A Molecular Dynamics Study of The Mechanical Properties of PLA-CNT Nanocomposites

Supervised By

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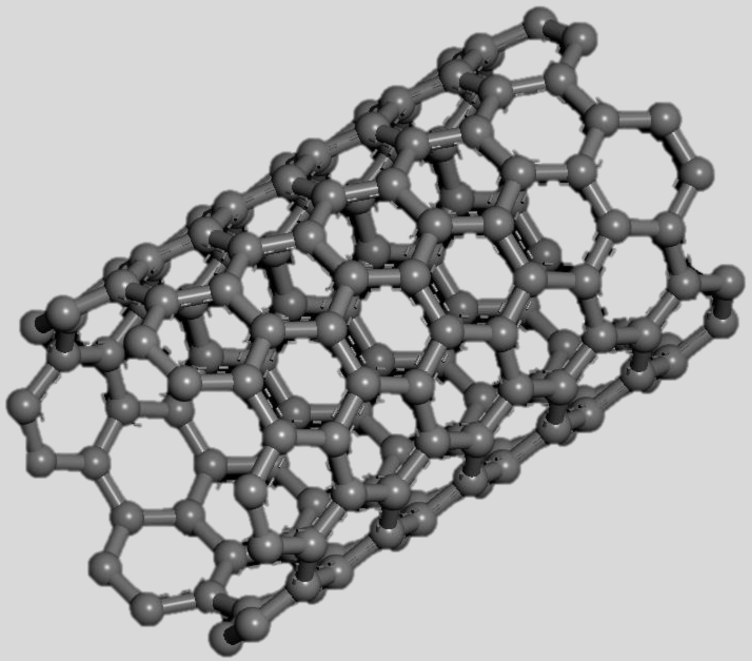
Introduction

Abstract

This thesis contains a non-destructive process of determining structural and mechanical property of a promising composite material named PLA-CNT. Polylactic Acid (PLA) is widely used as raw material of filler material of 3D printing additive manufacturing process. In order to perform molecular dynamics simulation PLA is modeled and packed in Materials Studio software package and validated in terms of Young’s modulus against mechanical testing value found in published literature of Kamthai and Magaraphan (2016). This PLA model is incorporated with CNT reinforcement and undergone molecular dynamics simulation of uniaxial tensile deformation through LAMMPS software package. Simulation resulted in significant improvement of mechanical properties such as Young’s modulus, tensile strength in PLA-CNT composite over PLA. Thus, enhanced mechanical property of raw material will result in similar enhancement in printed model.

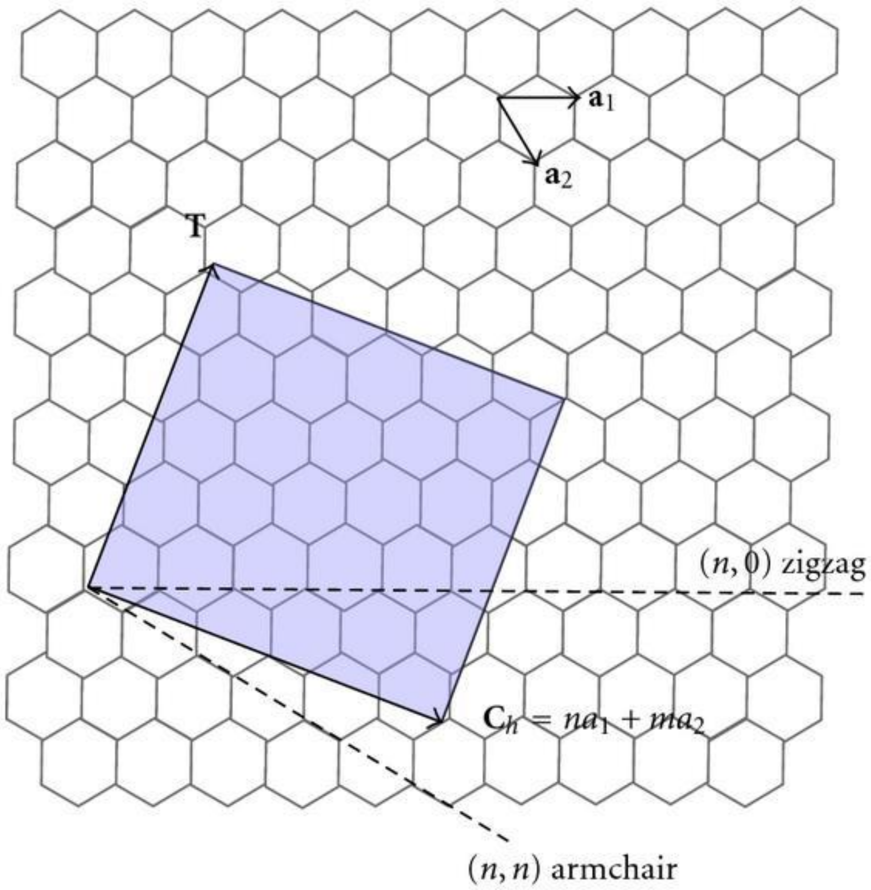
Carbon Nanotube

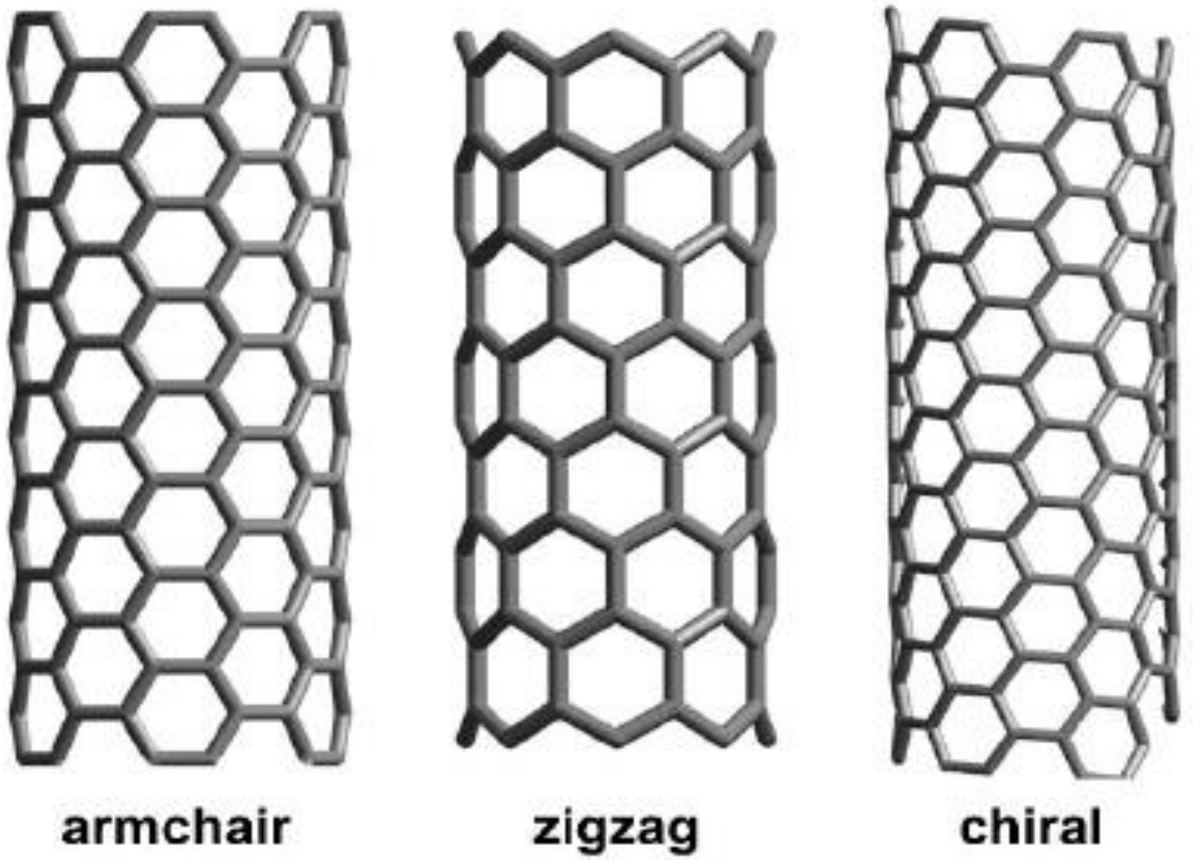
- Discovered by Ijima in 1991
- Two-dimensional hexagonal lattice of carbon atoms, bent and joined in one direction so as to form a hollow cylinder.
- Possess higher mechanical, electrical and thermal properties
- Potential reinforcement agents in composite materials for the upcoming ages



Carbon Nanotube

Different Chirality of CNT





Carbon Nanotube

Properties of CNT

Mechanical

- Young's modulus ranges from 270 to 950 Gpa (Ruoff RS et el (1993)
- tensile strength is also very high, in the range of 11–63 GPa.
- Yu et al. (2000) measured the Young's modulus of individual SWNTs, reporting values between 320 and 1470 GPa and determining a breaking strength of SWNTs on the perimeter of each rope ranging from 13 to 52 GPa.

