provides the researcher immense flexibility, due to variety of Force fields. Various systems can be effectively optimized and their energies can be calculated. Energy minimization and optimization of systems is based on single point energies [38].

It is an advanced molecular mechanics tool to predict molecular mechanical properties of wide range of system [38].

2.16.4 Sample Size in Molecular Dynamics Simulation

Atomistic level model system is built in classical molecular simulation, with defined potential i.e Force field acting between the atoms. These interactions are comparable from nano-scale to bulk model [32]. These site to site interactions between each atom is intra-molecular bonding interactions like chemical bonds, angle bending, dihedral torsional and non-bonding interaction such as Van der Waals forces and Coulombic forces.

Models typically consist in order of 1 to 100 nm, having specified boundary conditions. The term boundary condition defines structures consisting of identical sub-units. During course of the simulation atoms and molecule moves in the original cell, as it moves exactly the same way in bulk samples. Molecular and macroscopic properties can be averaged on a molecular dynamics (MD) trajectory, through a simpler integration of Newton's equations of motion for all of the atoms in the model system. Available computational expertise could routinely accessed systems in order of peco and nanoseconds [32, 33]. Distances as smaller up to nano-scale, interaction and forces are calculated through summation; using imposed boundary conditions [33].

For this study approximately atoms in range of 8000 – 10000 were used for each simulation and samples are simulate for peco seconds duration with time step variation of femto seconds; which equates to approximately millions samples.

In order to extract statistics; molecular dynamic simulation are performed as NPT which holds the number of atoms, pressure, and temperature of the system constant and NVT which hold the number of atoms, volume, and temperature of the system constant.

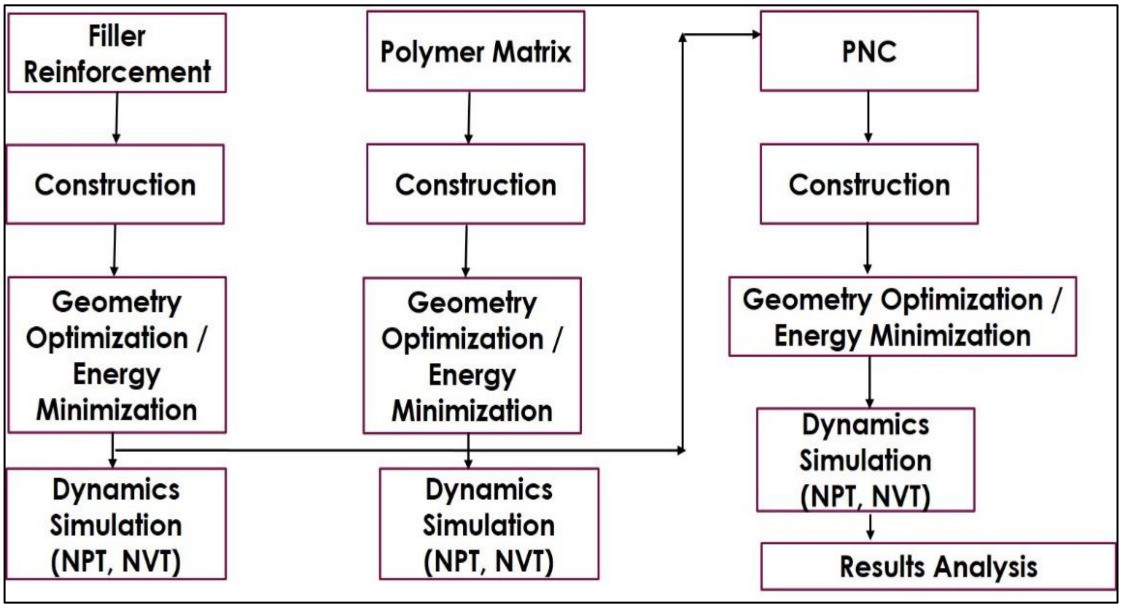


Figure 2-6: Systematic Approach for Simulation

Experimental technique is the conventional approach for obtaining properties of polymer nano composite but has its limitation due to time consuming and financial effects. The difficult has further exasperated because nano-scale material, as direct testing in existing testing capabilities is nearly impossible. Therefore, necessitating Computational approach (Molecular Dynamic Simulation) through Material Studio Software. Amorphous cell, Forcite and DFTB modules were used for Graphene Nano Sheet - Polyvinyl Alcohol and Boron Nitride Nano Sheet – Polyvinyl Chloride nao-composites.

Methodology for Simulation of Graphene Nano Sheet–Polyvinyl Alcohol Nano Composite

3.1 Introduction

In this chapter Molecular Dynamic simulation of Graphene Nano Sheet (GNS) – Polyvinyl Alcohol (PVA) based nano-composites are conducted by constructing and optimizing its structure and further its properties are analyzed. Various modules of Material Studio (2017) software were used for system building and calculations of desired properties.

3.2 Building of Graphene Structure

Graphene has 2-D hexagonal structure in which 6 carbon atoms are attached with one another through covalent bond.

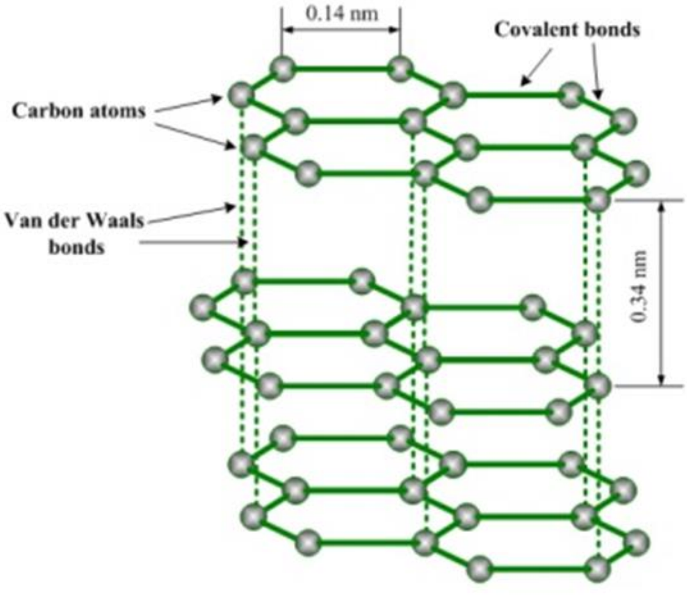


Figure 3-1: Graphene Structure

Graphene Nano Sheet and Optimization Structure

DFTB Module is used to create new project. The first step was to make a Graphene unit cell. From the Graphene unit cell Graphene nano wire was created.

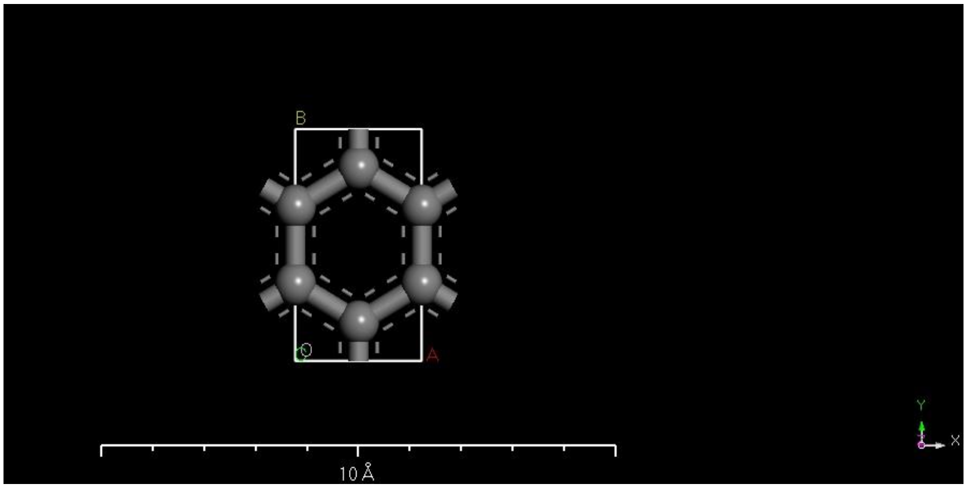


Figure 3-2: Graphene Unit Cell

Graphene Nano wire comprising 6 x Graphene cell was created with Hydrogen atoms added at the end to fulfill carbon atom valance [25].

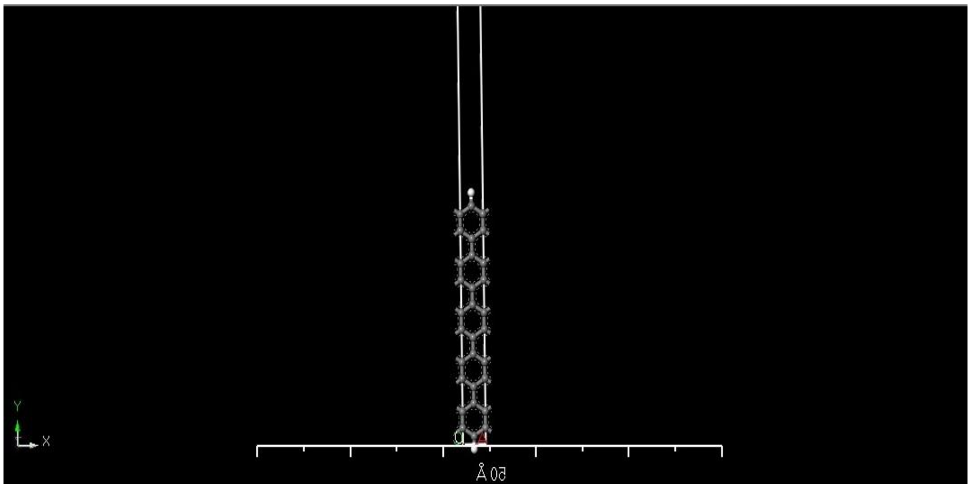
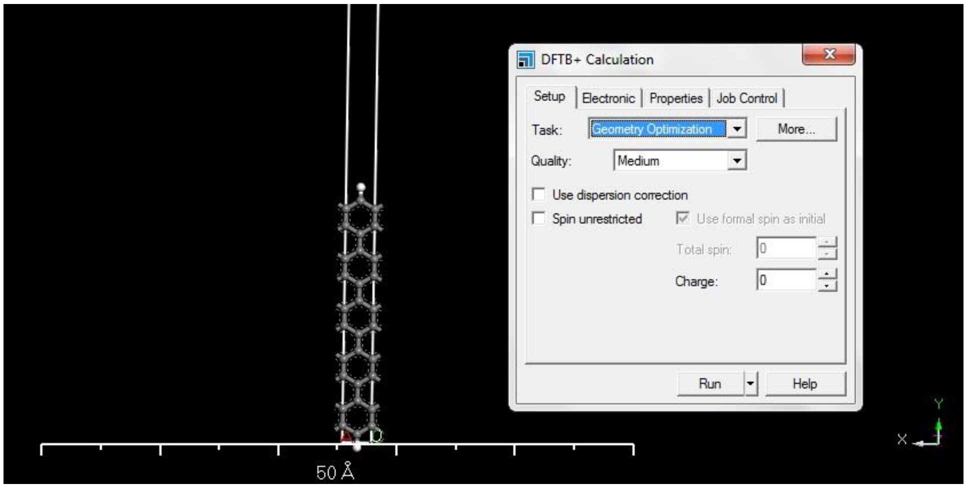


Figure 3-3: Graphene nano wire

Geometric optimization of Graphene Nano Wire was carried out through DFTB Geometry optimization. For geometric optimization Slater-Koster library was selected as mio (as it is specific for Carbon based systems) and for non-zero temperature calculation

Self-Consistent Charge (SCC) parameters that control the electronic minimization were set.



Task: Geometry Optimization

Quality: Medium

☐ Use dispersion correction

☐ Spin unrestricted

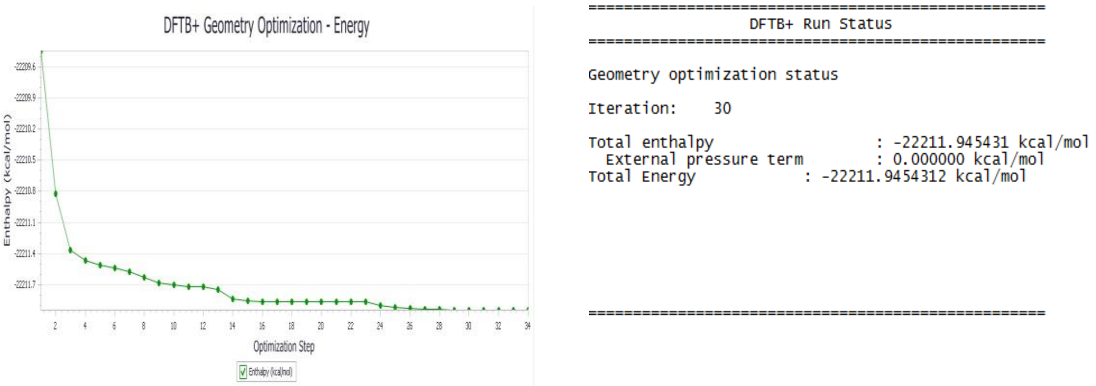
☑ Use formal spin as initial

Total spin: 0

Charge: 0

Figure 3-4: Geometric Optimization of Graphene Nano Wire

A folder was created and optimized structure with total energy after 30 iteration and convergence was achieved as - 22211.94 Kcal / mol



```
====================================================
                  DFTB+ Run Status
====================================================

Geometry optimization status

Iteration:    30

Total enthalpy                    : -22211.945431 kcal/mol
  External pressure term          : 0.000000 kcal/mol
Total Energy             : -22211.9454312 kcal/mol



====================================================
```

Figure 3-5: Geometric and Energy Optimization of Graphene Structure

Optimized structure of Graphene Nano Wire was used to create **Graphene Nano Sheet 7 x 7 unit cell**. The Graphene Nano sheet structure has been restricted to 4 nm (40 Armstrong) due to computational limitation and geometric optimization. Various structures with in range of 3 to 5 nm (30 to 50 Armstrong) has been reviewed for Polymer nano-composites [25, 26].

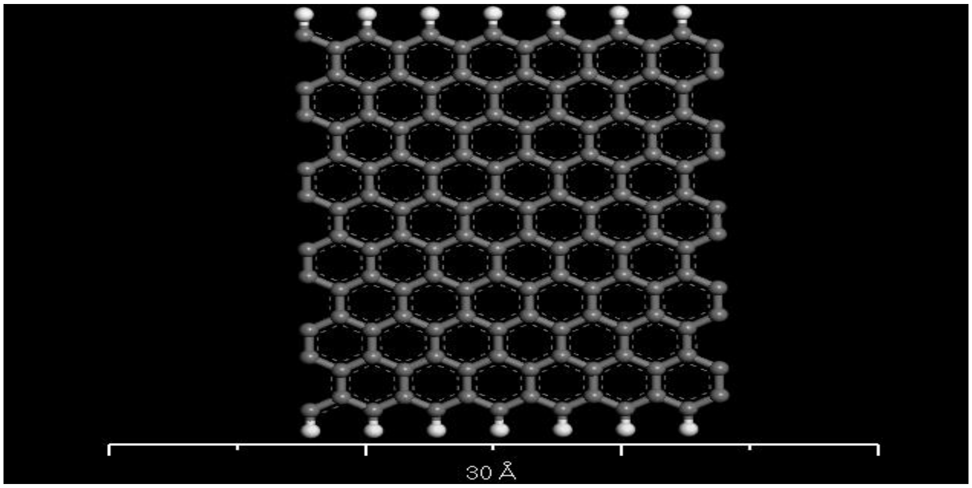
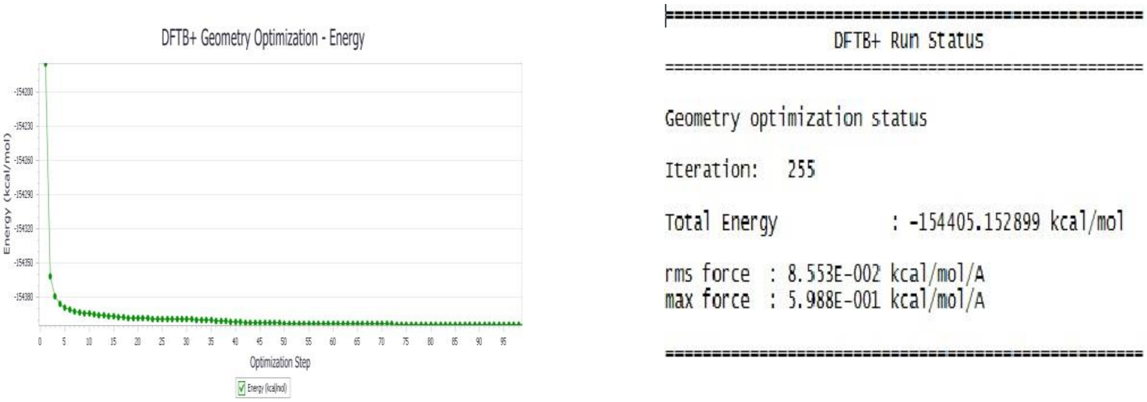


Figure 3-6: Graphene Nano Sheet 7 x 7 unit cell

Procedure mentioned above was repeated for geometric optimization of Graphene Nano Sheet. Optimized structure with total after 255 iteration and convergence is –154405.15 Kcal / mol



```
==================================================
                 DFTB+ Run Status
==================================================

Geometry optimization status

Iteration:   255

Total Energy          : -154405.152899 kcal/mol

rms force  : 8.553E-002 kcal/mol/A
max force  : 5.988E-001 kcal/mol/A

==================================================
```

Figure 3-7: Geometric optimization of GNS

Optimized Graphene Nano Sheet structure was subsequently used in construction of composite to evaluate Young Modulus of its nano-composites.

3.3 Building of polyvinyl alcohol structure

It is semi-crystalline homo-synthetic polymer; which is colorless and odorless. Chemical formula is as under:-

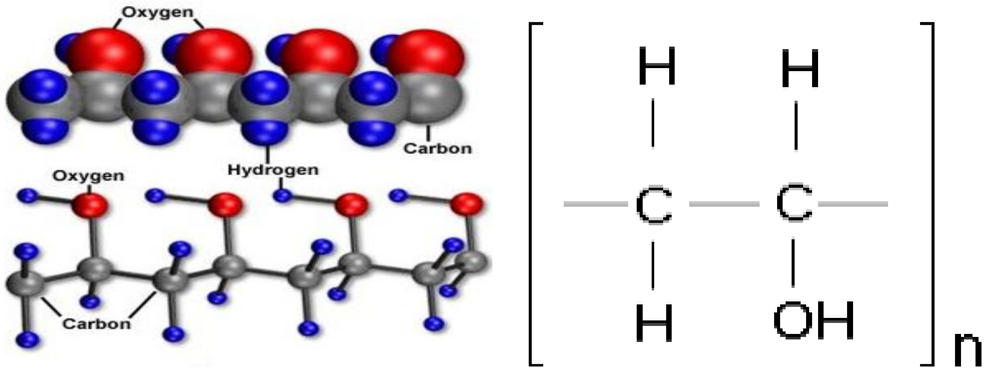


Figure 3-8: Polyvinyl Alcohol Molecular Structure

Construction of Polyvinyl Alcohol (PVA) Structure and Optimization

Initially Vinyl Alcohol (VA) monomer was constructed for construction of polymer chain structure.

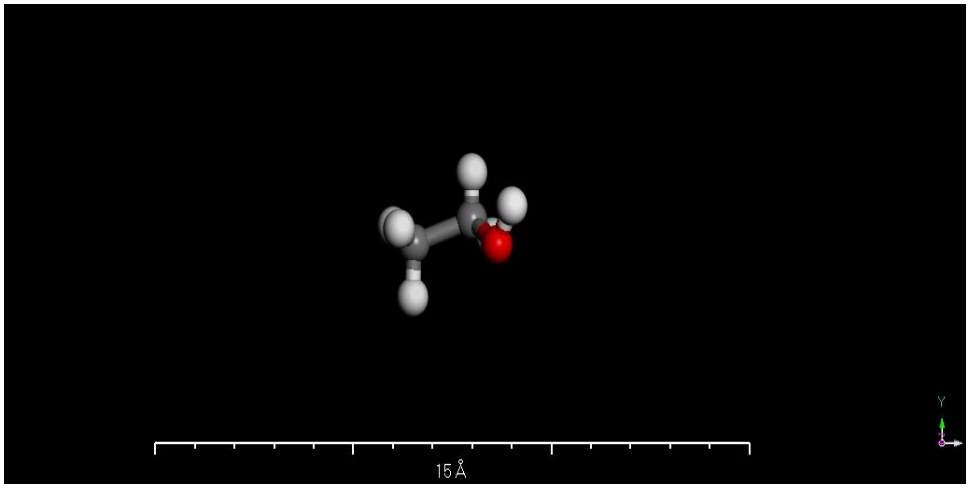


Figure 3-9: Vinyl alcohol

From monomer structure a polymer molecule with a chain length of 10 monomers was constructed.

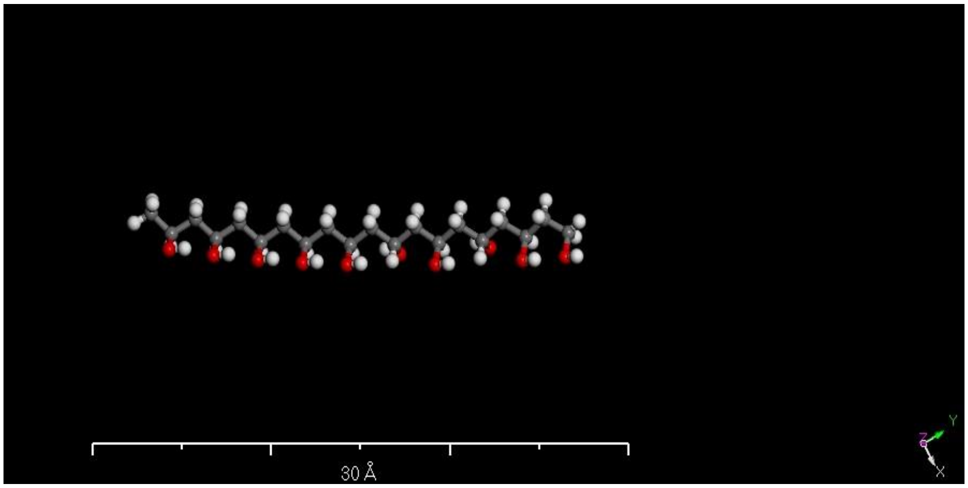
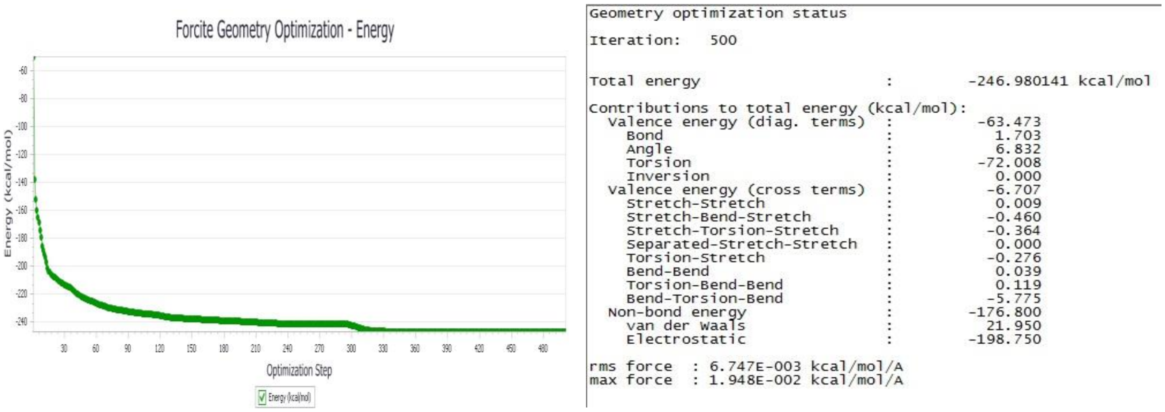


Figure 3-10: Polyvinyl alcohol (10 monomer repeated units)

For geometric optimization of structure | **Forcite** | module is used. Optimization resulted in stable low-energy structure. Force field used is COMPASS. It gave precise interactions description for Polymer and Graphene composite [28, 29]. Optimized structure after 500 iterations was achieved with total energy value – 246.98 Kcal / mol. Optimized Polyvinyl Alcohol structure was subsequently used in construction of composite



```
Geometry optimization status

Iteration:   500


Total energy                   :        -246.980141 kcal/mol

Contributions to total energy (kcal/mol):
  Valence energy (diag. terms)  :           -63.473
    Bond                        :             1.703
    Angle                       :             6.832
    Torsion                     :           -72.008
    Inversion                   :             0.000
  Valence energy (cross terms)  :            -6.707
    Stretch-Stretch             :             0.009
    Stretch-Bend-Stretch        :            -0.460
    Stretch-Torsion-Stretch     :            -0.364
    Separated-Stretch-Stretch   :             0.000
    Torsion-Stretch             :            -0.276
    Bend-Bend                   :             0.039
    Torsion-Bend-Bend           :             0.119
    Bend-Torsion-Bend           :            -5.775
  Non-bond energy               :          -176.800
    van der Waals               :            21.950
    Electrostatic               :          -198.750

rms force  : 6.747E-003 kcal/mol/A
max force  : 1.948E-002 kcal/mol/A
```

Figure 3-11: Geometric optimization of PVA

The construction and optimization of basic structure was a lengthy and cumbersome process as hours of simulation due to computational limitation.

3.4 Optimized Building Blocks for Nano Composites (GNS – PVA)

Optimized structures of Polyvinyl Alcohol (PVA) and Graphene Nano Sheet (GNS) were achieved. These optimized structures were found compatible with various samples already reviewed for simulation during various research works [25, 26, 27]. Few important details are tabulated below:-

Table 3-1: Properties of Optimized PVA

Parameter	**GNS**	**PVA**
Category	Allotrope form of Carbon	Synthetic homo polymer
Dimension	1.5 nm = 15 A° (Armstrong) for 7 x 7 unit cell Graphene sheet	3 nm = 30 A° (Armstrong) for 10 monomer repeated unit
Enthalpy	– 154405.15 Kcal / mol	– 246.98 Kcal / mol
No of Atoms in Structure	154 atoms in nano sheet	72 atoms in single molecule (10 monomer of Vinyl alcohol)

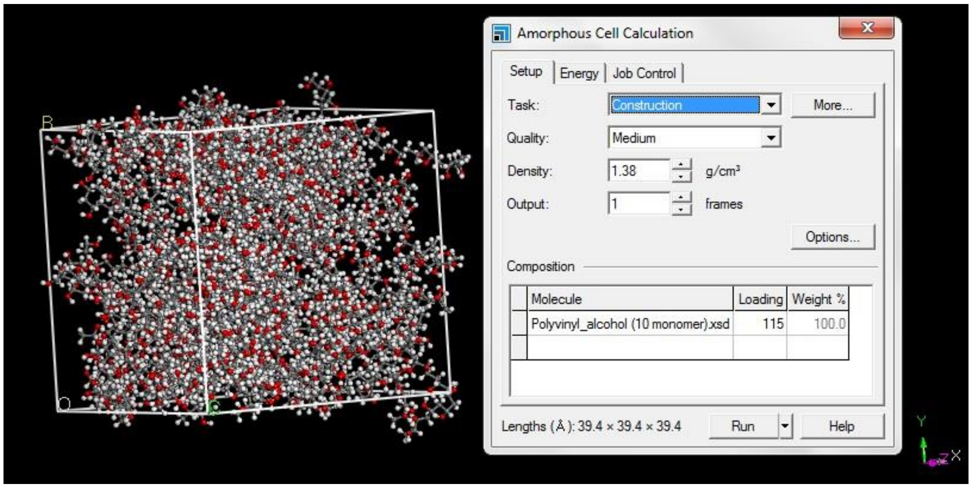
3.5 Construction of Poly Vinyl Alcohol (PVA) Super Cell in Material Studio

Amorphous Cell module was used to construct PVA Super cell. “Pack enclosed volume” and density were adjusted as 1.38 g/cm^3 with COMPASS as Force field [30, 31]. The construction of PVA (10 monomer repeated unit) system has been done through it.

Table 3-2: Properties of PVA Super Cell

PVA Cell Size	**PVA – Molecule**	**Total no of atoms**
39.4 A° x 39.4 A° x 39.4 A°	115 (10 monomer repeated units)	8280
37.6 A° x 37.6 A° x 37.6 A°	100 (10 monomer repeated units)	7200

Neat system of PVA was constructed in order to calculate and compare Young Modulus once composite systems were developed. The computational limitation and restriction of software module allows to build and optimize cell of maximum 115 PVA molecular structure.



Task: Construction

Quality: Medium

Density: 1.38 g/cm³

Output: 1 frames

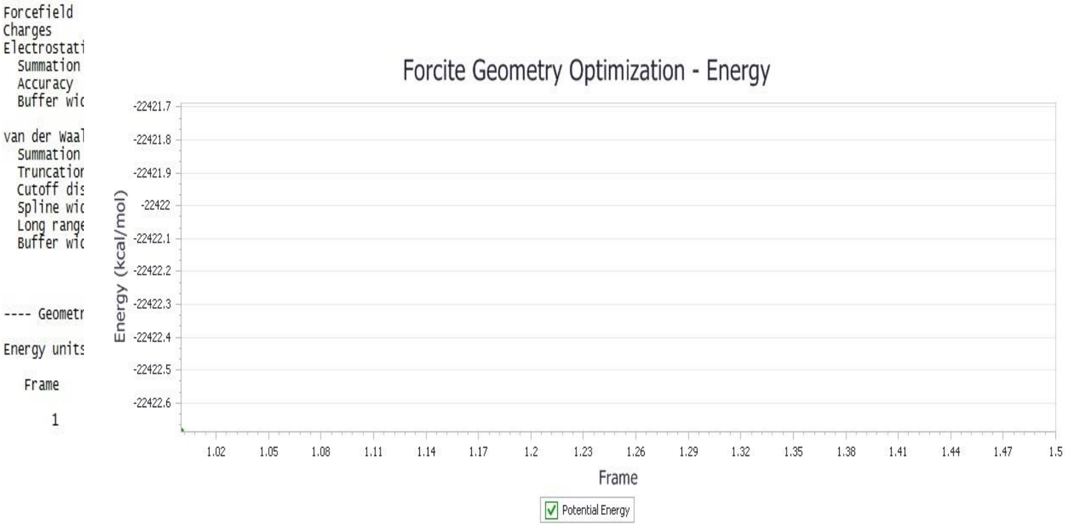
Molecule	Loading	Weight %
Polyvinyl_alcohol (10 monomer).xsd	115	100.0

Lengths (Å): 39.4 × 39.4 × 39.4

Figure 3-12: Polyvinyl Alcohol Cell

3.6 Geometric optimization of Poly Vinyl Alcohol (PVA) Super Cell

In order to optimize the structure, series of simulation were run on Forcite module for structure optimization. Force field used is COMPASS.



```
Forcefield
Charges
Electrostati
  Summation
  Accuracy
  Buffer wic

van der Waal
  Summation
  Truncatior
  Cutoff dis
  Spline wic
  Long range
  Buffer wic


---- Geometr

Energy units

   Frame

     1
```