Electrical

- Chandra B et el (2009) have demonstrated that CNTs exhibit unique conductive properties.
- SWNTs are metals with resistivities that range from 0.34 × 10–4 to 1.0 × 10–4 ohm·cm.
- Ebbesen TW et el (1996) showed that each carbon atom is covalently bonded to three neighbor carbons via sp2 molecular orbitals CNTs can be conducting or semi-conducting types depending on the type of chirality**.** Thus, CNTs can be conducting or semi-conducting types depending on the type of chirality

Carbon Nanotube

Properties of CNT

Thermal

- Ruoff RS et el (1995) found that, as rolled graphitic structures, CNTs are of great importance and interest not only for their electronic and mechanical properties, but also for their thermal properties.
- Although their size is very small, the quantum effects are important and the low temperature specific heat and thermal conductivity show direct evidence of the 1-D quantization of the phonon band structure in CNTs.
- The incorporation of pristine and functionalized nanotubes to different materials can double the thermal conductivity for a loading of only 1%, showing that nanotube composite materials may be useful for thermal management applications in industries.

Polylactic Acid (PLA)

- Polylactic acid or polylactide (PLA) is a biodegradable and bioactive polyester made up of lactic acid building blocks
- discovered in 1932 by Wallace Carothers by heating lactic acid under vacuum while removing condensed water.
- PLA is manufactured from renewable sources and is compostable, addressing problems in solid waste disposal and lessening our dependence on petroleum-based raw materials.
- It is currently the second most produced and consumed bioplastic in the world in terms of volume
- A raw material for current blooming additive manufacturing technology like 3D printing.

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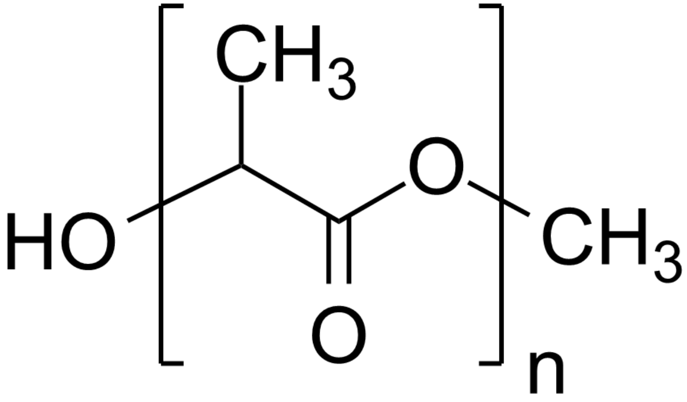


Chemical Formula of PLA

Polylactic Acid (PLA)

Properties of PLA

Mechanical Properties

The mechanical properties of lactic acid-based polymers can be varied to a large extent ranging from soft and elastic plastics to stiff and high strength materials. Semi crystalline PLA is preferred over the amorphous polymer when higher mechanical properties are desired. Sodergard and Stolt (2002) showed that semi crystalline PLA has an approximate tensile modulus of 3 GPa, tensile strength of 50–70 MPa, flexural modulus of 5 GPa, flexural strength of 100 MPa, and an elongation at break of about 4%. Farah et el (2016) showed that Young's modulus for PLA can vary 3.7 GPa to 4.1 Gpa. Desa et al (2014) showed the Young's modulus as 1.18 GPa. Also, Wang et al (2002) showed for different starch ratio it can vary 1.1 GPa to 1.78 GPa. Kamthai and Magaraphan (2016) found the value to be around 2.0043 GPa.

Polylactic Acid (PLA)

Properties of PLA

Physical Properties

In the solid state, PLA can be either amorphous or semi crystalline, depending on the stereochemistry and thermal history. For amorphous PLAs, Heton et al (2005) stated that the Tg determines the upper use temperature for most commercial applications. For semi crystalline PLAs, both the Tg (~58 °C) and Tm, (130– 230 °C, depending on structure) are important for determining the use temperatures across various applications. Both of these transitions, Tg and Tm, are strongly affected by overall optical composition, primary structure, thermal history, and Mw. Above Tg amorphous PLAs transition from glassy to rubbery and will behave as a viscous fluid upon further heating. Below Tg, PLA behaves as a glass with the ability to creep until cooled to its β-transition temperature of approximately−45 °C. Below this temperature PLA will only behave as a brittle polymer.

Rheological Properties

PLA is a pseudoplastic, non-Newtonian fluid. This means that its viscosity (resistance to flow) will change depending on the stress that it is subjected to. Specifically, PLA is a shear-thinning material, which means that the viscosity decreases with applied stress

Polylactic Acid (PLA)

Potentiality of PLA

PLA is an ecofriendly product with better features for use in the human body (nontoxicity). Farah et al (2016) found that PLA is the first commodity polymer produced from annually renewable resources. It is classified as generally recognized as safe (GRAS) by the United State Food and Drug Administration (FDA) and is safe for all food packaging applications. The research on lactic acid-based polymers intended for medical applications has accelerated since FDA approval that during the last two decades an increasing utilization of large scale industrial lactic acid-based polymers for other uses has occurred.

Lasprilla et al (2012) showed that as a bioabsorbable polymer, PLA, is one of the most promising biopolymers due to the fact that the monomers may be produced from non-toxic renewable feedstock as well as due to being a naturally occurring organic acid. Lactic acid (2-hydroxypropionic acid, LA), a PLA constituent unit, since it is a chiral molecule, exists as two enantiomers, L- andD-lactic acid, PLA has stereoisomers, such as poly(L-lactide) (PLLA), poly(D-lactide) (PDLA), and poly(DL-lactide) (PDLLA).

In comparison to other biopolymers, the production of PLA has numerous advantages, including: 1) Eco-friendly — apart from being derived from renewable resources (e.g., corn, wheat, or rice), PLA is biodegradable, recyclable, and compostable. Its production also consumes carbon dioxide. 2) Biocompatibility — the most attractive aspect of PLA, especially with respect to biomedical applications. A biocompatible material should not produce toxic or carcinogenic effects in local tissues. Also, the degradation products should not interfere with tissue healing. PLA hydrolyzes to its constituent α-hydroxy acid when implanted in living organisms, including the human body. It is then incorporated into the tricarboxylic acid cycle and excreted. Moreover, PLA degradation products are non-toxic (at a lower composition) making it a natural choice for biomedical applications.

Methodology

Methodology

Generation of Single Polymer Chain and CNT

↓

Packing of Polymer chain around CNT

↓

Msi2lmp software to convert material studio pdb file to LAMMPS compatible data file

↓

LAMMPS software to perform MD simulation

↓

Methodology

Forcefield selection

The Consistent-Valence Force Field (CVFF) is a generalized valence forcefield. the original forcefield provided with the *Discover* program, developed by Dauber-Osguthorpe (1988). Parameters are provided for amino acids, water, and a variety of other functional groups. It is also a family of forcefields adapted to a broad variety of organic compounds, includes force fields for polymers, metals, etc. The CVFF forcefield supplied by Biosym/MSI defines atom types for the 20 commonly occurring amino acids, most hydrocarbons, and many other organic molecules. Atom types CVFF covers hydrogen, carbon ,nitrogen, oxygen, sulfur, phosphorus, halogens, ions, argon, silicon. However, in the CVFF forcefield, hydrogen bonds are a natural consequence of the standard van der Waals and electrostatic parameters, and special hydrogen bond functions do not improve the fit of CVFF to experimental data showed by Haglar et el (1997). It was based on the Polymer Consistent Force Field (PCFF). Although the exact parameters of this force-field are proprietary (hence unavailable), it is known and referenced that it was parameterized, tested and validated for most of the common organic and inorganic materials.

Methodology

Forcefield selection

$$E_{pot} = E_{valence} + E_{nonbond}$$
$$E_{valence} = E_{diagonal} + E_{coupling}$$
$$E_{diagonal} = E_{bond} + E_{angle} + E_{torsion} + E_{out\text{-}of\text{-}plane}$$
$$E_{nonbond} = E_{elec} + E_{vdw}$$

Evalence is the valence component energy.
Ediagonal is the diagonal term energy.
Ecoupling is the coupling term energy.
Ebond is the bond stretching energy.
Eangle is the angle energy.
Etorsion is the torsion energy.
Eout-of-plane is the out-of plane deformation energy.
Enon-bpnd is the non-bond energy between atoms in different molecules and atoms separated by three or more bonded atoms.
Eelec is the term for Coulombic electrostatic interaction
EvdW is the term for Van der walls energies.

Methodology

Forcefield selection

$$E_{bond} = \sum_{b} D_b[1 - e^{-a}(b - b_0)]^4$$

$$E_{angle} = \sum_{\theta} H_\theta(\theta - \theta_0)^2$$

$$E_{torsion} = \sum_{\varphi} H\varphi\,[1 - \cos(n\varphi)]$$

$$E_{out-of-plane} = \sum_{\chi} H_x X^2$$

$$E_{elect} = \sum \frac{q_i q_j}{\varepsilon r_{ij}}$$

$$E_{vdW} = \sum \varepsilon\,[\left(\frac{r^0}{r}\right)^{12} - 2\left(\frac{r^0}{r}\right)^{6}]$$

$$E_{coupling}$$
$$= \sum_{b}\sum_{b'} F_{bb'}(b - b_0)\,(b' - b'_0) + \sum_{\theta}\sum_{\theta'} F_{\theta\theta'}(\theta - \theta_0)\,(\theta' - \theta'_0)$$
$$+ \sum_{b}\sum_{\theta} F_{b\theta}(b - b_0)\,(\theta - \theta_0) + \sum_{\varphi} F_{\varphi\theta'\theta}\cos(\theta - \theta_0)(\theta' - \theta'_0)$$
$$+ \sum_{X}\sum_{X'} F_{XX'} X X'$$

Methodology

Rule of Mixture

Volume of Fraction Calculation by Rule of Mixture:

$$f_{CNT} = \frac{\pi\left(R_{CNT} + \frac{h_{vdw}}{2}\right)}{A_{cell}}$$

Methodology

Input Structure of LAMMPS Input Script

LAMMPS input script contains 4 parts

i) Initialization

First all the parameter required for simulation is defined before the creation of atoms or read in from a file. The units of simulation, periodic boundary condition or non-periodic boundary condition, atom style and force filed parameter are set in this step.

ii) Atom definition

The atoms can generate using different software and their co-ordinate is created in a data file which contains molecular topology information. The data file read in the LAMMPS input script using *read_data* command.

iii) Setting

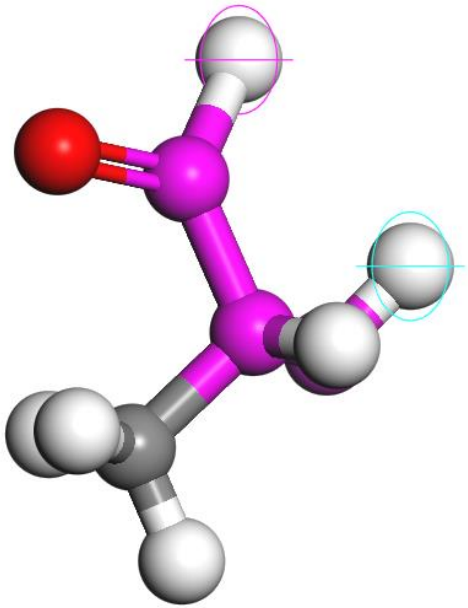
After defining atoms, angles, bonds, dihedrals necessary setting for simulation is specified. The force field coefficient, temperature of simulation, energy minimization criteria, time steps is specified in this step. Boundary conditions, time integrations and diagnostics are imposed by *fix* command.

iv) Simulation runs

Model Formulation

Model Formulation

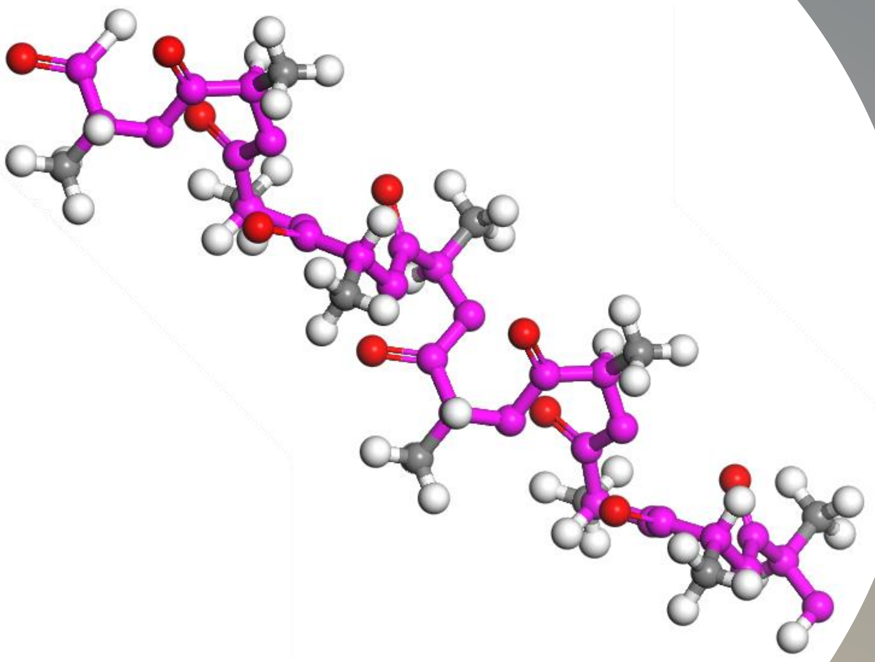
Material Modeling of PLA



Of all available software BIOVIA Materials Studio 2017 is used to create material modeling PLA-CNT nano composites. In order to create PLA polymer a repeat unit of Lactic Acid is created.

Model Formulation

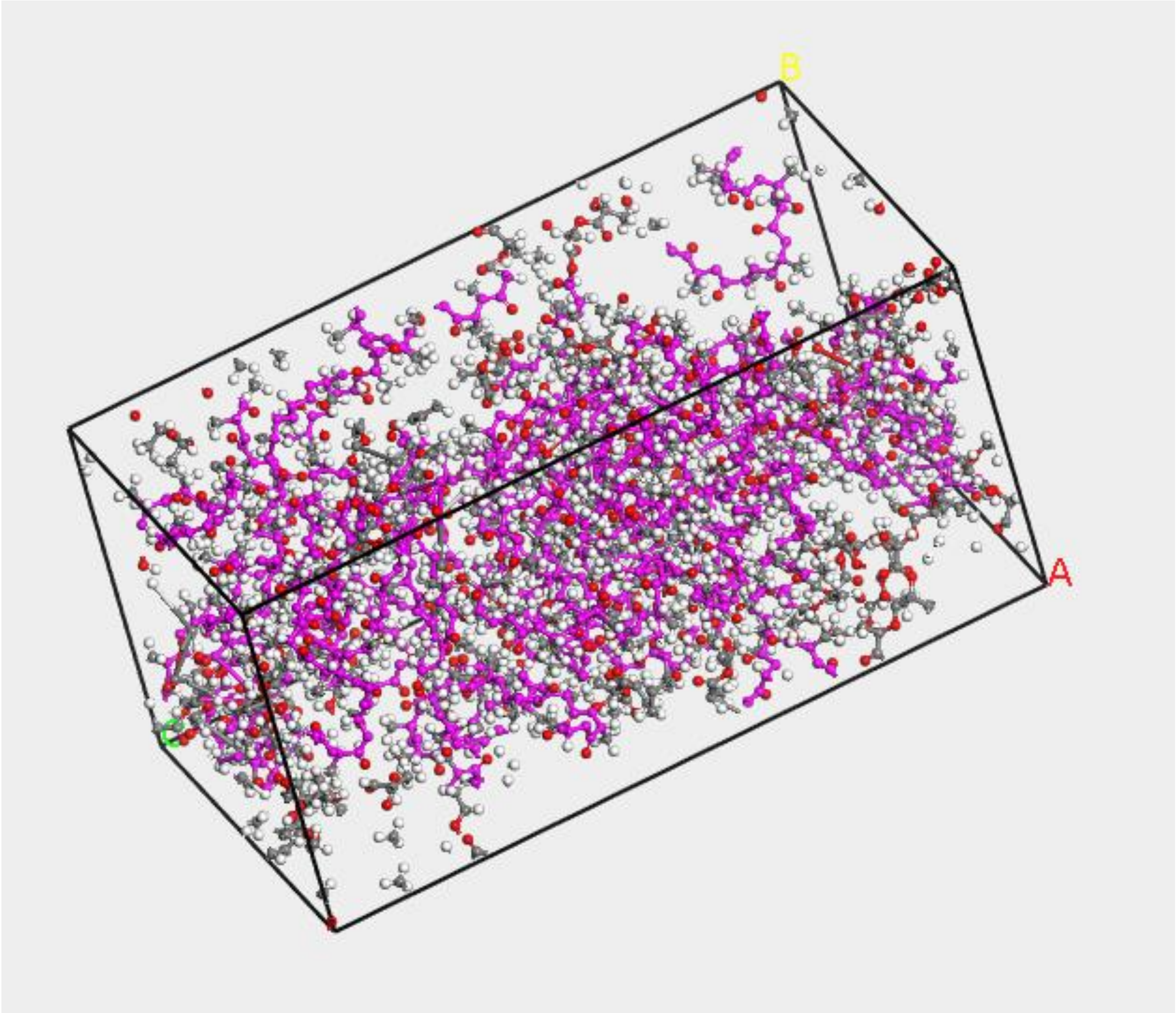
Material Modeling of PLA



For purpose of simulation different length of Polylactic acid is created using above structure as a repeat unit.