Figure 3-13: PVA Cell Optimization

In Molecular Dynamics simulation, potential functions define the atomistic interactions between the atoms. Potential function is of two kinds; bonded potential due to covalent bonds and non-bonded potential due to van dar waals forces. For polymeric chain structure system COMPASS force field is most suitable [29]. Computed total energy after IForciteI geometric optimization calculation is tabulated below:-

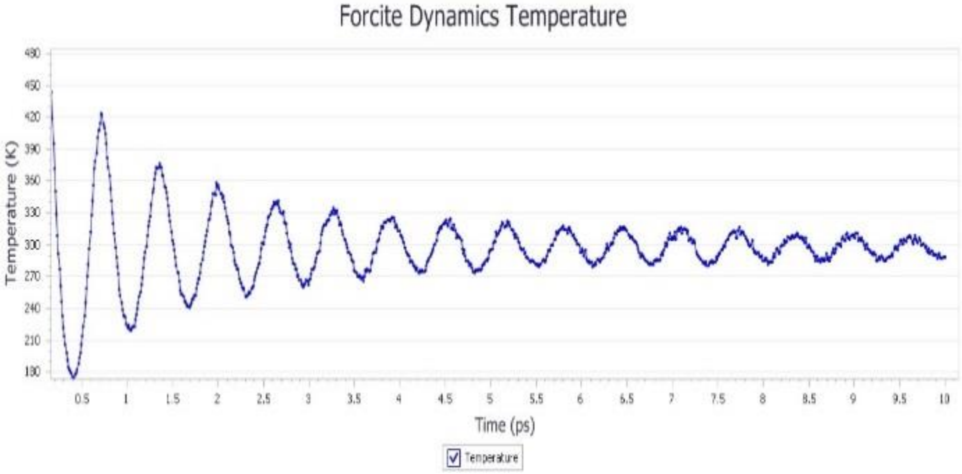
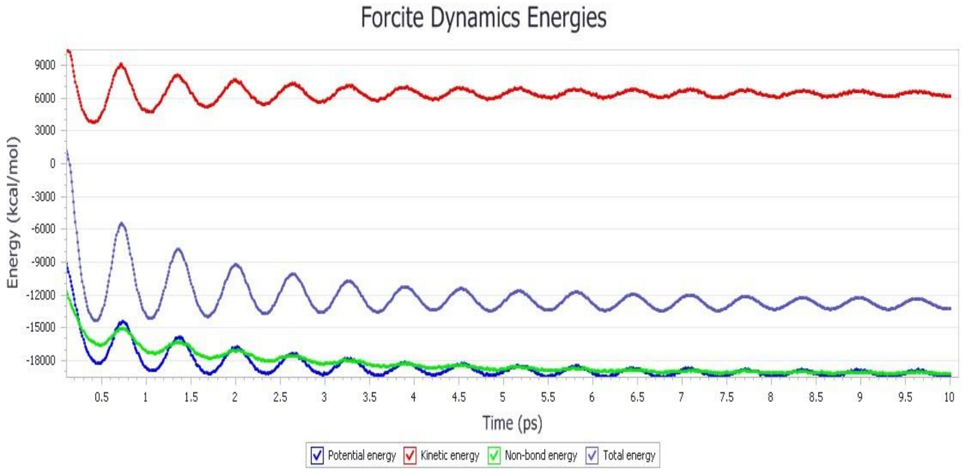


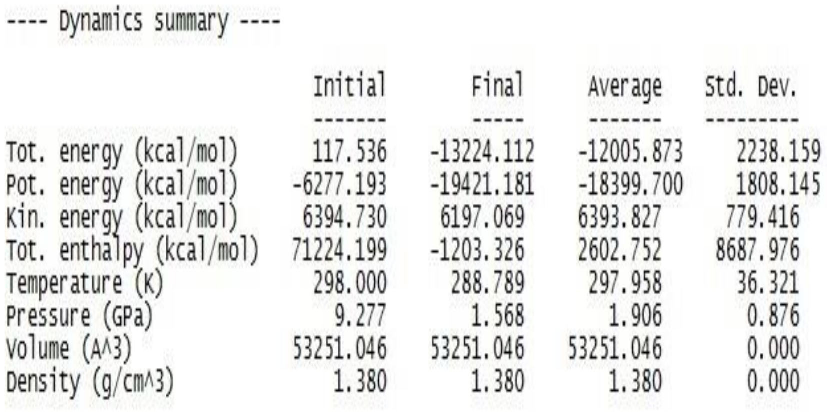
Table 3-3: Computed Total Energy after IForciteI Geometric Optimization

PVA Cell Size	**Total no of atoms**	**Total Energy (Kcal /mol)**
39.4 A° x 39.4 A° x 39.4 A°	8280	-22422.688
37.6 A° x 37.6 A° x 37.6 A°	7200	-6291.333

3.7 Molecular Dynamics (MD) Simulation of PVA Nano Composite

To calculate realistic results/ properties Molecular Dynamics simulation was used as it brings real time effects and stabilizes the system. The system contains molecule of 115 PVA molecules and periodic boundary condition was added to the unit cell. An energy minimization was carried out before the MD simulation again through **I Forcite I**. Series of MD simulations were performed NVT simulation 10 ps with a time step of 1 fs with temperature of 298 K and NPT simulation of 10 ps with a time step of 1 fs with temperature of 298 K (Pressure = 1 atm). After these MD simulations both PVA cell were found stable. Final Temperature and energy is tabulated below:-





```
---- Dynamics summary ----

                          Initial      Final      Average    Std. Dev.
                          -------      -----      -------    ---------
Tot. energy (kcal/mol)    117.536   -13224.112  -12005.873    2238.159
Pot. energy (kcal/mol)  -6277.193   -19421.181  -18399.700    1808.145
Kin. energy (kcal/mol)   6394.730     6197.069    6393.827     779.416
Tot. enthalpy (kcal/mol) 71224.199  -1203.326    2602.752    8687.976
Temperature (K)           298.000     288.789     297.958      36.321
Pressure (GPa)              9.277       1.568       1.906       0.876
Volume (A^3)            53251.046   53251.046   53251.046       0.000
Density (g/cm^3)            1.380       1.380       1.380       0.000
```

Figure 3-14: Molecular Dynamic Simulation of PVA Cell

Table 3-4: Properties of PVA Cell after MD Simulation

PVA – GNS Cell Size	Total no of atoms	Final Energy (Kcal /mol)	Avg Temperature K
39.4 A° x 39.4 A° x 39.4 A°	8280	-15324.112	300
37.6 A° x 37.6 A° x 37.6 A°	7200	-13324.112	298

3.8 Mechanical Properties Calculation of PVA System in Forcite Material Studio

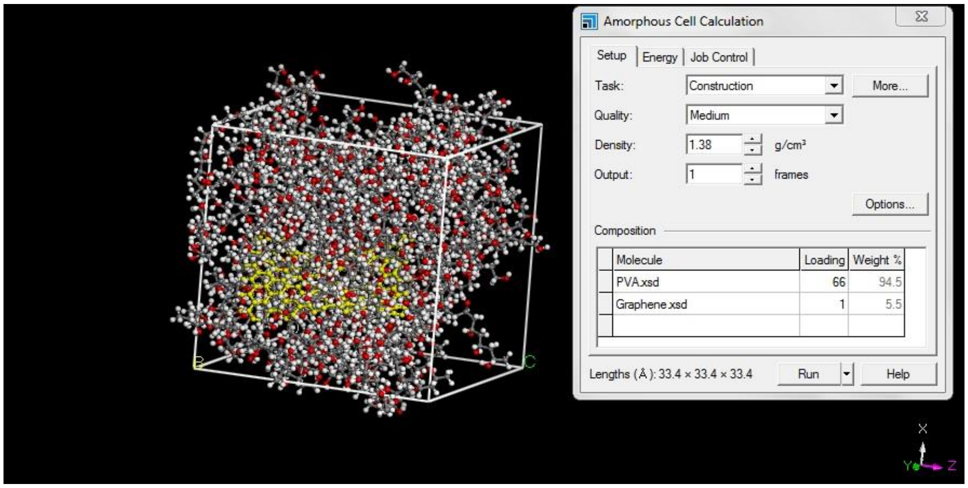
Forcite Module was used to calculate the Young Modulus of PVA. The results are tabulated below for a pure PVA matrix (PVA system) with a density of 1.38 g/cm^3.

Table 3-5: Young Modulus of PVA Cell

PVA Cell Size	Young Modulus – Giga Pascal (GPa)
39.4 A° x 39.4 A° x 39.4 A°	3.22
37.6 A° x 37.6 A° x 37.6 A°	3.19

3.9 Construction of PVA – GNS Nano Composite in Material Studio

Amorphous Cell module was used to construct the PVA and GNS structure modelled in a composite material. The construction of PVA (10 monomer repeated unit) and GNS sheet (7 x 7 Graphene unit) was done through it.



Task: Construction
Quality: Medium
Density: 1.38 g/cm³
Output: 1 frames

Composition

Molecule	Loading	Weight %
PVA.xsd	66	94.5
Graphene.xsd	1	5.5

Lengths (Å): 33.4 × 33.4 × 33.4

Figure 3-15: PVA – GNS Nano Composite

In order to calculate mechanical properties numbers of systems were developed with various loading of PVA and GNS.

Table 3-6: Different Iterations of PVA and GNS

PVA – GNS Cell Size	Cell Configuration	Weight percentage of GNS	Total no of atoms
38.7 A° x 38.7 A° x 38.7 A°	105 molecule (10 monomer repeated units) 1 Graphene Nano sheet	3.5	7714
37.2 A° x 37.2 A° x 37.2 A°	93 molecule (10 monomer repeated units) 1 Graphene Nano sheet	4	6850
35.8 A° x 35.8 A° x 35.8 A°	82 molecule (10 monomer repeated units) 1 Graphene Nano sheet	4.5	6058
34.5 A° x 34.5 A° x 34.5 A°	73 molecule (10 monomer repeated units) 1 Graphene Nano sheet	5	5410
33.4 A° x 33.4 A° x 33.4 A°	66 molecule (10 monomer repeated units) 1 Graphene Nano sheet	5.5	4906
32.4 A° x 32.4 A° x 32.4 A°	60 molecule (10 monomer repeated units) 1 Graphene Nano sheet	6.0	4474

In order to optimize the structure series, simulation was run on Forcite module. Force field used is COMPASS. Tabulated value of Total Energy for Nano composite is below:-

Table 3-7: Total Energy for Nano Composite

PVA – GNS Cell Size	Cell Configuration	Total Energy (kcal/mol)
38.7 A° x 38.7 A° x 38.7 A°	105 PVA molecule (10	-13574.8

	monomer repeated units) 1 Graphene Nano sheet	
37.2 A° x 37.2 A° x 37.2 A°	93 PVA molecule (10 monomer repeated units) 1 Graphene Nano sheet	-13374.7
35.8 A° x 35.8 A° x 35.8 A°	82 PVA molecule (10 monomer repeated units) 1 Graphene Nano sheet	-13463.7
34.5 A° x 34.5 A° x 34.5 A°	73 PVA molecule (10 monomer repeated units) 1 Graphene Nano sheet	-11212.78
33.4 A° x 33.4 A° x 33.4 A°	66 PVA molecule (10 monomer repeated units) 1 Graphene Nano sheet	-9586.7
32.4 A° x 32.4 A° x 32.4 A°	60 PVA molecule (10 monomer repeated units) 1 Graphene Nano sheet	-8416.8

3.10 Molecular Dynamics (MD) Simulation of PVA – GNS Nano Composite

IForciteI was used to carry out MD of the composite systems. The system contains single Graphene nano sheet randomly surrounded by 105 PVA molecules in unit cell. The periodic boundary condition was added to the unit cell. An energy minimization was carried out before the MD simulation again through IForciteI. A 10 ps NVT simulation at Temperature of 360 K (Glass Transition Temperature of PVA [23]) with a time step of 1 fs and a 10 ps NPT simulation (T = 360 K and P= 1 atm) with a time step of 1 fs was carried out. After MD simulations the GNS sheet was well dispersed inside the PVA matrix. A similar procedure was implemented on the all PVA-GNS system. The initial value for simulation was kept at 5ps however later it was enhanced to 10ps to further converge temperature and total energy.

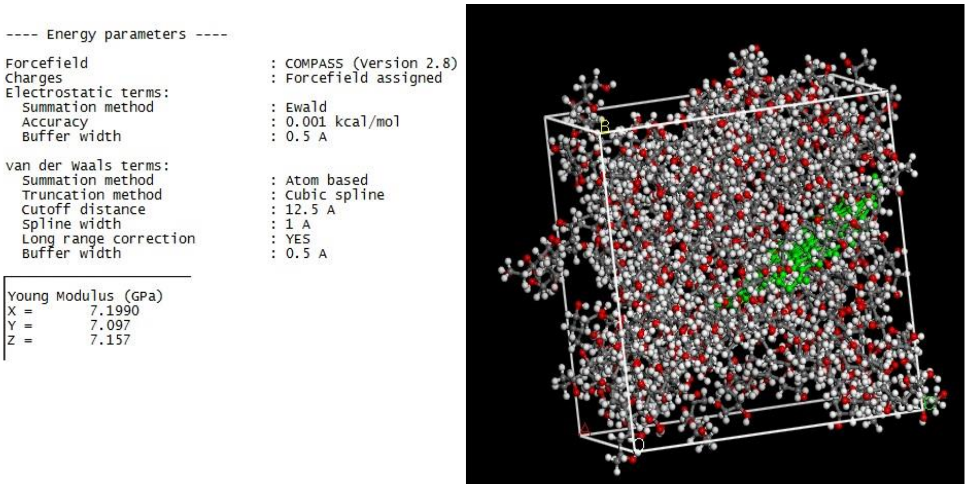
3.11 Mechanical Properties Calculation of PVA – GNS Nano Composite

IForciteI was used to calculate Young Modulus. Constant strain method was used to calculate the mechanical properties as this method is most suited to Polymer composites. Calculations results showed that Young’s moduli of GNS - PVA has enhanced after in cooperation of GNS. The value of Young Modulus for all PVA-GNS achieved through above mentioned process is tabulated below:-

Table 3-8: Value of Young’s Modulus for all PVA-GNS

PVA – GNS Cell Size	**Cell Configuration**	**Weight percentage of GNS**	**Young Modulus (GPa)**
38.7 A° x 38.7 A° x 38.7 A°	105 PVA molecule (10 monomer repeated units) 1 Graphene Nano Sheet	3.5	5.37
37.2 A° x 37.2 A° x 37.2 A°	93 PVA molecule (10 monomer repeated units) 1 Graphene Nano Sheet	4	5.97
35.8 A° x 35.8 A° x 35.8 A°	82 PVA molecule (10 monomer repeated units) 1 Graphene Nano Sheet	4.5	6.38
34.5 A° x 34.5 A° x 34.5 A°	73 PVA molecule (10 monomer repeated units) 1 Graphene Nano Sheet	5	6.97
33.4 A° x 33.4 A° x 33.4 A°	66 PVA molecule (10 monomer repeated units) 1 Graphene Nano Sheet	5.5	7.07
32.4 A° x 32.4 A° x 32.4 A°	60 PVA molecule (10 monomer repeated units) 1 Graphene Nano Sheet	6.0	7.18

I Forcite I Mechanical properties predicts the Young Modulus.



```
---- Energy parameters ----

Forcefield                    : COMPASS (Version 2.8)
Charges                       : Forcefield assigned
Electrostatic terms:
  Summation method            : Ewald
  Accuracy                    : 0.001 kcal/mol
  Buffer width                : 0.5 A

van der Waals terms:
  Summation method            : Atom based
  Truncation method           : Cubic spline
  Cutoff distance             : 12.5 A
  Spline width                : 1 A
  Long range correction       : YES
  Buffer width                : 0.5 A

Young Modulus (GPa)
X =       7.1990
Y =       7.097
Z =       7.157
```

Figure 3-16: Single GNS – PVA Nano Composite

Methodology for Simulation of Graphene Nano Sheet– Polyvinyl Chloride Nano Composite

4.1 Introduction

In this chapter Molecular Dynamic simulation of Graphene Nano Sheet (GNS) – Polyvinyl chloride (PVC) based nano-composites is conducted by constructing and optimizing its structure and further its properties are analyzed. Various modules of Material Studio (2017) software were used for system building and calculations of desired properties.

4.2 Building of Polyvinyl Chloride structure

It is a semi-crystalline homo-synthetic polymer; Chemical formula is as under:-

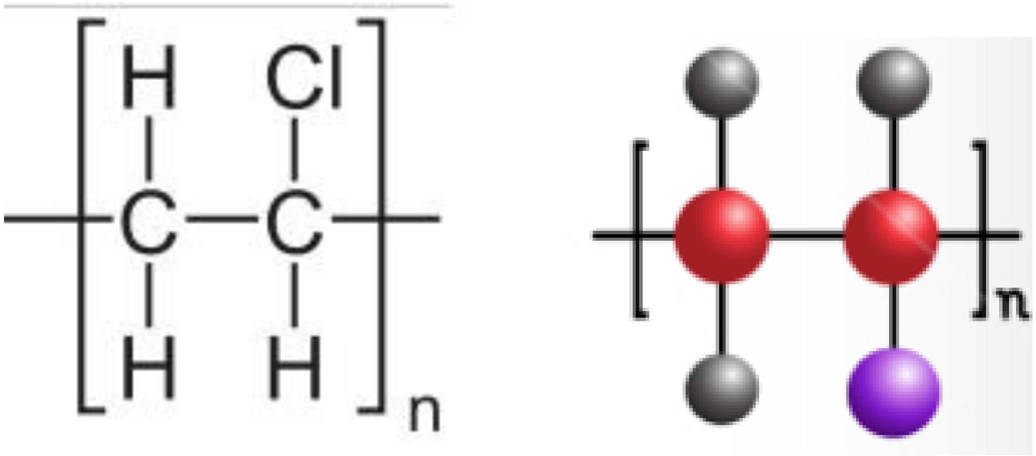


Figure 4-5: Polyvinyl Chloride Structure

Construction of Polyvinyl Chloride (PVC) Structure and Optimization

Initially Vinyl Chloride (VC) monomer was constructed for construction of polymer chain structure.

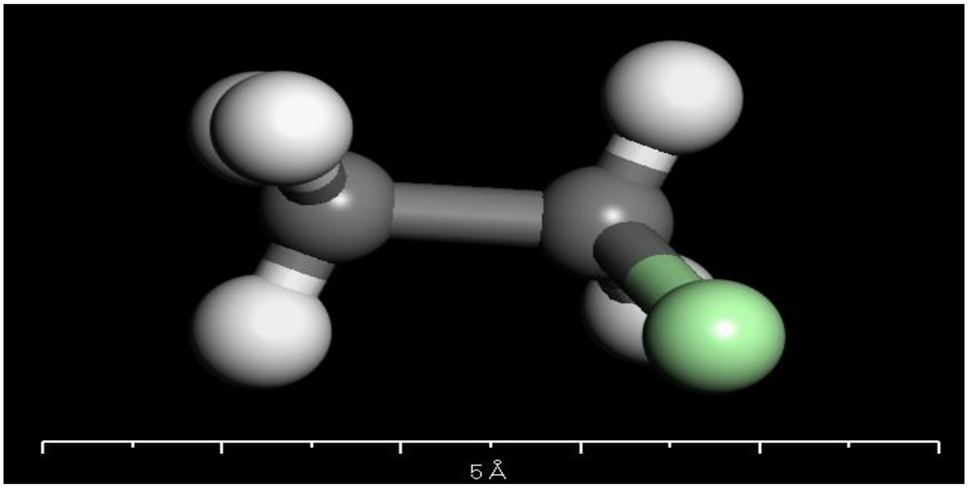


Figure 4-1: Vinyl Chloride

From monomer structure a polymer molecule with a chain length of 10 monomers was constructed.

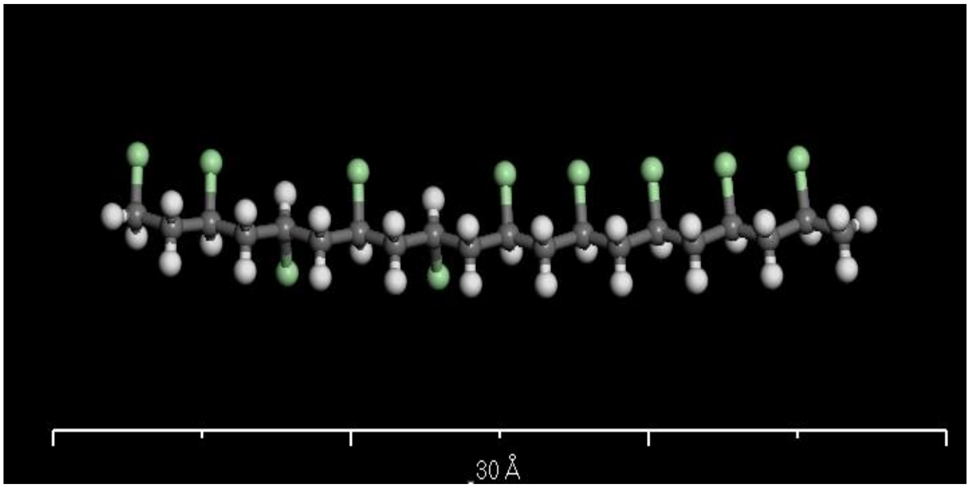
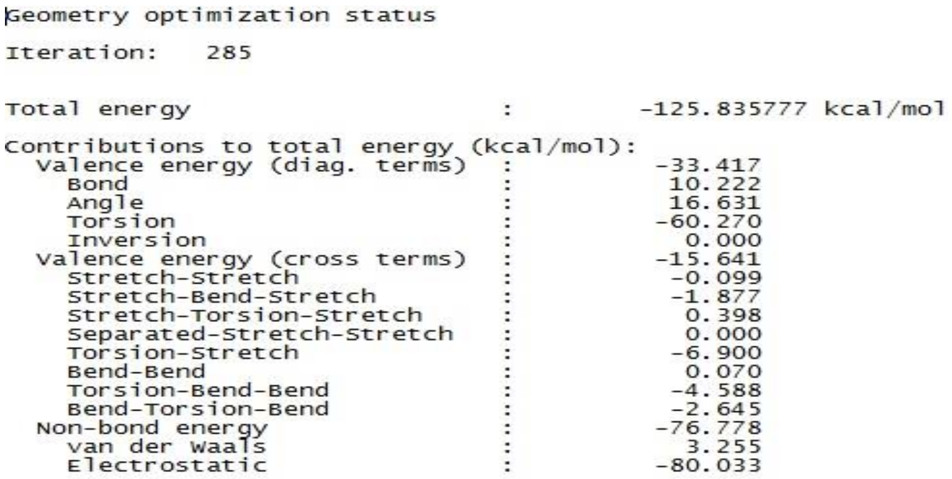


Figure 4-2: Polyvinyl Chloride (10 monomer repeated units)

| Forcite | module was used for geometric optimization resulted in stable low-energy structure. Force field used is COMPASS. Optimized structure after 285 iterations was achieved with total energy value – 125.84 Kcal / mol. Optimized Polyvinyl Chloride structure was subsequently used in construction of composite.



```
Geometry optimization status
Iteration:   285

Total energy                        :        -125.835777 kcal/mol

Contributions to total energy (kcal/mol):
  Valence energy (diag. terms)      :          -33.417
    Bond                            :           10.222
    Angle                           :           16.631
    Torsion                         :          -60.270
    Inversion                       :            0.000
  Valence energy (cross terms)      :          -15.641
    Stretch-Stretch                 :           -0.099
    Stretch-Bend-Stretch            :           -1.877
    Stretch-Torsion-Stretch         :            0.398
    Separated-Stretch-Stretch       :            0.000
    Torsion-Stretch                 :           -6.900
    Bend-Bend                       :            0.070
    Torsion-Bend-Bend               :           -4.588
    Bend-Torsion-Bend               :           -2.645
  Non-bond energy                   :          -76.778
    van der Waals                   :            3.255
    Electrostatic                   :          -80.033
```

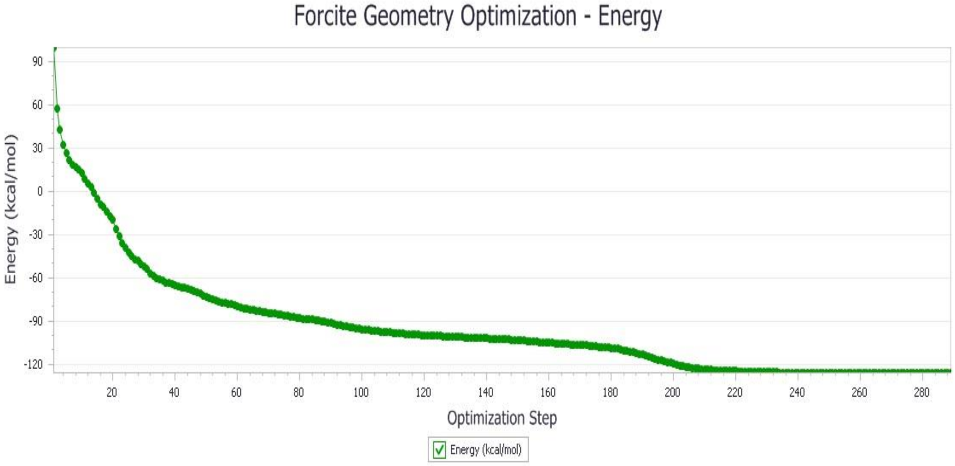


Figure 4-3: Geometric optimization of PVC

4.3 Optimized Building Blocks for Nano Composites (PVC)

Optimized structures of Poly vinyl Alchol were achieved. This optimized structure was found compatible with various samples already reviewed for simulation during various research works [25, 26, 27]. Few important details are tabulated below:-

Table 4-1: Optimized Structures of PVC

Parameter	PVC
Category	Synthetic homo polymer
Dimension	3 nm = 30 A° (Armstrong) for 10 monomer repeated unit
Enthalpy	– 125.84 Kcal / mol
No of Atoms in Structure	62 atoms in single molecule (10 monomer of Vinyl alcohol)

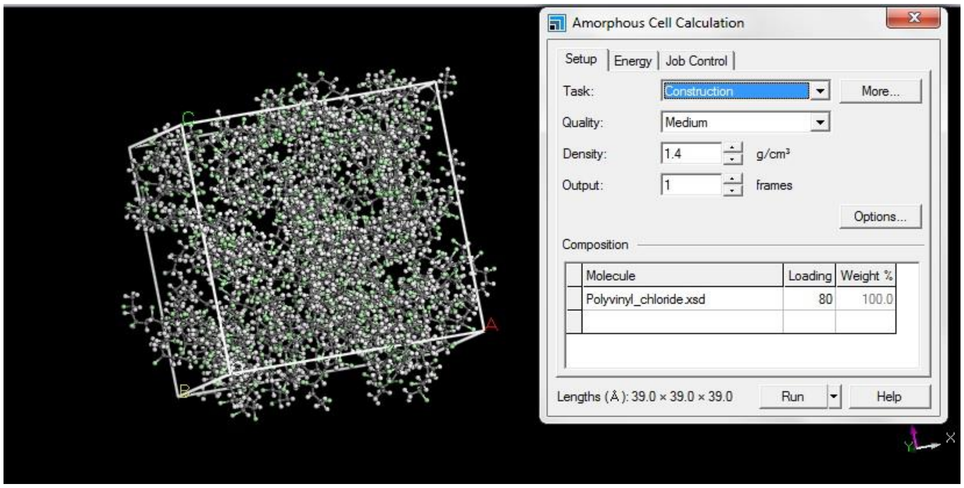
4.4 Construction of Poly Vinyl Chloride (PVC) Super Cell in Material Studio

Amorphous Cell module was used to construct PVC Super cell. “Pack enclosed volume” and density were adjusted as 1.4 g/cm^3 with COMPASS as Force field [30, 31]. The construction of PVA (10 monomer repeated unit) system has been done through it.

Table 4-2: Construction of PVC through Amorphous Cell Module

PVC Cell Size	PVC – Molecule	Total no of atoms
39 A° x 39 A° x 39 A°	80	4960

Neat system of PVC was constructed in order to calculate and compare Young Modulus once composite systems were developed. The computational limitation and restriction of software module allows to build and optimize cell of maximum 80 PVC molecular system.



Task: Construction

Quality: Medium

Density: 1.4 g/cm³

Output: 1 frames

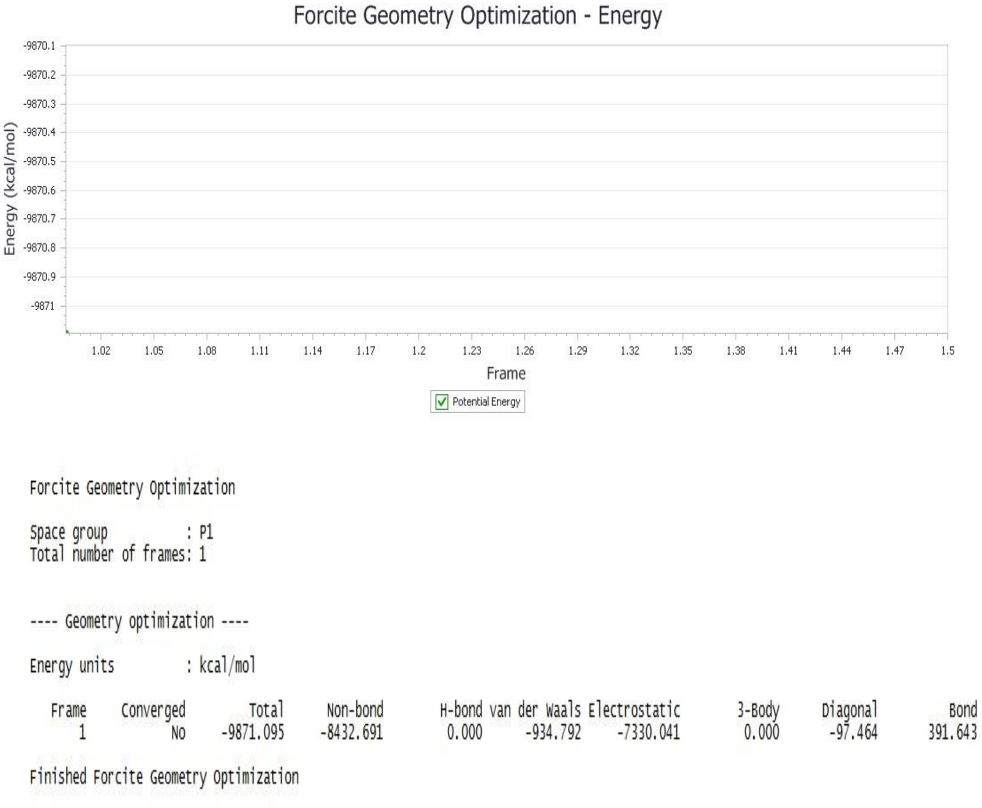
Molecule	Loading	Weight %
Polyvinyl_chloride.xsd	80	100.0