Model Formulation

Material Modeling of PLA

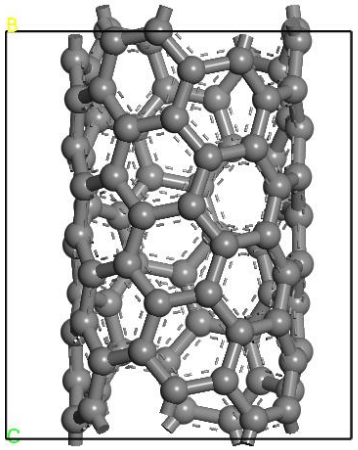


Using suitable forcefield, in this case CVFF and the packing density of 1.23 g/cm^3 polylactic acid is packed into an amorphous cell. The lattice type used are 3D triclinic with lengths A=30 Å, B=30 Å, C=60 Å.

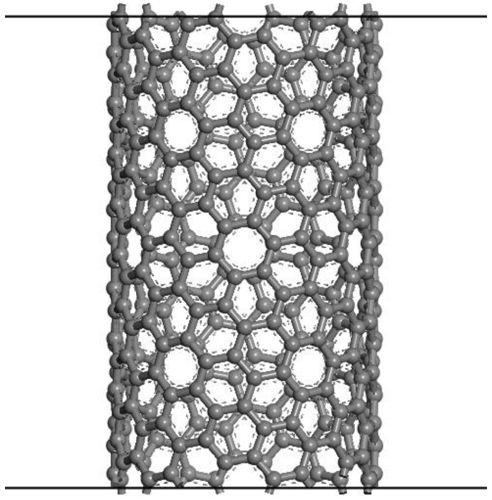
Model Formulation

Material Modeling of CNT

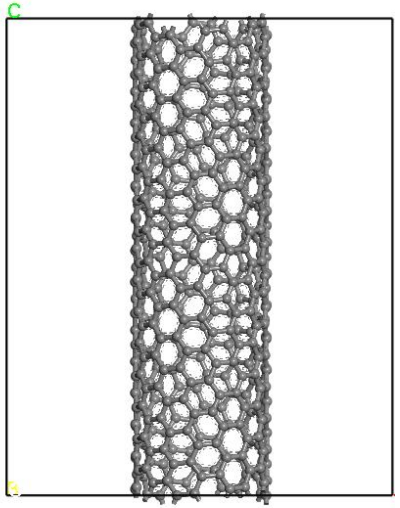
In order to prepare PLA-CNT nanocomposite model, Single walled carbon nanotube (SWNT) of chirality (3,6), (6,9), (6,12) are modeled.



3,6



6,9



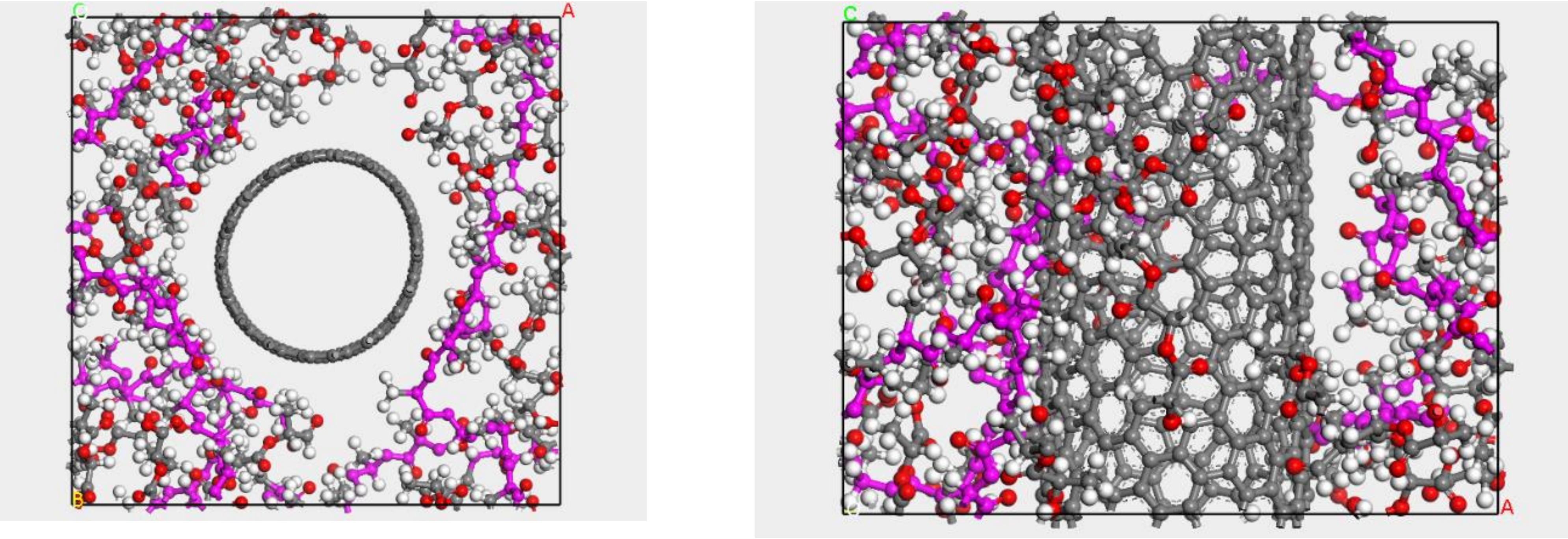
6,12

Chirality	Length (Å)	Diameter (Å)	Lattice Parameter ($Å^3$)
(3,6)	22.54	6.12	31×31×22.54
(6,12)	22.54	12.43	25×25×22.54
(6,9)	37.14	10.24	30×30×37.14

Model Formulation

Material Modeling of CNT

Using suitable forcefield, in this case CVFF and the packing density of 0.9g/cm^3 polylactic acid and SWNT are packed into amorphous cell. Lattice parameter is used as mentioned in Table 1.



Amorphous Packing of PLA-CNT Nanocomposite

Model Formulation

Transforming Model to Simulation Data Cell

In order to create suitable input dataset for LAMMPS simulation from molecular model generated in Materials studio, msi2lmp is used. The input dataset summery is listed below table

Packing	CNT volume fraction	Atoms	Bonds	Angles	Dihedrals	Impropers
PLA	0%	2116	2093	3680	4554	230
PLA-SWNT (3, 6)	12.76%	1484	1540	2744	3724	308
PLA-SWNT (6, 9)	13.60%	2336	2524	4568	6616	656
PLA-SWNT(6,12)	19.60%	1511	1654	3008	4441	461

Simulation Details

Material Modeling of CNT

Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is a molecular dynamics program was selected to carry out molecular dynamics simulation. Amorphous cell containing different composition of PLA-CNT nanocomposites and Polylactic acid undergone simulation process of a uniaxial deformation using CVFF potential. Periodic boundary condition is applied to x, y and z direction. For Atom style *full* is chosen for polylactic acid being bio-molecular. Bond style *morse* bond, angle style *harmonic,* improper style *cvff* are selected according to LAMMPS documentation suitable for the simulation dataset. For simulation efficiency neighbor *0.4 bin* is used as designated neighbor cutoff.

The initial structure is inserted into the molecular dynamics code where an equilibration sequence is performed prior to deforming the amorphous cell. The equilibration sequence relaxes any high energy configurations that are artificially created due to the lattice used to generate the amorphous polymer structure. The relaxation involves four different steps. Initially, the simulation ran for 10,000 timesteps (Δt=1 fs) using NVT dynamics at 500 K followed by relaxation for 50,000 timesteps (Δt=0.5 fs) using NPT dynamics at 500 K. The next relaxation cooled the structure down to the desired temperature for 50,000 timesteps followed by further relaxation of 50,000 timesteps at the desired temperature.

Uniaxial tensile deformation is simulated at NPT with deformation of 0.0001 engineering strain rate along z axis. During this process pressure tensor of every step are stored against its strain. This provided enough information to construct a stress-strain diagram and harness desired mechanical properties in the form of Young’s modulus.