Lengths (Å): 39.0 × 39.0 × 39.0

Figure 4-4: Polyvinyl Chloride Cell

4.5 Geometric optimization of Poly Vinyl chloride (PVC) Super Cell

In order to optimize the structure, series of simulation were run on Forcite module for structure optimization. Force field used is COMPASS.



```
Forcite Geometry Optimization

Space group          : P1
Total number of frames: 1


---- Geometry optimization ----

Energy units         : kcal/mol

   Frame    Converged       Total     Non-bond       H-bond van der Waals Electrostatic      3-Body    Diagonal        Bond
     1             No   -9871.095   -8432.691       0.000      -934.792     -7330.041       0.000     -97.464     391.643

Finished Forcite Geometry Optimization
```

Figure 4-5: PVC Cell Optimization

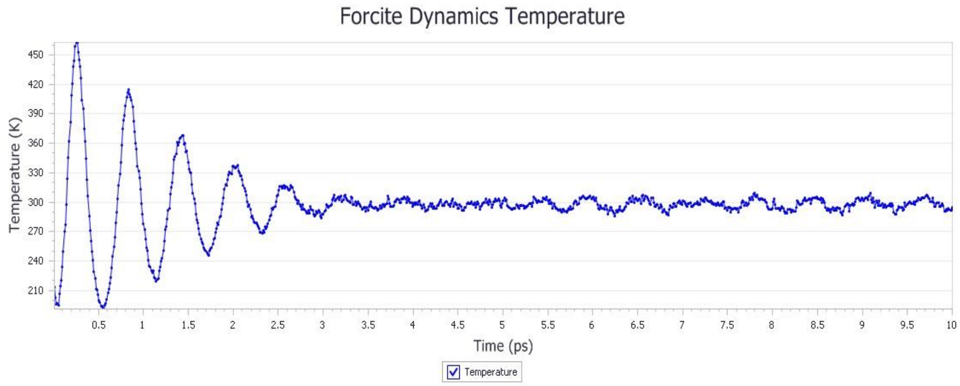
For polymeric chain structure system COMPASS force field is most suitable [29]. Computed total energy after IForciteI geometric optimization calculation is tabulated below:-

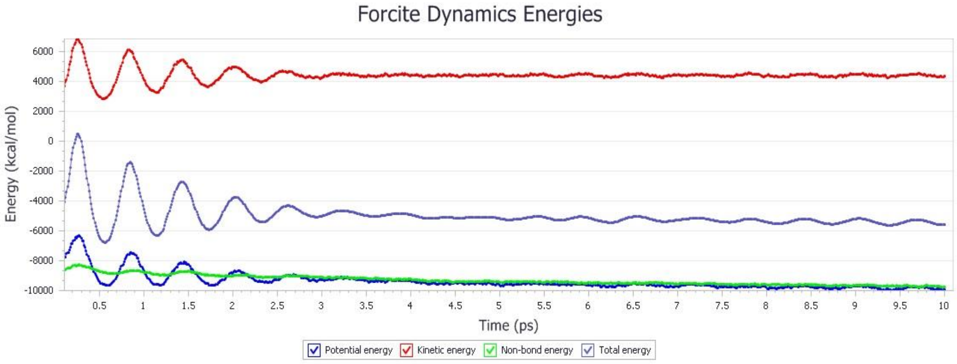
Table 4-3: Computed Total Energy after IForciteI Geometric Optimization

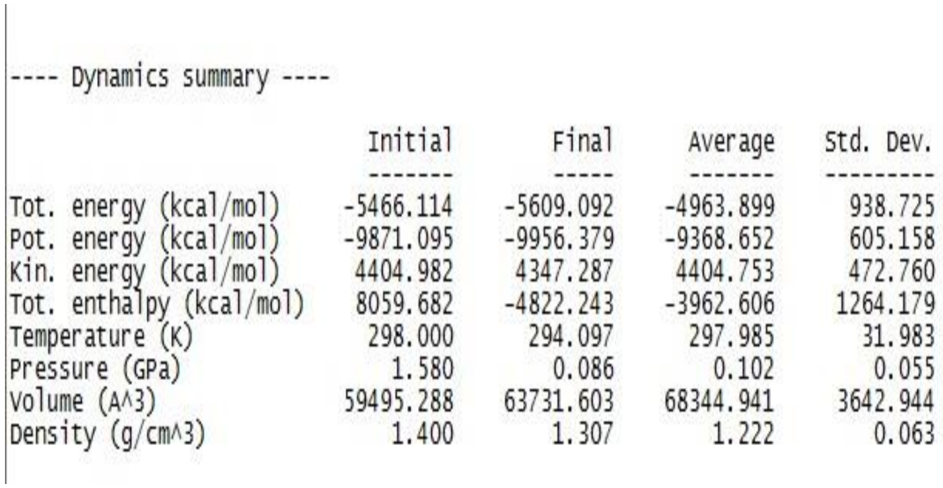
PVC Cell Size	Total numbers of atoms	Total Energy (Kcal /mol)
39 A° x 39 A° x 39 A°	4960	-9871

4.6 Molecular Dynamics (MD) Simulation of PVC Nano Composite

To calculate realistic results/ properties Molecular Dynamics simulation was used as it brings real time effects and stabilizes the system. The system contains molecule of 80 PVC molecules and periodic boundary condition was added to the unit cell. An energy minimization was carried out before the MD simulation again through **I Forcite I**. Series of MD simulations were performed NVT simulation 10 ps with a time step of 1 fs with temperature of 298 K and NPT simulation of 10 ps with a time step of 1 fs with temperature of 298 K (Pressure = 1 atm). After these MD simulations both PVC cell were found stable.







```
---- Dynamics summary ----

                              Initial      Final    Average   Std. Dev.
                              -------      -----    -------   ---------
Tot. energy (kcal/mol)      -5466.114  -5609.092  -4963.899     938.725
Pot. energy (kcal/mol)      -9871.095  -9956.379  -9368.652     605.158
Kin. energy (kcal/mol)       4404.982   4347.287   4404.753     472.760
Tot. enthalpy (kcal/mol)     8059.682  -4822.243  -3962.606    1264.179
Temperature (K)               298.000    294.097    297.985      31.983
Pressure (GPa)                  1.580      0.086      0.102       0.055
Volume (A^3)                59495.288  63731.603  68344.941    3642.944
Density (g/cm^3)                1.400      1.307      1.222       0.063
```

Figure 4-6: MD Simulation of PVC Cell

Final Temperature and energy is tabulated below:-

Table 4-3: Temperature and Energy of MD Simulation of PVC Cell

PVC Cell Size	**Total numbers of atoms**	**Final Energy (Kcal /mol)**	**Average Temperature (K)**
39 A° x 39 A° x 39 A°	4960	-5609.09	297.98

4.7 Mechanical Properties Calculation of PVC System in Forcite Material Studio

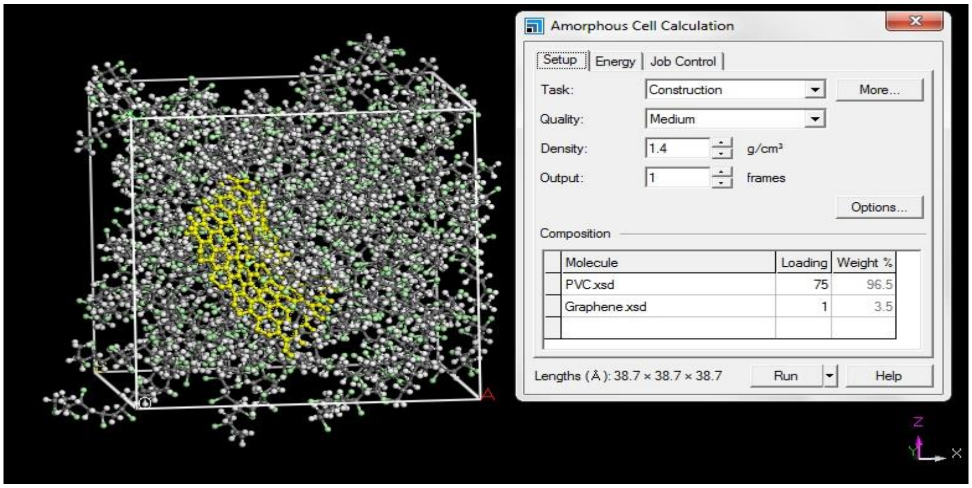
Forcite Module was used to calculate the Young Modulus of PVC. The results are tabulated below for a pure PVC matrix (PVC system) with a density of 1.4 g/cm^3 [39].

Table 4-4: Young Modulus of PVC

PVC Cell Size	**Young Modulus (GPa)**
39 A° x 39 A° x 39 A°	2.9

4.8 Construction of PVC – GNS Nano Composite in Material Studio

Amorphous Cell module was used to construct the PVC and GNS structure modelled in a composite material. The construction of PVC (10 monomer repeated unit) and GNS sheet (7 x 7 Graphene unit) was done through it.



Task: Construction

Quality: Medium

Density: 1.4 g/cm³

Output: 1 frames

Composition

Molecule	Loading	Weight %
PVC.xsd	75	96.5
Graphene.xsd	1	3.5

Lengths (Å): 38.7 × 38.7 × 38.7

Figure 4-7: PVC – GNS Nano Composite

In order to calculate mechanical properties numbers of systems were developed with various loading of PVC and GNS.

Table 4-5: Various Loading of PVC and GNS

PVC – GNS Cell Size	Cell Configuration	Weight percentage of GNS	Total no of atoms
38.7 A° x 38.7 A° x 38.7 A°	75 molecule PVC (10 monomer repeated units) 1 Graphene Nano sheet	3.5	4804
36.9 A° x 36.9 A° x 36.9 A°	65 molecule PVC (10 monomer repeated units) 1 Graphene Nano sheet	4	4184
35.5 A° x 35.4 A° x 35.4 A°	57 molecule PVC(10 monomer repeated units) 1 Graphene Nano sheet	4.5	3688
34.2 A° x 34.2 A° x 34.2 A°	51 molecule PVC(10 monomer repeated units) 1 Graphene Nano sheet	5	3266
33.3 A° x 33.3 A° x 33.3 A°	47 molecule PVC(10	5.5	3068

	monomer repeated units) 1 Graphene Nano sheet		
32.2 A° x 32.2 A° x 32.2 A°	42 molecule PVC(10 monomer repeated units) 1 Graphene Nano sheet	6.0	2758

In order to optimize the structure series, simulation was run on Forcite module. Force field used is COMPASS. Tabulated value of Total Energy for Nano composite is below:-

Table 4-6: Total Energy for Nano Composite

PVC – GNS Cell Size	**Cell Configuration**	**Total Energy (kcal/mol)**
38.7 A° x 38.7 A° x 38.7 A°	75 molecule (10 monomer repeated units) 1 Graphene Nano sheet	-6315.03
36.9 A° x 36.9 A° x 36.9 A°	65 molecule (10 monomer repeated units) 1 Graphene Nano sheet	-4569.1
35.5 A° x 35.4 A° x 35.4 A°	57 molecule (10 monomer repeated units) 1 Graphene Nano sheet	-4252.9
34.2 A° x 34.2 A° x 34.2 A°	51 molecule (10 monomer repeated units) 1 Graphene Nano sheet	-3990.2
33.3 A° x 33.3 A° x 33.3 A°	47 molecule (10 monomer repeated units) 1 Graphene Nano sheet	-3208.9
32.2 A° x 32.2 A° x 32.2 A°	42 molecule (10 monomer repeated units) 1 Graphene Nano sheet	-2568.1

4.9 Molecular Dynamics (MD) Simulation of PVC – GNS Nano Composite

IForciteI was used to carry out MD of the composite systems. The system contains single Graphene nano sheet randomly surrounded by 75 PVC molecules in unit cell. The periodic boundary condition was added to the unit cell. An energy minimization was carried out before the MD simulation again through IForciteI. A 10 ps NVT simulation at Temperature of 360 K (Glass Transition Temperature of PVA [23]) with a time step of 1 fs and a 10 ps NPT simulation (T = 360 K and P= 1 atm) with a time step of 1 fs was carried out. After MD simulations the GNS sheet was well dispersed inside the PVC matrix. A similar procedure was implemented on the all PVC-GNS system. The value for simulation was kept at 10ps to converge temperature and total energy.

4.10 Mechanical Properties Calculation of PVC – GNS Nano Composite

IForciteI was used to calculate Young Modulus. Constant strain method was used to calculate the mechanical properties as this method is most suited to Polymer composites. Calculations results showed that Young’s moduli of GNS - PVC has enhanced after in cooperation of GNS. The value of Young Modulus for all PVC - GNS achieved through above mentioned process is tabulated below:-

Table 4-7: Various Loading of PVC and GNS

PVC – GNS Cell Size	Cell Configuration	Weight percentage of GNS	Young Modulus (GPa)
38.7 A° x 38.7 A° x 38.7 A°	75 molecule (10 monomer repeated units) 1 Graphene Nano sheet	3.5	3.1
37.2 A° x 37.2 A° x 37.2 A°	65 molecule (10 monomer repeated units) 1 Graphene Nano sheet	4	3.23
35.8 A° x 35.8 A° x 35.8 A°	57 molecule (10	4.5	3.53

	monomer repeated units) 1 Graphene Nano sheet		
34.5 A° x 34.5 A° x 34.5 A°	51 molecule (10 monomer repeated units) 1 Graphene Nano sheet	5	4.23
33.4 A° x 33.4 A° x 33.4 A°	47 molecule (10 monomer repeated units) 1 Graphene Nano sheet	5.5	4.37
32.4 A° x 32.4 A° x 32.4 A°	42 molecule (10 monomer repeated units) 1 Graphene Nano sheet	6.0	4.42

Methodology for Simulation of Boron Nitride Nano Sheet– Polyvinyl Chloride Nano Composite

5.1 Introduction

In this chapter simulation result of Boron Nitride Nano Sheet and Polyvinyl Chloride based Nano-composites through construction and optimization will be discussed and its properties will be analyzed. Various modules of Material Studio (2017) software were used for system building and calculations of desired properties.

5.2 Building of Boron Nitride Structure

In Boron and Nitride, 2D Boron is arranged one after the other in a honeycomb structure, forming hexagonal lattice formation. Boron Nitride bond are formed through sp2 hybridization.

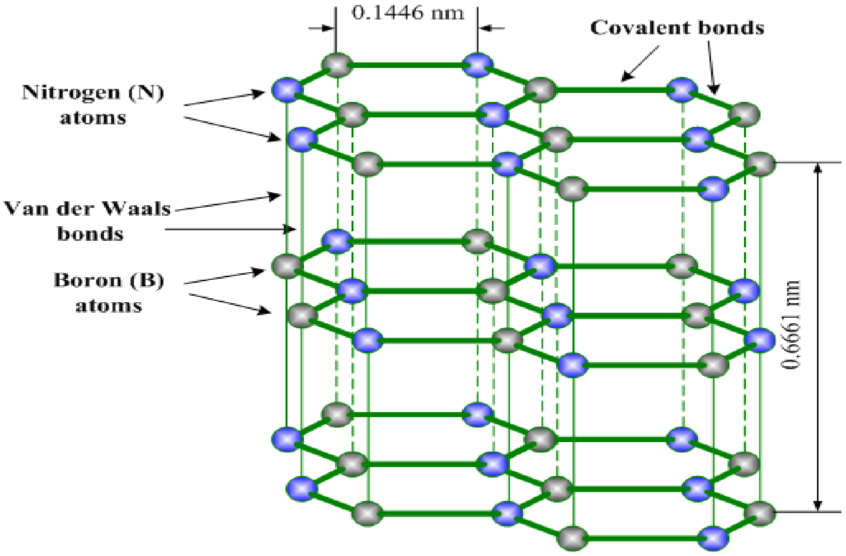


Figure 5-1: Hexagonal Boron Nitride

Boron Nitride Nano Sheet and Optimization Structure

Atomistic tool used to create new project. First step was to make a Hexagonal Boron Nitride unit cell. From the unit cell Hexagonal Boron Nitride Nano Sheet was created.