Result and Analysis

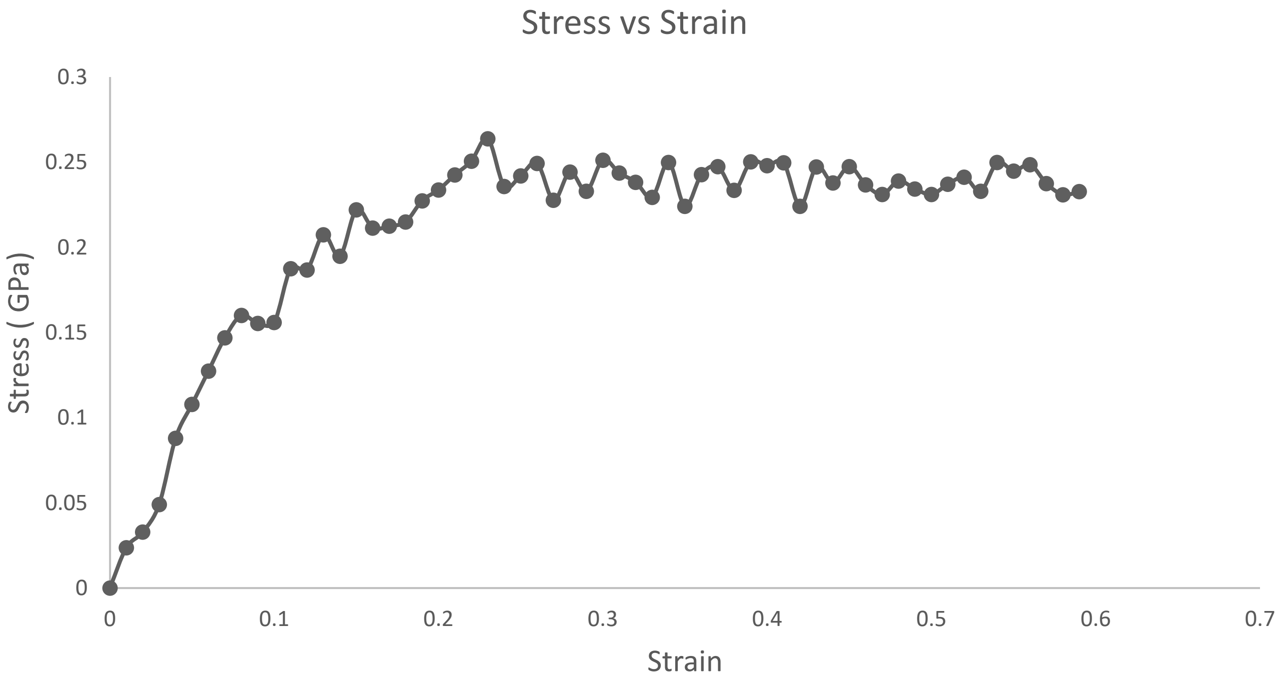
Mechanical Properties of PLA

This analysis focused on the increment of Young’s modulus of PLA polymer by reinforcing carbon nanotube. Molecular dynamics simulations were used to study deformation mechanisms during uniaxial tensile deformation of amorphous PLA and PLA CNT nanocomposite. From this simulation process the value of Young’s modulus and tensile strength is obtained.

Mechanical properties of PLA such us Young’s modulus, tensile strength vary within significant range. Farah et al (2016) showed that Young’s modulus for PLA can vary 3.7 GPa to 4.1 GPa. Desa et al (2014) showed the Young’s modulus as 1.18 GPa. Also, Wang et al (2002) showed for different starch ratio it can vary 1.1 GPa to 1.78 GPa. Kamthai and Magaraphan (2016) found the value to be around 2.0043 GPa.

Result and Analysis

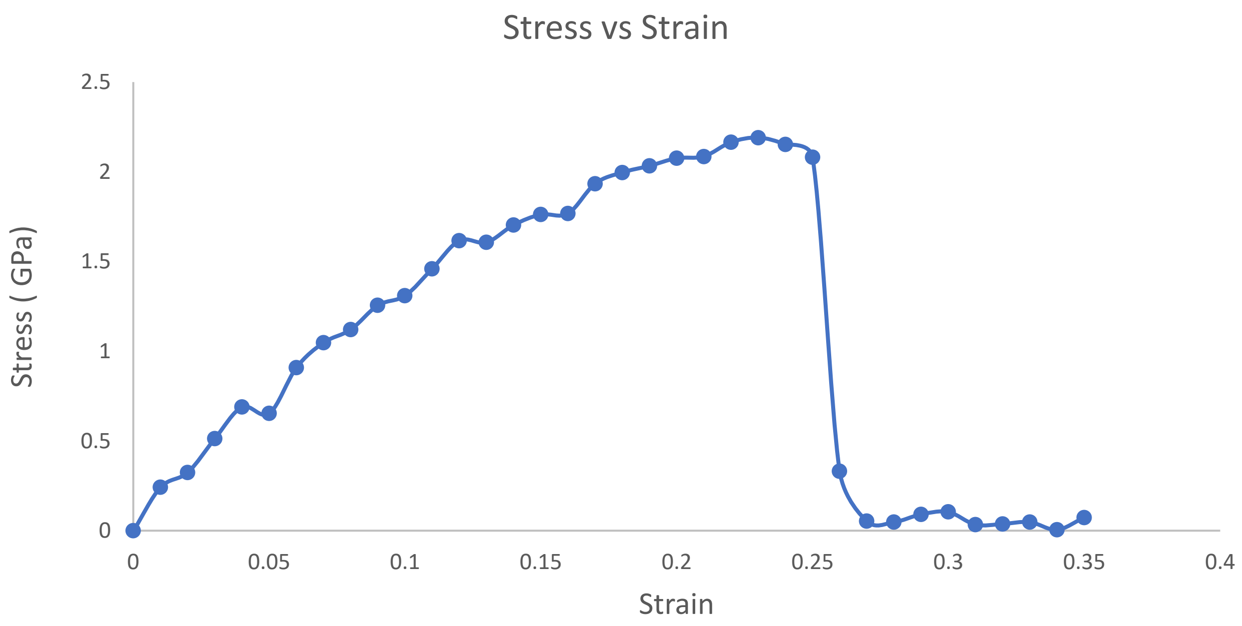
Mechanical Properties of PLA



From simulation, the PLA has shown young's modulus of 2.085 GPa and tensile strength of .26 GPa obtained from the stress strain diagram (fig 13). Diagram is generated from the dataset of strain and pressure tensor obtained from the simulation (Appendix A). This graph shows that, the elastic region of PLA continues up to around .15 GPa. From this point onward plastic region of PLA continues.

Result and Analysis

Mechanical Properties of PLA-CNT Nanocomposite

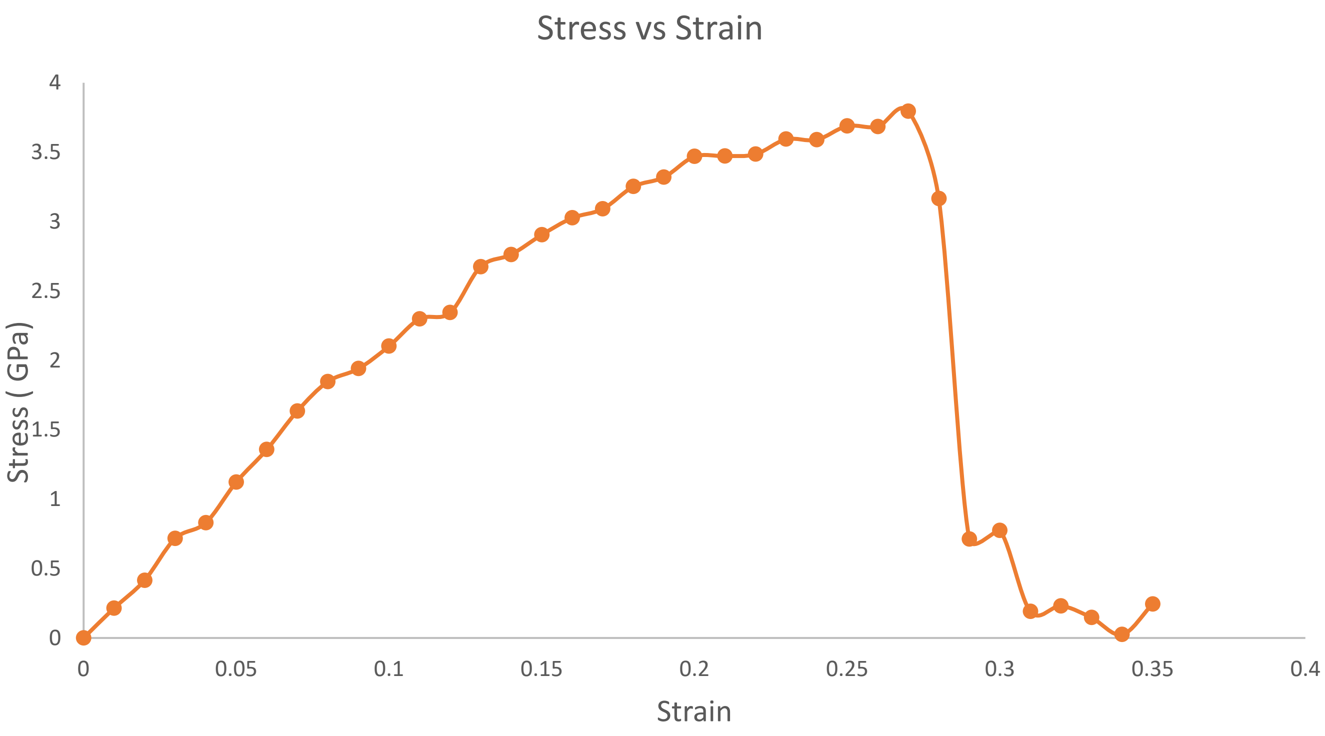


12.76% PLA-SWNT (3,6):

Amorphous packing of PLA and (3,6) SWNT undergoing simulation resulted in 14.811 GPa of young's modulus and 2.19 GPa of tensile strength. Result is obtained from the stress strain diagram is (fig 14) constructed from dataset of strain and pressure tensor obtained from the simulation (Appendix A). A catastrophic failure occurred at 0.25 strain thus the stress-strain curve is formed.