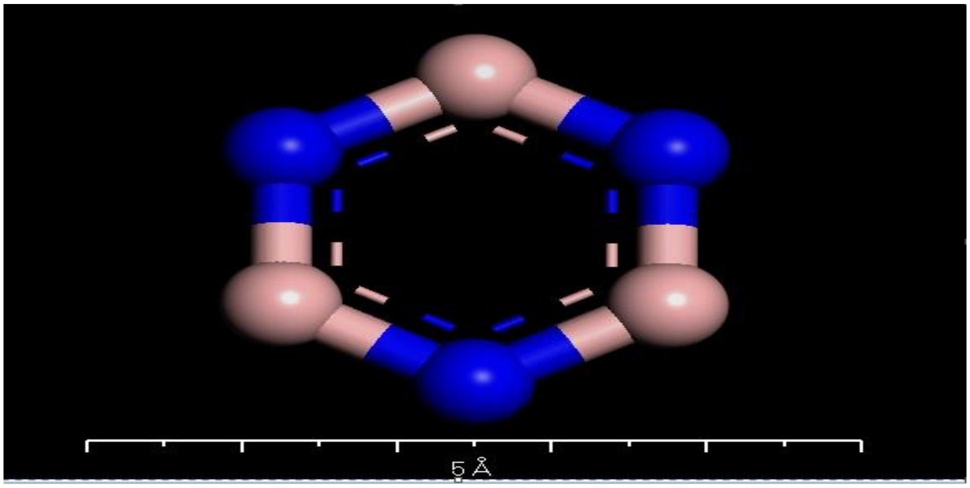


Figure 5-2: Boron Nitride Unit Cell

Hexagonal Boron Nitride comprising 7 x 7 unit cell attached together to form Boron Nitride Nano sheet (BNNS).

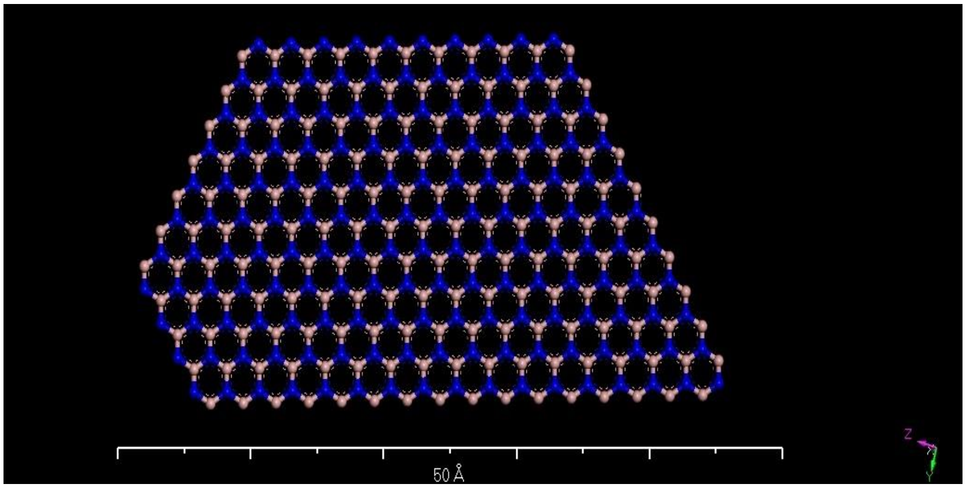
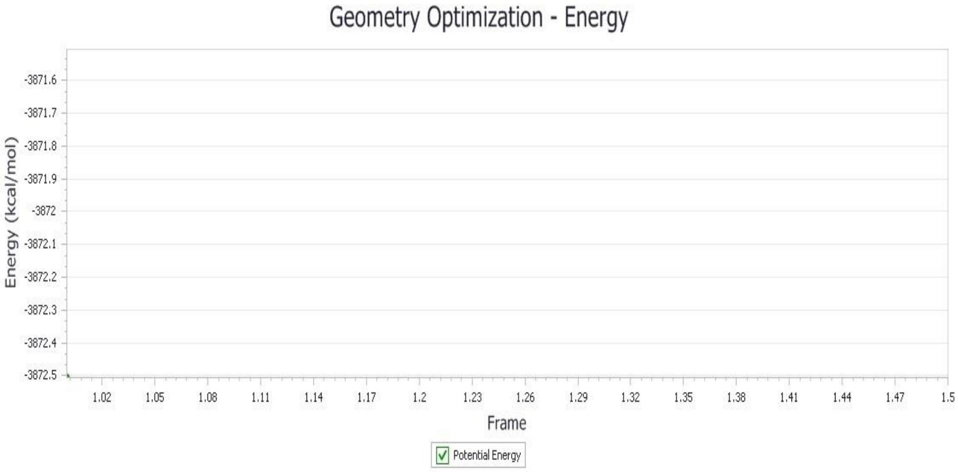
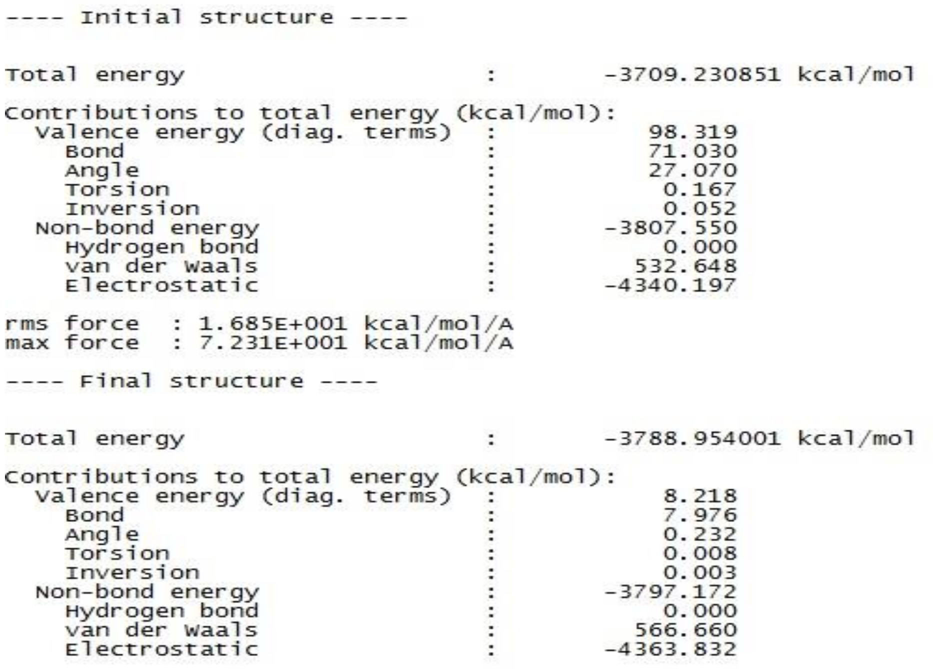


Figure 5-3: Boron Nitride Nano Sheet

Geometric optimization of Boron Nitride Nano Sheet was carried out through Forcite geometry optimization. Force filed used is Dreiding. A folder was created and optimized structure with total energy after 500 iteration and convergence was achieved as -3788.95 Kcal / mol





```
---- Initial structure ----

Total energy                    :       -3709.230851 kcal/mol

Contributions to total energy (kcal/mol):
  Valence energy (diag. terms)  :           98.319
    Bond                        :           71.030
    Angle                       :           27.070
    Torsion                     :            0.167
    Inversion                   :            0.052
  Non-bond energy               :        -3807.550
    Hydrogen bond               :            0.000
    van der Waals               :          532.648
    Electrostatic               :        -4340.197

rms force  : 1.685E+001 kcal/mol/A
max force  : 7.231E+001 kcal/mol/A

---- Final structure ----

Total energy                    :       -3788.954001 kcal/mol

Contributions to total energy (kcal/mol):
  Valence energy (diag. terms)  :            8.218
    Bond                        :            7.976
    Angle                       :            0.232
    Torsion                     :            0.008
    Inversion                   :            0.003
  Non-bond energy               :        -3797.172
    Hydrogen bond               :            0.000
    van der Waals               :          566.660
    Electrostatic               :        -4363.832
```

Figure 5-4: Geometric Optimization of Boron Nitride Nano Sheet Structure

Boron Nitride Nano sheet structure was restricted to 4 nm (40 Armstrong) due to computational limitation and geometric optimization. Various structures of nano-fillers within range of 3 to 5 nm (30 to 50 Armstrong) have been reviewed [25, 26]. Optimized Boron Nitride Nano Sheet structure was used introduced in polymer to evaluate Young Modulus of its nano-composites.

5.3 Building of Polyvinyl Chloride structure

It is a semi-crystalline homo-synthetic polymer; Chemical formula is as under:-

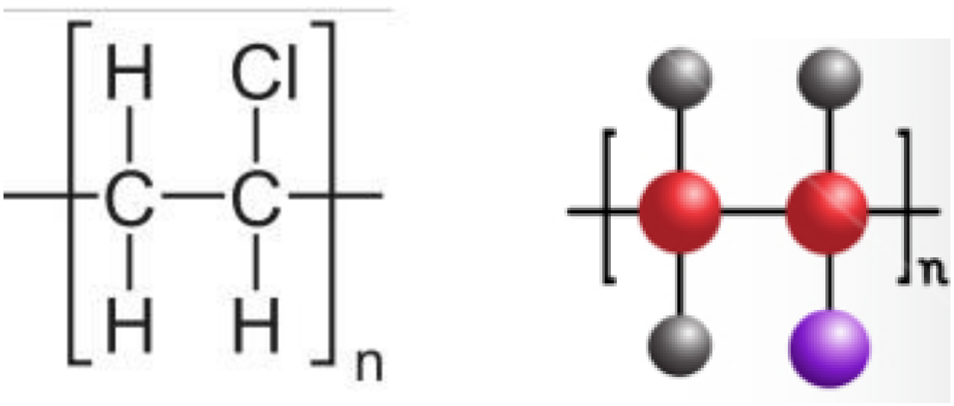


Figure 5-5: Polyvinyl Chloride Structure

Construction of Polyvinyl Chloride (PVC) Structure and Optimization

Initially Vinyl Chloride (VC) monomer was constructed for construction of polymer chain structure.

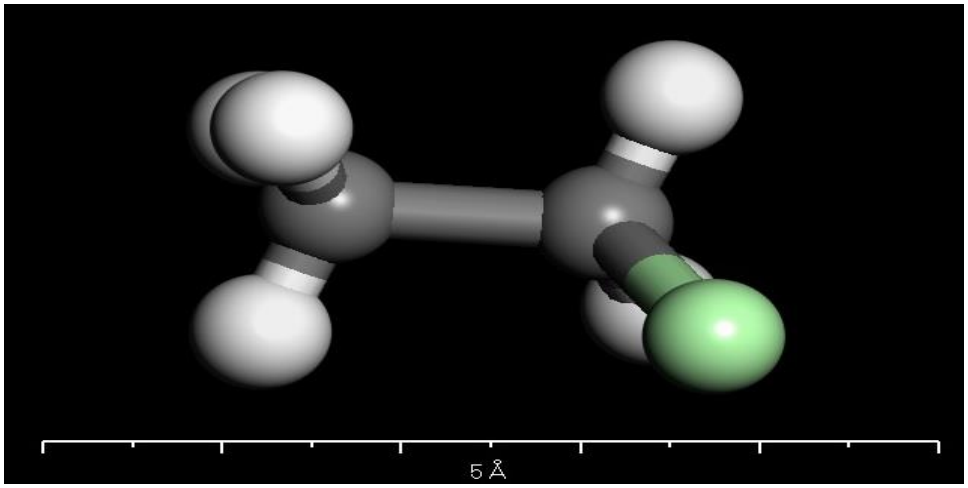


Figure 5-6: Vinyl Chloride

From monomer structure a polymer molecule with a chain length of 10 monomers was constructed.

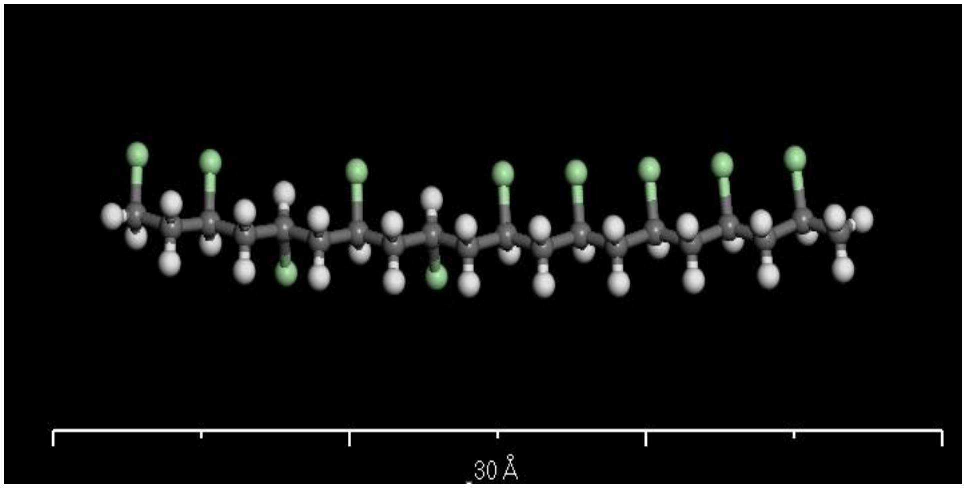
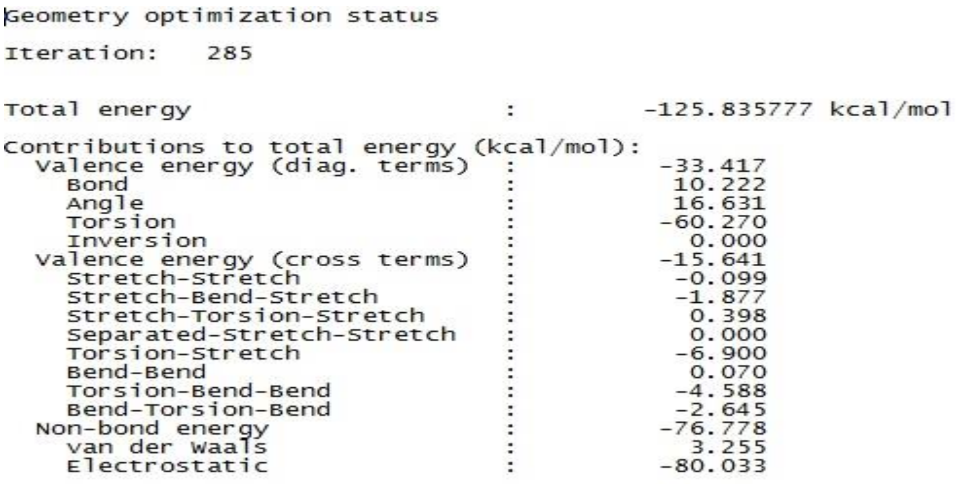