Result and Analysis

Mechanical Properties of PLA-CNT Nanocomposite

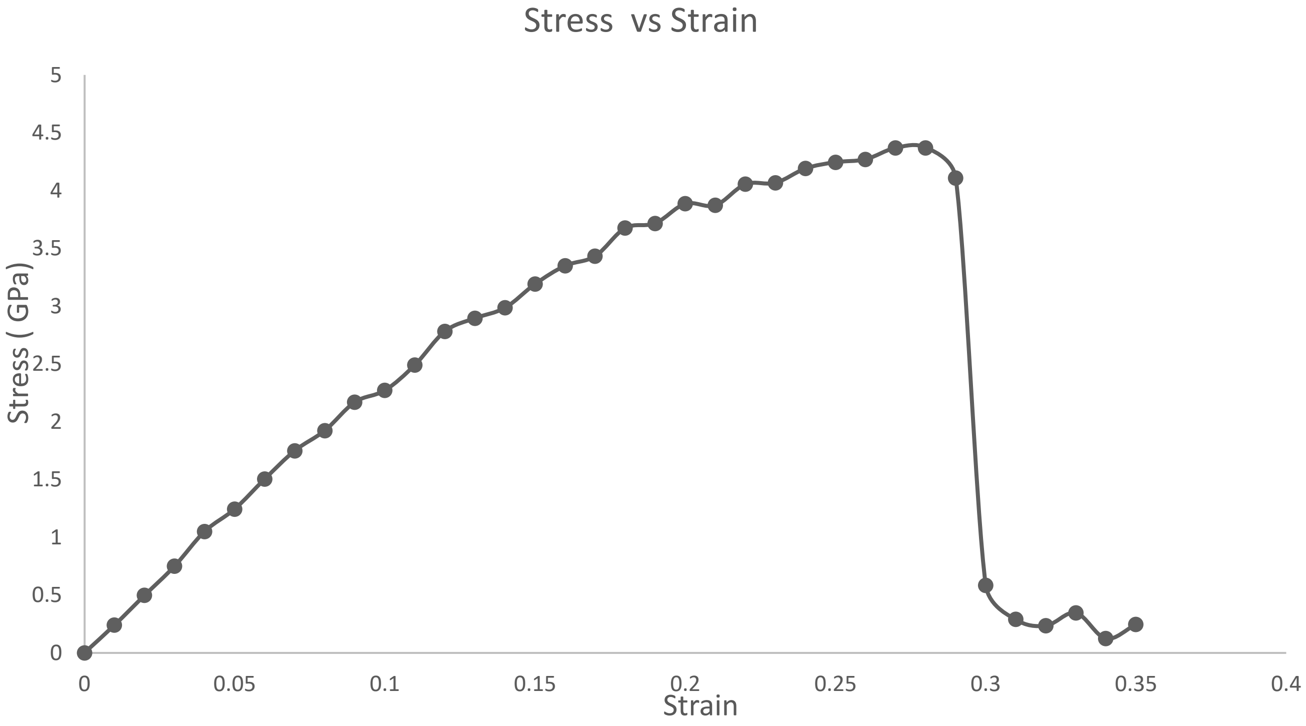


13.60% PLA-SWNT (6,9):

Amorphous packing of PLA and (6,9) SWNT undergoing simulation resulted in 22.795 GPa of young's modulus and 3.79 GPa of tensile strength. Result is obtained from stress strain diagram (fig-15) constructed from dataset of strain and pressure tensor obtained from the simulation (Appendix A). A catastrophic failure occurred at 0.28 strain thus the stress-strain curve is formed.

Result and Analysis

Mechanical Properties of PLA-CNT Nanocomposite



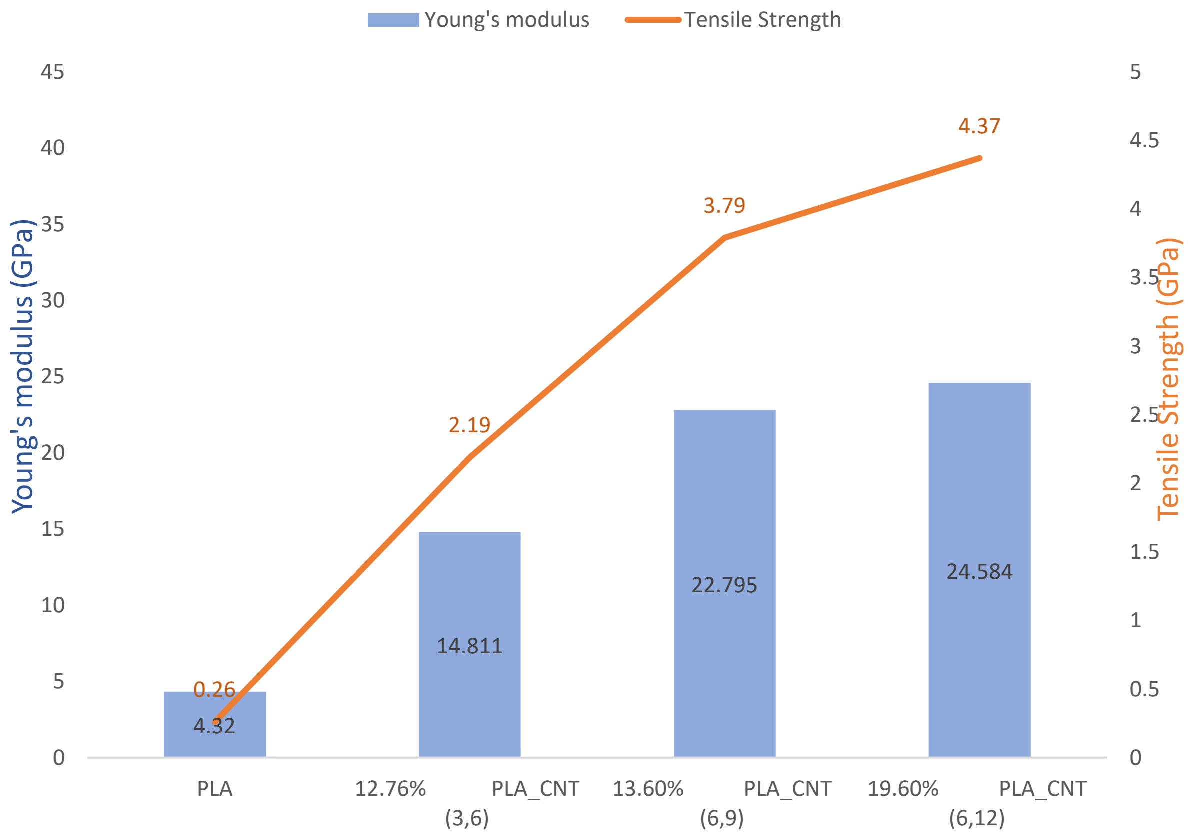
19.60% PLA-SWNT (6,12):

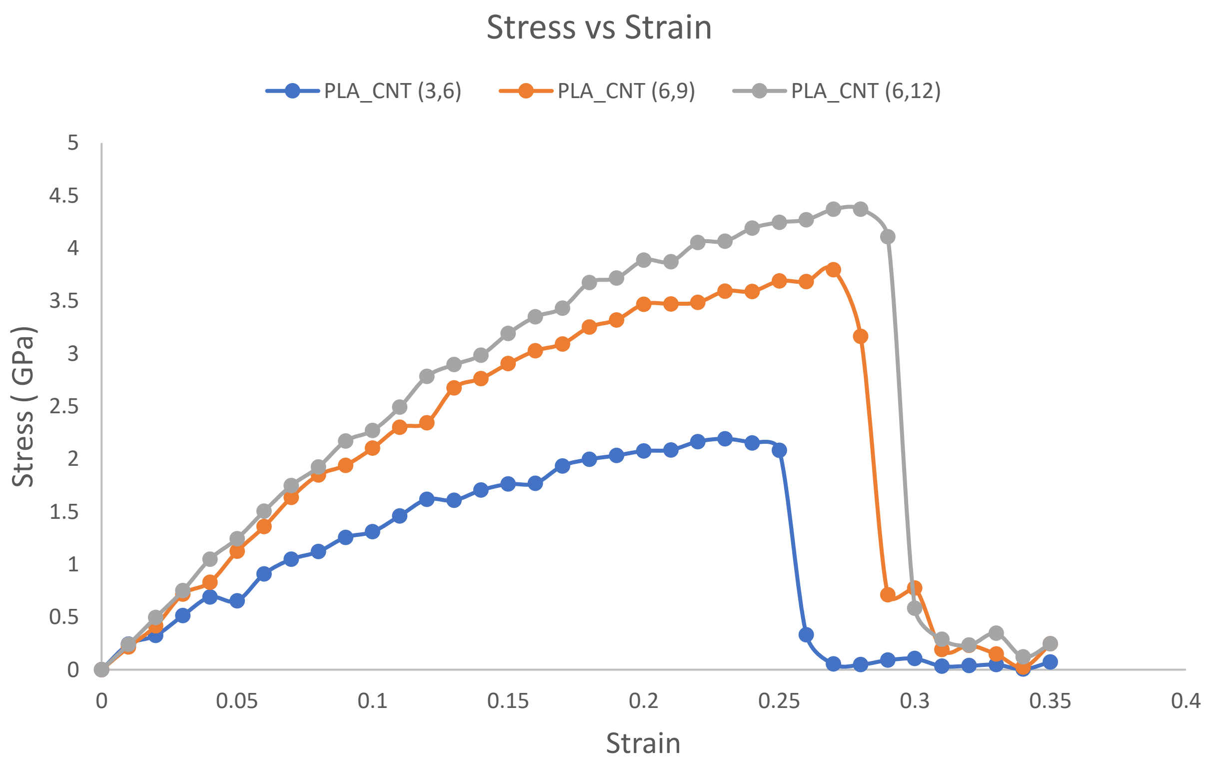
Amorphous packing of PLA and (6,12) SWNT undergoing simulation resulted in 24.583 GPa of young's modulus and 4.37 GPa of tensile strength. Result is obtained from stress strain diagram (fig-16) constructed from dataset of strain and pressure tensor obtained from the simulation (Appendix A). A catastrophic failure occurred at 0.29 strain thus the stress-strain curve is formed.