Figure 5-7: Polyvinyl Chloride (10 monomer repeated units)

| Forcite | module was used for geometric optimization resulted in stable low-energy structure. Force field used is COMPASS. Optimized structure after 285 iterations was achieved with total energy value – 125.84 Kcal / mol. Optimized Polyvinyl Chloride structure was subsequently used in construction of composite.



```
Geometry optimization status

Iteration:   285

Total energy                     :        -125.835777 kcal/mol

Contributions to total energy (kcal/mol):
  Valence energy (diag. terms)   :          -33.417
    Bond                         :           10.222
    Angle                        :           16.631
    Torsion                      :          -60.270
    Inversion                    :            0.000
  Valence energy (cross terms)   :          -15.641
    Stretch-Stretch              :           -0.099
    Stretch-Bend-Stretch         :           -1.877
    Stretch-Torsion-Stretch      :            0.398
    Separated-Stretch-Stretch    :            0.000
    Torsion-Stretch              :           -6.900
    Bend-Bend                    :            0.070
    Torsion-Bend-Bend            :           -4.588
    Bend-Torsion-Bend            :           -2.645
  Non-bond energy                :          -76.778
    van der Waals                :            3.255
    Electrostatic                :          -80.033
```

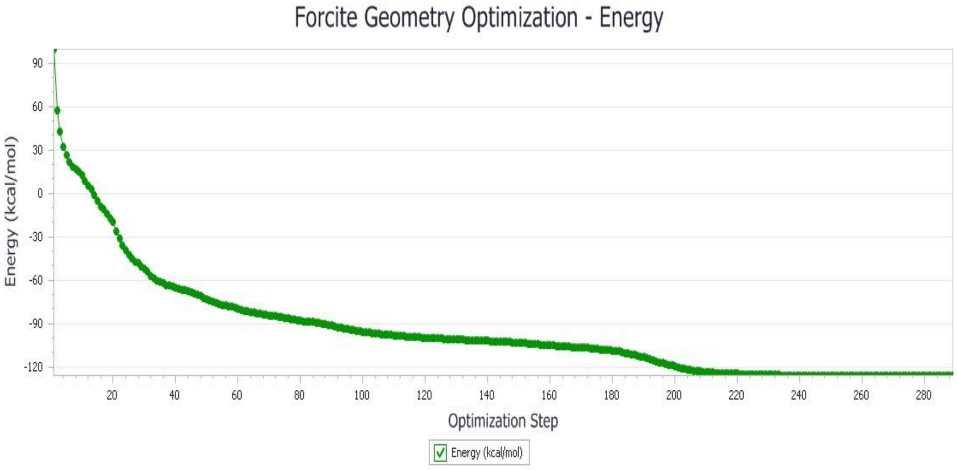


Figure 5-8: Geometric optimization of PVC

5.4 Optimized Building Blocks for Nano Composites (BNNS – PVC)

Optimized structures of Boron Nitride Nano Sheet (BNNS) and Poly vinyl Alchol were achieved. These optimized structures were found compatible with various samples already reviewed for simulation during various research works [25, 26, 27]. Few important details are tabulated below:-

Table 5-1: Properties of Boron Nitride Nano Sheet

Parameter	BNNS	PVC
Category	Synthetic material	Synthetic homo polymer
Dimension	4 nm = 40 A° (Armstrong)	3 nm = 30 A° (Armstrong) for 10 monomer repeated unit
Enthalpy	- 3788.95 Kcal / mol	– 125.84 Kcal / mol
No of Atoms in Structure	324 atoms	62 atoms in single molecule (10 monomer of Vinyl alcohol)

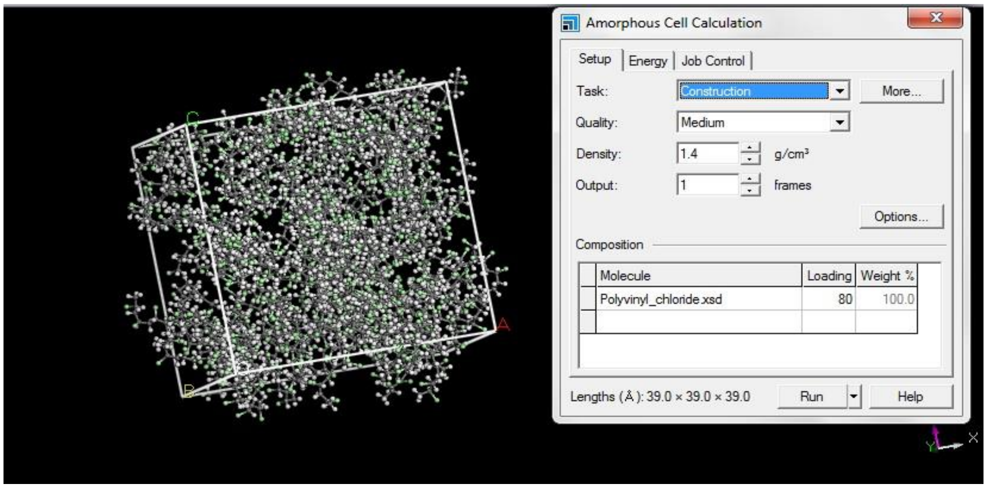
5.5 Construction of Poly Vinyl Chloride (PVC) Super Cell in Material Studio

Amorphous Cell module was used to construct PVC Super cell. “Pack enclosed volume” and density were adjusted as 1.4 g/cm^3 with COMPASS as Force field [30, 31]. The construction of PVA (10 monomer repeated unit) system has been done through it.

Table 5-2: PVC through Amorphous Cell Module

PVC Cell Size	PVC – Molecule	Total no of atoms
39 A° x 39 A° x 39 A°	80	4960

Neat system of PVC was constructed in order to calculate and compare Young Modulus once composite systems were developed. The computational limitation and restriction of software module allows to build and optimize cell of maximum 80 PVC molecular system.



Amorphous Cell Calculation

Task: Construction

Quality: Medium

Density: 1.4 g/cm³

Output: 1 frames

Composition

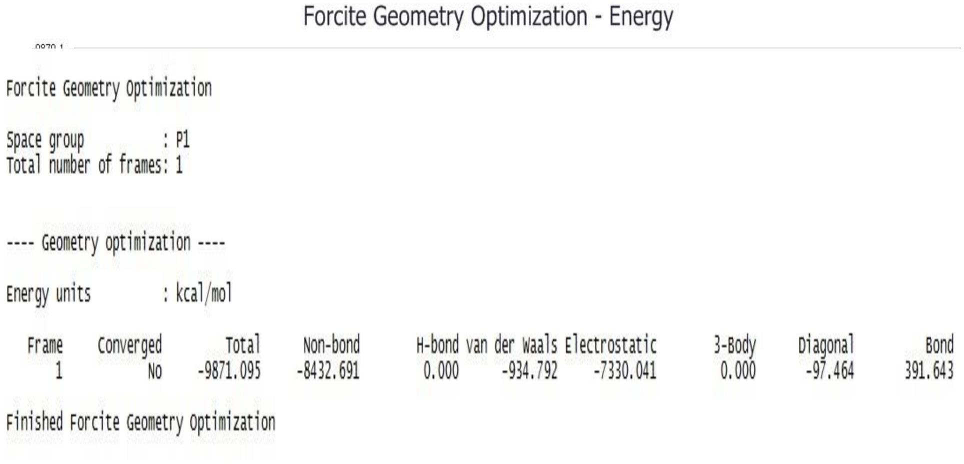
Molecule	Loading	Weight %
Polyvinyl_chloride.xsd	80	100.0

Lengths (Å): 39.0 × 39.0 × 39.0

Figure 5-9: Polyvinyl Chloride Cell

5.6 Geometric optimization of Poly Vinyl chloride (PVC) Super Cell

In order to optimize the structure, series of simulation were run on Forcite module for structure optimization. Force field used is COMPASS.



Forcite Geometry Optimization - Energy

```
Forcite Geometry Optimization

Space group          : P1
Total number of frames: 1


---- Geometry optimization ----

Energy units         : kcal/mol

  Frame    Converged       Total      Non-bond       H-bond van der Waals Electrostatic       3-Body     Diagonal        Bond
      1           No   -9871.095     -8432.691        0.000      -934.792     -7330.041        0.000      -97.464     391.643

Finished Forcite Geometry Optimization
```

Figure 5-10: PVC Cell Optimization

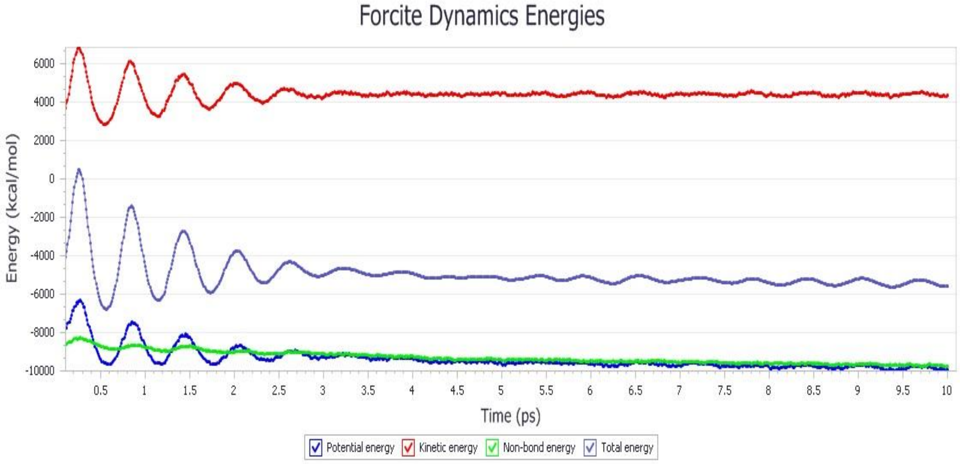
For polymeric chain structure system COMPASS force field is most suitable [29]. Computed total energy after IForciteI geometric optimization calculation is tabulated below:-

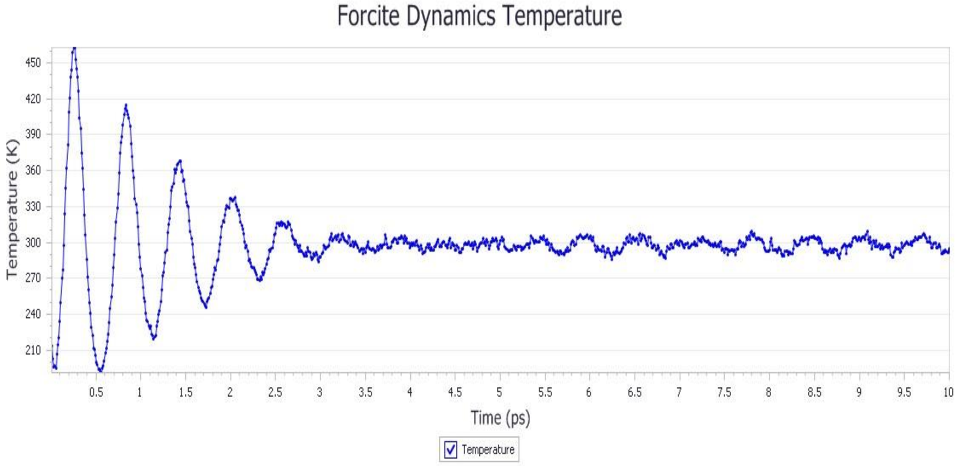
Table 5-3: Total Energy after IForciteI Geometric Optimization

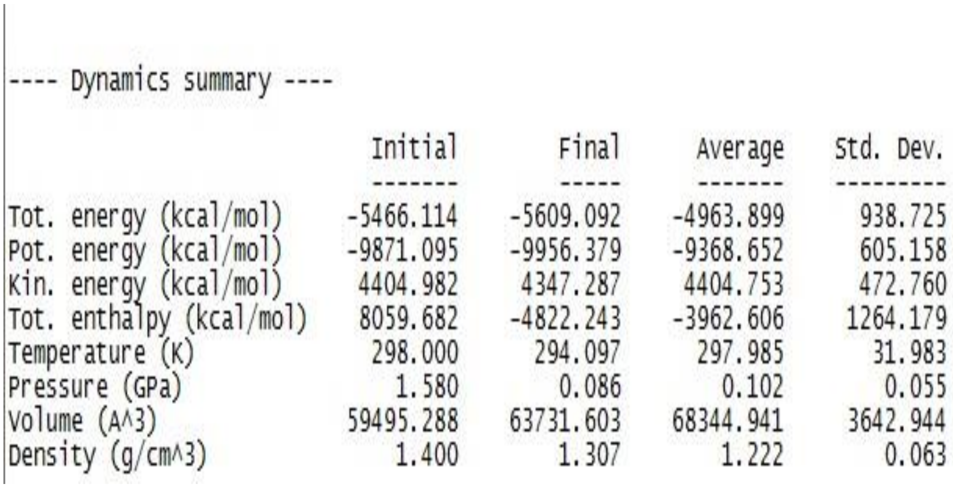
PVC Cell Size	Total numbers of atoms	Total Energy (Kcal /mol)
39 A° x 39 A° x 39 A°	4960	-9871

5.7 Molecular Dynamics (MD) Simulation of PVC Nano Composite

To calculate realistic results/ properties Molecular Dynamics simulation was used as it brings real time effects and stabilizes the system. The system contains molecule of 80 PVC molecules and periodic boundary condition was added to the unit cell. An energy minimization was carried out before the MD simulation again through **I Forcite I**. Series of MD simulations were performed NVT simulation 10 ps with a time step of 1 fs with temperature of 298 K and NPT simulation of 10 ps with a time step of 1 fs with temperature of 298 K (Pressure = 1 atm). After these MD simulations both PVC cell were found stable.







```
---- Dynamics summary ----

                            Initial       Final     Average    Std. Dev.
                            -------       -----     -------    ---------
Tot. energy (kcal/mol)    -5466.114   -5609.092   -4963.899      938.725
Pot. energy (kcal/mol)    -9871.095   -9956.379   -9368.652      605.158
Kin. energy (kcal/mol)     4404.982    4347.287    4404.753      472.760
Tot. enthalpy (kcal/mol)   8059.682   -4822.243   -3962.606     1264.179
Temperature (K)             298.000     294.097     297.985       31.983
Pressure (GPa)                1.580       0.086       0.102        0.055
Volume (A^3)              59495.288   63731.603   68344.941     3642.944
Density (g/cm^3)              1.400       1.307       1.222        0.063
```

Figure 5-11: MD Simulation of PVC Cell

Final Temperature and energy is tabulated below:-

Table 5-4: Temperature and Energy of PVC Cell

PVC Cell Size	Total numbers of atoms	Final Energy (Kcal /mol)	Average Temperature (K)
39 A° x 39 A° x 39 A°	4960	-5609.09	297.98

5.8 Mechanical Properties Calculation of PVC System in Forcite Material Studio

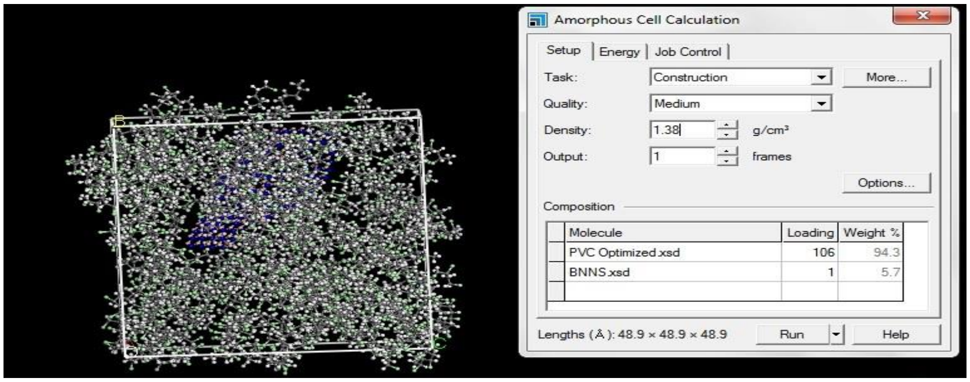
Forcite Module was used to calculate the Young Modulus of PVC. The results are tabulated below for a pure PVC matrix (PVC system) with a density of 1.4 g/cm^3 [39].