Result and Analysis

Result Comparison

The values of Young's modulus and tensile strength increased in composite from the polymer. The value of Young's modulus and tensile strength increased with the increment of CNT reinforcement denoted as volume fraction. The comparison is illustrated in fig-1 and fig-2.





Result and Analysis

Discussion

PLA polymer resulted 2.085 GPa in young’s modulus and .26 GPa in tensile strength. In PLA-CNT nanocomposite the Young’s modulus resulted in 14.811 Gpa, 22.795 GPa, 24.583 GPa and the tensile strength resulted in 2.19 GPa, 3,79 GPa, 4,37 GPa. The young’s modulus increased around 7.1 to 11.79 times and tensile strength increased around 8.4 to 16.8 to the value of PLA polymer which is the result of incrementing the volume fraction of CNT reinforcement in PLA. This indicates enhancement of mechanical property in terms of young’s modulus and tensile strength when the PLA is reinforced with Carbon nanotube.

Conclusion and Recommendation

PLA-CNT nanocomposite is constructed and packed in amorphous cell to perform uniaxial tensile deformation by molecular dynamics simulation. MD simulation showed that, compared to pure PLA, the Young's modulus of the composite greatly improved by the factors of 7.1 to 11.79 and tensile strength increased by the factors of 8.4 to 16.8 with incorporating different volume fraction of CNT. With the increment of volume fraction the contact surface area of CNT with PLA increases, which is responsible for significant enhancements in mechanical properties.

This study indicates that, different types of PLA-CNT nanocomposites with desired load carrying capacity can be manufactured. This creates an opportunity to perform new use of PLA. In the field of bio-medical healthcare sector and additive manufacturing, application of PLA will obtain a new dimension in the form of PLA CNT nanocomposite with this enhanced mechanical property.

However, thermal and electrical properties of PLA CNT nanocomposite are considered before making filament out of it. To implement this mechanically enhanced composite in 3D printing technology those properties are also important to explore.

The composition of the nanocomposite is another important factor. Cost of CNT and the method of mixing compared with the overall improvement of the nanocomposite is to be considered. An optimum ratio considering all above stated factor is the key to achieve the goal.

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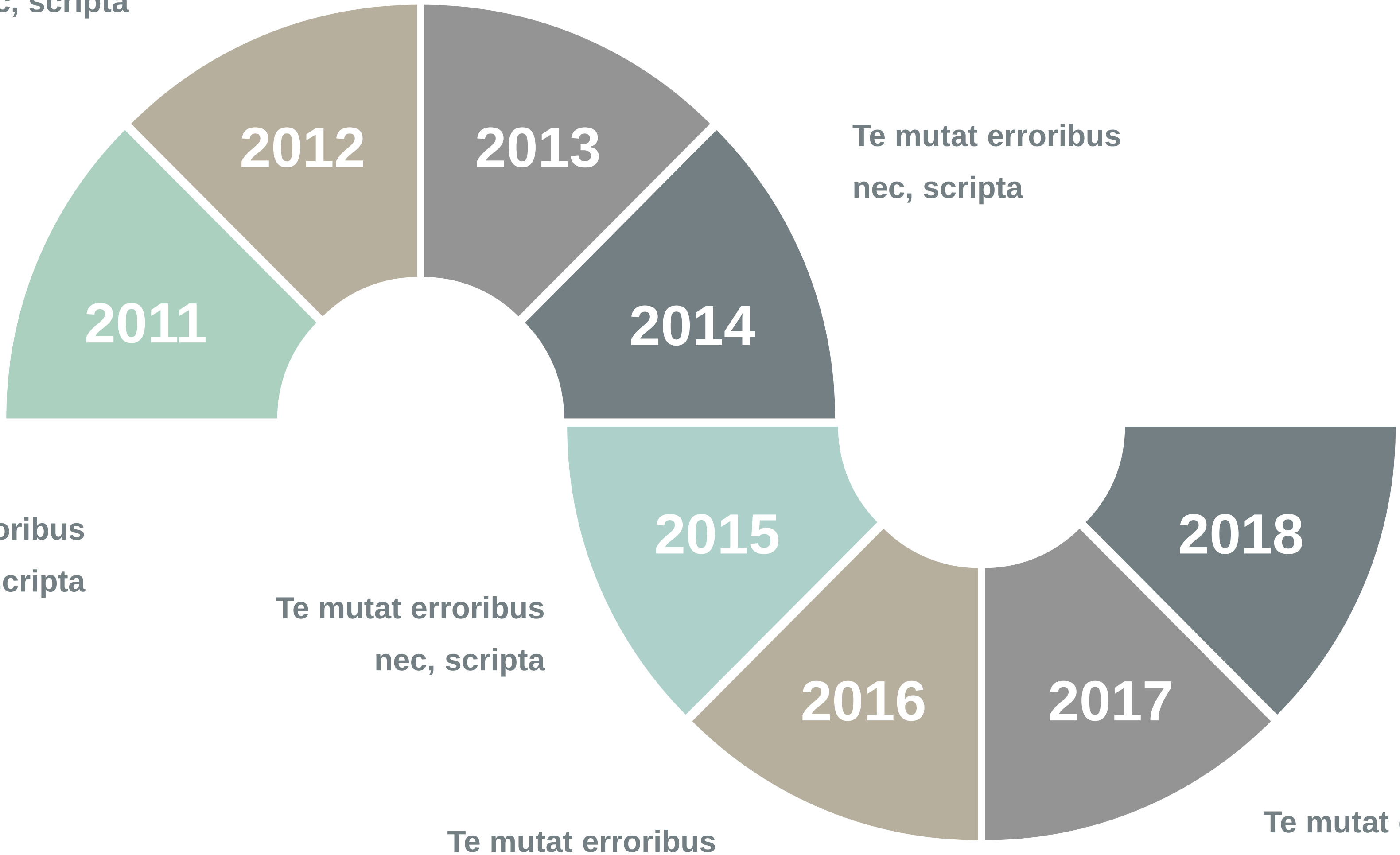

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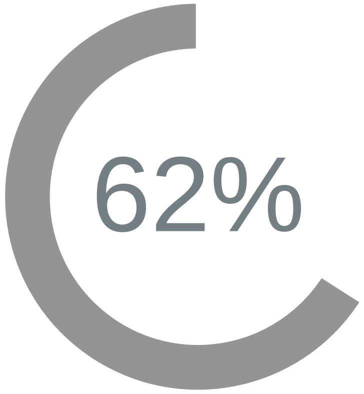

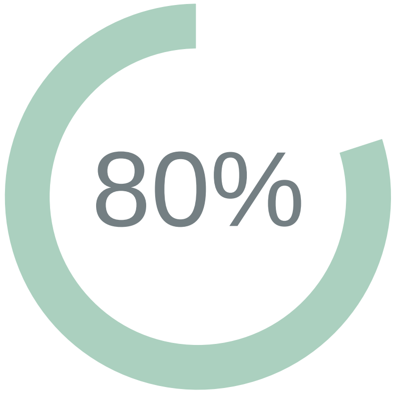

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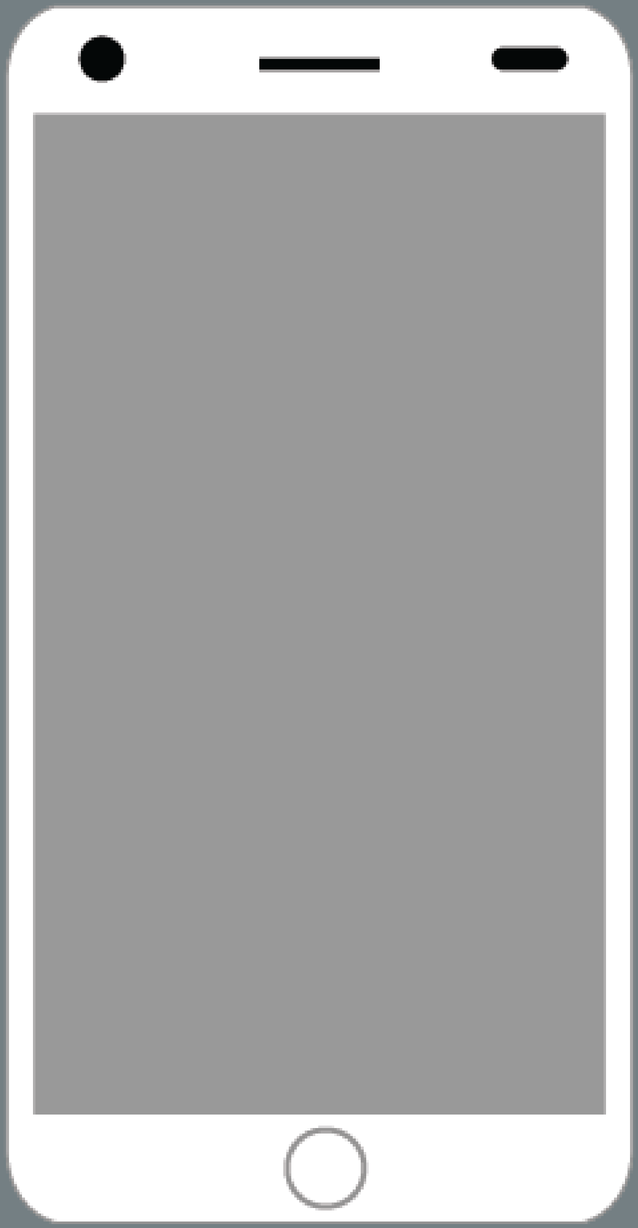

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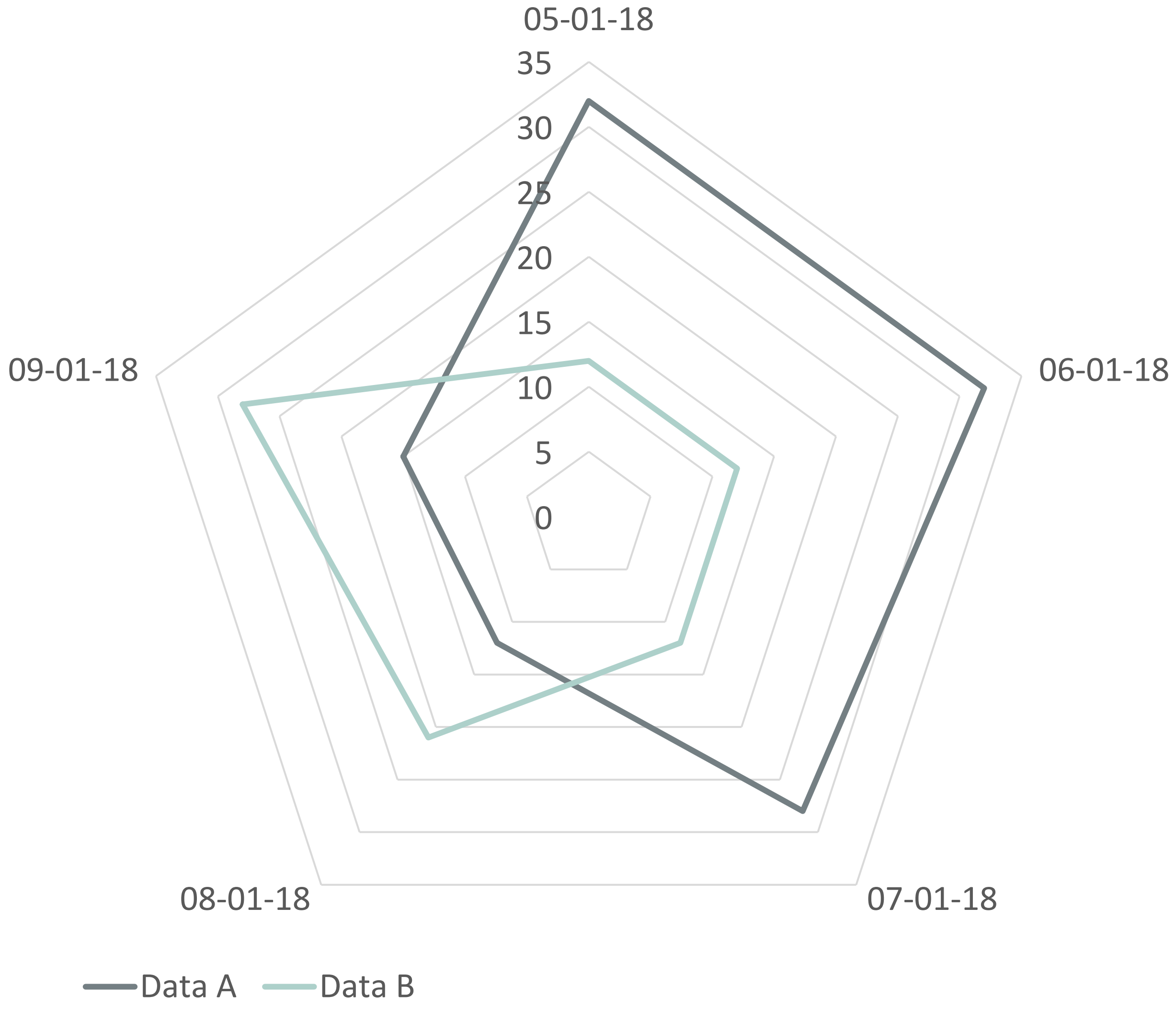

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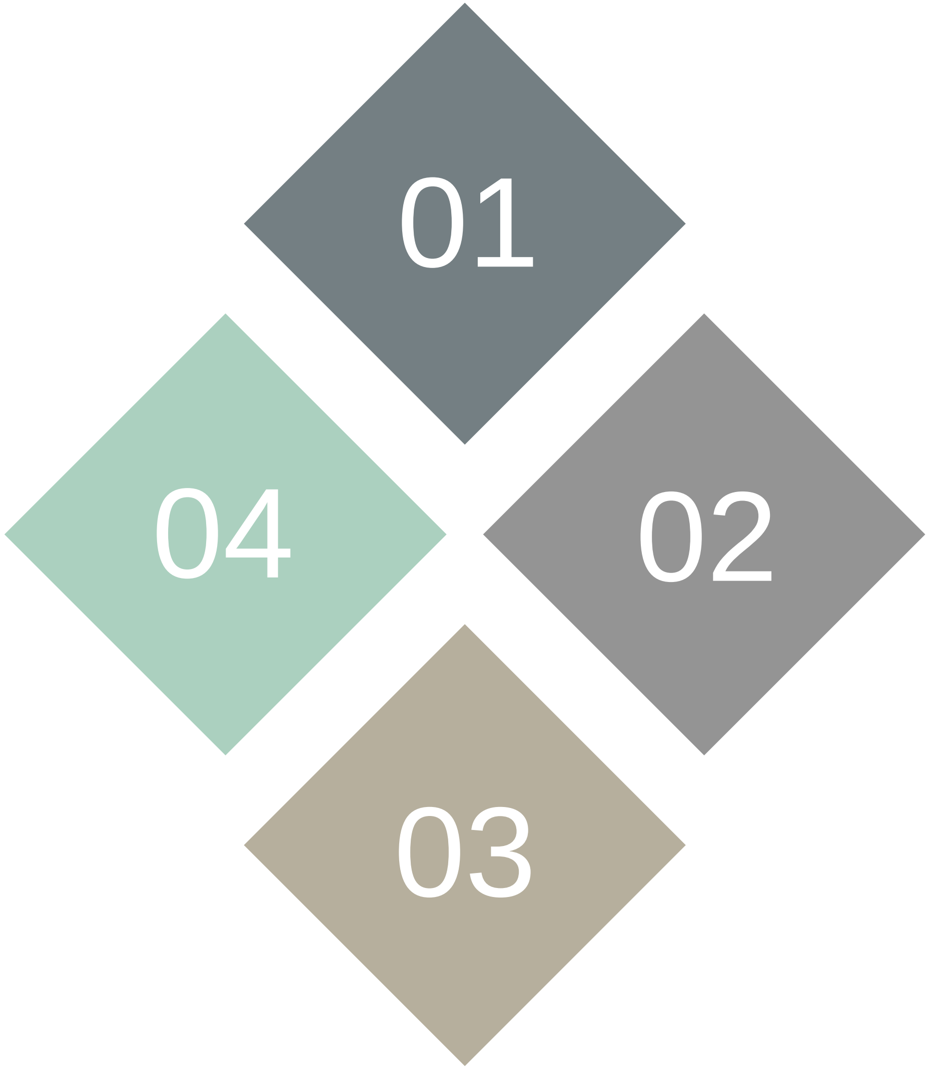

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