Table 5-5: Young Modulus of PVC

PVC Cell Size	Young Modulus (GPa)
39 A° x 39 A° x 39 A°	2.9

5.9 Construction of PVC – BNNS Nano Composite in Material Studio

Amorphous Cell module was used to construct the PVC and BNNS structure modelled in a composite material. The construction of PVC (10 monomer repeated unit) and BNNS was carried out.



Task: Construction

Quality: Medium

Density: 1.38 g/cm³

Output: 1 frames

Composition

Molecule	Loading	Weight %
PVC Optimized.xsd	106	94.3
BNNS.xsd	1	5.7

Lengths (Å): 48.9 × 48.9 × 48.9

Figure 5-12: PVC – BNNS Nano Composite

In order to calculate mechanical properties system was developed with loading of PVC and BNNS.

Table 5-6: Mechanical Properties of PVC

PVC – BNNS Cell Size	**Cell Configuration**	**Weight percentage of BNNS**	**Total no of atoms**
48.9 A° x 48.9 A° x 48.9 A°	106 molecule (10 monomer repeated units) 1 Boron Nitride Nano sheet	5.7	6896

In order to optimize the structure series, simulation was run on Forcite module. Force field used was Dreiding. Tabulated value of Total Energy for Nano composite is a below:-

Table 5-7: Total Energy for Nano Composite

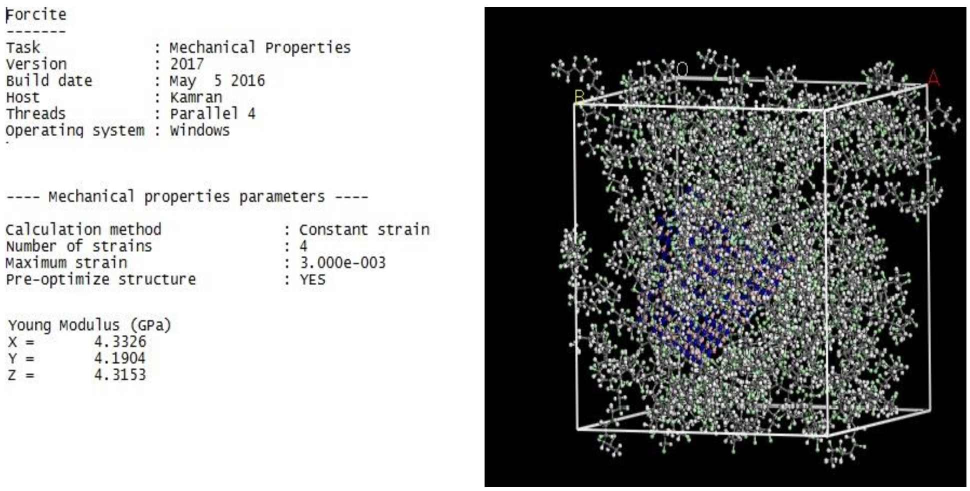
PVC – BNNS Cell Size	**Total Energy (kcal/mol)**	**Total no of atoms**
48.9 A° x 48.9 A° x 48.9 A°	-3872	6896

5.10 Molecular Dynamics (MD) Simulation of PVC – BNNS Nano Composite

IForciteI was used to carry out MD of the composite systems. The system contains single Boron Nitride Nano Sheet randomly surrounded by 106 PVC molecules in unit cell. The periodic boundary condition was added to the unit cell. An energy minimization was carried out before the MD simulation again through IForciteI. A 10 ps NVT simulation at Temperature of 360 K (Glass Transition Temperature of PVA [23]) with a time step of 1 fs and a 10 ps NPT simulation (T = 360 K and P= 1 atm) with a time step of 1 fs was carried out. After MD simulations the BNNS sheet was well dispersed inside the PVC matrix.

5.11 Mechanical Properties Calculation of PVC – BNNS Nano Composite

IForciteI was used to calculate Young Modulus. Constant strain method was used to calculate the mechanical properties as this method is most suited to Polymer composites. Calculations results showed that Young’s moduli of PVC - BNNS has enhanced to 4.33 GPa after in cooperation of BNNS.



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Forcite
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Task             : Mechanical Properties
Version          : 2017
Build date       : May  5 2016
Host             : Kamran
Threads          : Parallel 4
Operating system : Windows


---- Mechanical properties parameters ----

Calculation method             : Constant strain
Number of strains              : 4
Maximum strain                 : 3.000e-003
Pre-optimize structure         : YES

Young Modulus (GPa)
X =       4.3326
Y =       4.1904
Z =       4.3153
```

Figure 5-13: BNNS – PVC Nano Composite

Results and Discussion

6.1 Introduction

Atomistic simulations using Material Studio 2017 software were performed in order to model Poly Vinyl Alcohol - Graphene Nano Sheet and Polyvinyl Chloride Boron Nitride Nano Sheet nano-composite.

6.2 Polyvinyl Alcohol and Graphene Nano Sheet Nano-Composite

The Poly Vinyl Alcohol chain models were constructed by linking 10 structural repeat units through **Atomistic I Structural Building I**. The structure was subjected to Series of Molecular Dynamics simulations; NVT simulation 10 ps with a time step of 1 fs with temperature of 298 K and NPT simulation of 10 ps with a time step of 1 fs with temperature of 298 K (Pressure = 1 atmospheric) through **Forcite I Geometric Optimization I**. The force field applied in the Molecular Dynamics simulation was COMPASS. Structural stabilizing and energy of polymer chain was achieved. The Young Modulus was calculated through **Forcite** I **Mechanical properties I** was 3.2 GPa. The value is more than the experimental value as the structure of PVA is constructed without any defects however; defect is inherent in case of experimental systems.

The Graphene Nano sheet was manually constructed, and energy was minimized in order to obtain a stable structure **DFTB Module**.

The Polyvinyl Alcohol and Graphene Nano Sheet atomic cell model has been constructed through **Amorphous Cell module** and further equilibrated and reaches low energy derivative through **Forcite I Geometric Optimization I**.

Forcite Module simulates time dependent behavior through point masses and point charge of a molecular system in classic regime. Basic idea is to track motion of all atoms in a molecular arrangement by resolving Newton's equation of motions.

Amorphous Cell module was used to construct number of computational models of PVA-GNS Supercell of 3.5, 4, 4.5, 5, 5.5 and 6 weight percentage of Graphene. Different concentration of Graphene is in-cooperated in order to determine its influence on the mechanical behavior of the composite.

Forcite Mechanical Properties is used to accurately predict Young Modulus of nano-composite. The increase in Young Modulus is evident as its increase from 67 % up to 124 % from initial value of 3.2 GPa with in-cooperation Graphene Nano Sheet. The in-cooperation of Graphene Nano Sheet has increased the elastic properties of the polymeric material.

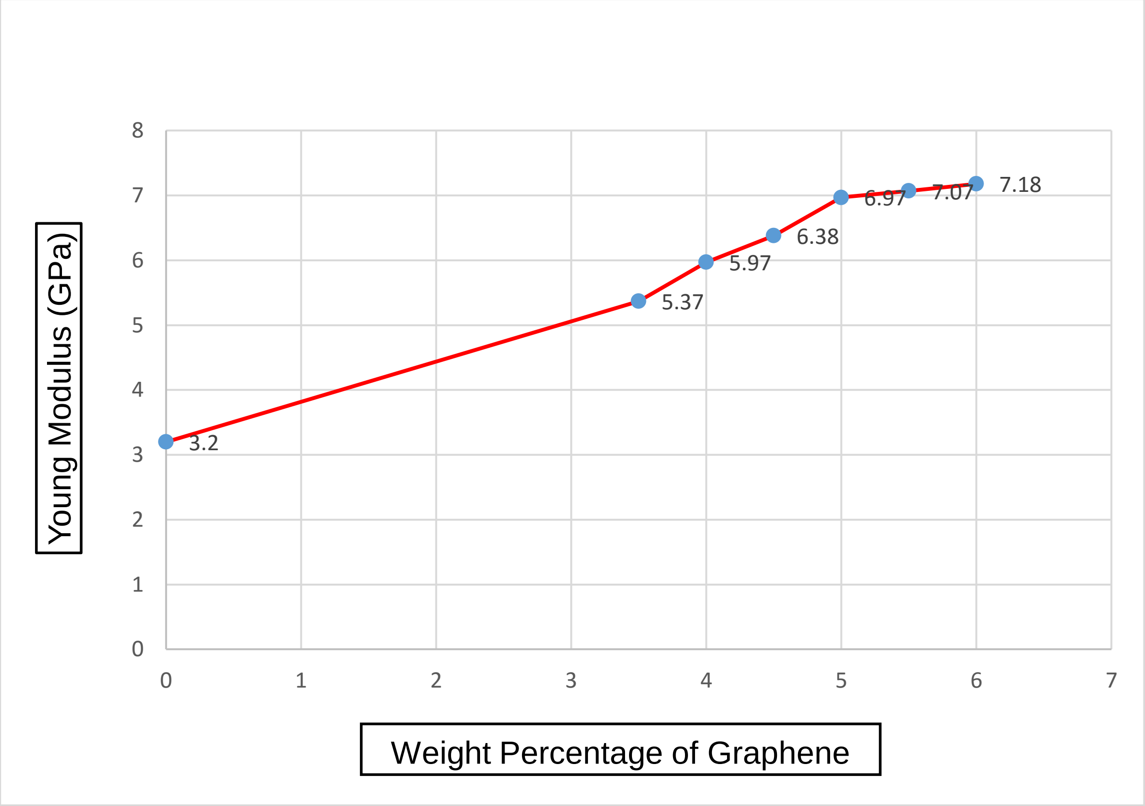

Figure 6.1 Young Modulus vs Weight Percentage (PVA – GNS)

In light of various above referred statistics obtained through scholar researches the graph plotted after obtaining Young Modulus value through simulation shows linear increase in Young Modulus is observed with increase of weight percentage of Graphene from 3.5 to 5 weight percent whereas after 5.1 to 6 weight percent the increases in not linear. The maximum achieved value is approximately 124 percent increase which is within various above referred research work.

6.3 Polyvinyl Alcohol and Graphene Nano Sheet Nano-Composite

Value of Young Modulus obtained through Forcite Module at various weight loading on plotted in graph depicted below:-

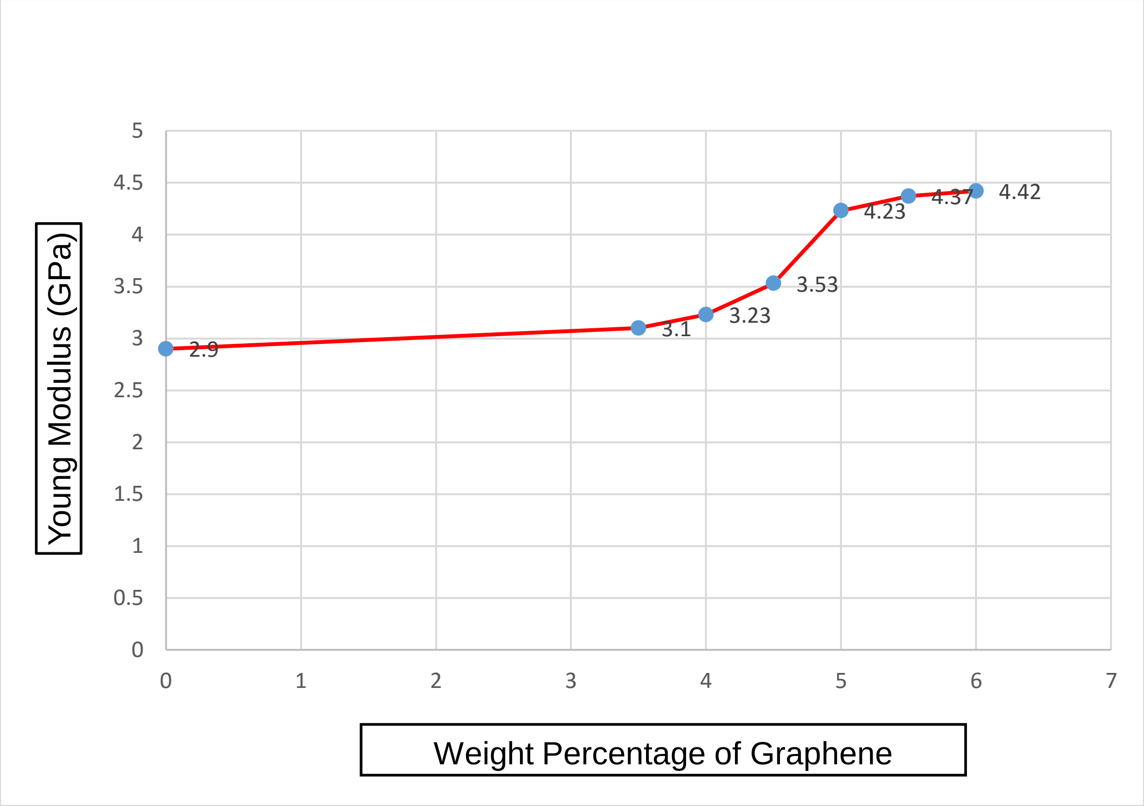

Figure 6.2 Young Modulus vs Weight Percentage (PVC – GNS)

The maximum value observed after increase weight percent is 4.42 GPa which is almost 53 percent increase with incorporation of Graphene Nano Sheet.

6.4 Polyvinyl Chloride and Boron Nitride Nano Sheet Nano-Composite

The Poly Vinyl Alcohol chain models were constructed by linking 10 structural repeat units **Atomistic I Structural Building I**. The structure was subjected to Series of Molecular Dynamics simulations; NVT simulation 10 ps with a time step of 1 fs with temperature of 298 K and NPT simulation of 10 ps with a time step of 1 fs with temperature of 298 K (Pressure = 1 atmospheric) through **Forcite I Geometric Optimization I**. The force field applied in the Molecular Dynamics simulation was

Dreiding. Structural stabilizing and energy of polymer chain was achieved. The Young Modulus was calculated through Forcite Mechanical Properties was 2.9 GPa.

The Boron Nitride Nano sheet was manually constructed, and energy was minimized in order to obtain a stable structure **Forcite Module**. The Polyvinyl Vinyl Chloride and Boron Nitride Nano Sheet atomic cell model has been constructed through **Amorphous Cell module** and further equilibrated and reaches low energy derivative through **Forcite I Geometric Optimization I**.

Forcite Mechanical properties accurately predict Young Modulus for the studies of nano-composite. The value Young Modulus increase from 2.9 to 4.33 GPa.

CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusion

Graphene a 2-D hexagonal single atom thick sheet of carbon has revolutionize the material industry due to its electrical and thermal properties. The nano-composites of Graphene have achieved a remarkable success in materials industry. The synthesis of nano-composites is a challenging and complicated task because when we talk about nano-composites. We are talking about a very small length and time scale. At such a small dimension it becomes difficult to find out results and analyze them. We have seen from results, in chapter 4, 5 that the interface of Graphene sheet with PVA ad PVC has extraordinarily increased the Young’s Modulus. Carbon based nano-composites has advanced the aerospace industry. Computational method is a less difficult and fast method to find out the properties of nano-composites and provide a source to verify the results with experimental results.

7.2 Recommendations

Simulation work through Material Studio Software may be encouraged for other material compositions for MS Students. Most of the properties were calculated by taking nano sheet as device configuration these properties may also be calculated as bulk configuration. The synthesis of nano-composites may be done after having confidence in computational results.

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