ADDIS ABABA UNIVERSITY

ADDIS ABABA INSTITUTE OF TECHNOLOGY

SCHOOL OF MECHANICAL AND INDUSTRIAL ENGINEERING

NUMERICAL DETERMINATION OF THE EFFECT OF FILLER VOLUME FRACTION, GEOMETRY, AND TEMPERATURE ON THERMAL AND MECHANICAL PROPERTY OF POLYMER NANOCOMPOSITES.

The thesis was submitted to the school of Mechanical and Industrial Engineering of Addis Ababa University in partial fulfillment of the requirements for the degree of Masters of Science (MSc.) in Mechanical Engineering (Mechanical Design Stream).

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Declarations

This is to certify that the thesis presented by Abrahaley Eukubay entitled "**numerical determination of the effect of filler volume fraction, geometry, and temperature on thermal and mechanical property of polymer nanocomposites"** and submitted to the school of Mechanical and Industrial Engineering of Addis Ababa University in partial fulfillment of the requirements for the award of the degree of Masters of Science (MSc.) in Mechanical Design Engineering with the regulation of the University, and meet the accepted standards concerning of the originality and quality.

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ABSTRACT

Some of the engineering materials cannot be standalone for specific applications due to certain limitations of their property. To overcome this limitation, different constitutes mix with other materials to produce a composite material with a shared property for desired engineering applications. For example, polymer material's low thermal and mechanical property is solved by incorporating nanofillers with different volume fraction and shapes. In such cases, the performance is determined by the combined effect of the inclusion's geometry, volume fraction, and operating temperatures. Understanding the role of nanoparticle distribution, size, geometry, and temperature on polymer nanocomposites' thermal and mechanical properties help to design materials with infallible mechanical and thermal behaviors.

In this work, the role of nano silicate particle volume fraction, geometries/aspect ratio, and the working temperature on the effective thermal conductivity and elastic modulus of the epoxy matrix composites are analyzed numerically using the finite element method and mean-field homogenization approaches. The result furtherly validates with analytical models and experimental results taken from the literature.

The effective thermal conductivity and young modulus of the polymer nanocomposite material are increased with the increasing of the nano silicate volume fraction within the epoxy matrix. Besides, ellipsoid nano silicate particles give more improved properties than spherical nanoscopic inclusion of the same volume fraction. The proposed finite element method was effective in estimating the effective thermal conductivity of the composite material for both spherical and ellipsoidal geometries of nanoscopic fillers. On the other hand, the analytical model better predicted the composite material's effective young modulus of spherical inclusions.

The effect of temperature on the nanocomposite's effective thermal conductivity and modulus of elasticity is also estimated following similar approaches. The nanocomposite's effective thermal conductivity of the polymer composite material increases with temperature, but the effective modulus of elasticity/stiffness decreases with temperature.

Keywords: numerical, nanocomposite, filler volume fraction, thermo-mechanical property.

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NOMENCLATURE

PNCM - Polymer nanocomposite material

ITR - Interphase thermal resistance

K_{cm} - Effective thermal conductivity

K_i - Thermal conductivity of the interphase

ψ - a factor that determines the maximum possible amount of particle,

ϕ - Volume fraction,

C - Shape factor of particle or constants that depends on the shape, orientation, and aspect ratio,

ϕ_{max} - Maximum packing fraction,

r_p - Radius of the filler

t - Thickness of the polymer layer around the particle.

ϕ_f - Filler volume fraction of

ϕ_i - Volume fraction of the interphase layer around the filler in the composite particle.

E - Elastic modulus,

B - Constant take into account the relative elastic modulus of the particle and the base material,

k_e - Einstein`s coefficient

α- Aspect ratio

RVE - Representative volume element

MFH - Mean-field homogenization

FEM - Finite element method

$\langle\varepsilon\rangle^{(m)}$ - Average strain tensors of matrix phases

$\langle\varepsilon\rangle^{(p)}$ - Average strain tensors of particle phases

$\langle\sigma\rangle^{(m)}$ - Average stress tensors of matrix phases

$\langle\sigma\rangle^{(p)}$ - Average strain tensors of particle phases

$\langle\varepsilon\rangle$ - Macroscopic strain tensor

$\langle\sigma\rangle$ - Macroscopic stress tensor

$\overline{A}_{MT}^{(m)}$ - Mori -Tanaka matrix strain concentration tensor

$\overline{B}_{MT}^{(m)}$ - Mori -Tanaka matrix stress concentration tensor

$\overline{A}_{dil}^{(p)}$ - Dilute strain concentration tensor.

$\overline{B}_{dil}^{(p)}$ - Dilute stress concentration tensor

∇T - Thermal gradient vector

q - Heat flux vector

$\overline{A}$ - Thermal gradient concentration tensor

$\overline{B}$ - Heat flux concentration tensor.

I - Identity tensor

E_p - Elastic modulus tensor of the particle

E_m - Elastic modulus tensor of the matrix

S - Eshelby's stiffness tensor

E_{cm} = Effective elastic modulus tensor of the composite material

K_p - Thermal conductivity tensor of particle

K_m - Thermal conductivity tensor of matrix

R_m - Resistivity tensor

K_{CM} - Effective thermal conductivity tensor of the composite material

α - Coefficient of thermal expansion

$\overline{\alpha}$ - Coefficient of thermal expansion tensor

ΔT - Temperature change.

CHAPTER ONE

1. INTRODUCTION

1.1. Background

Some of the engineering materials cannot be standalone for specific applications due to certain limitations of their property. To overcome this limitation, different constitutes mix with other materials to produce a composite material that imparts a shared property for required specific engineering applications [1]. Based on the type of constituents, the composite material can be a polymer, ceramic, or metal matrix particle reinforced composite material [2]. Moreover, polymer materials are weak in their properties, then they are filled with nano inclusions to produce polymer nanocomposites [3]. Polymer nanocomposites are composite material in which the nanoscopic inorganic particles are spread in the polymer matrices to improve their mechanical, and thermal properties. Meanwhile, the type, geometry, property, state of dispersion, filler-matrix interaction, and loading of filler material determine the specific application required to accomplish, the type of matrices used, and the desired property of polymer nanocomposite [4].

Different type of nanofillers was used by many researchers to enhance the property of polymer composite. The silica nanoparticle, carbon nanotube, and copper oxide are the most commonly used fillers. One of the crucial parameters used to estimate the enhancement of the desired property of polymer nanocomposite is the scattering state of a nanoscopic particle in the given polymer matrix. Depending on that, the formation of polymer nanocomposite can be classified into three possible structures of polymer composites. A separate phase is obtained for not intercalated the polymer chain between the nanofiller and this has a similar property with traditional polymer composite. But, when the nanofiller dispersed between the polymer chain and creates a well-ordered layer, an intercalated nanocomposite is obtained with the improved property. However, the exfoliated structure of nanocomposite is obtained by uniformly dispersed the nanoscopic filler in the matrix and yields the best property over other types of composites [2]–[5].

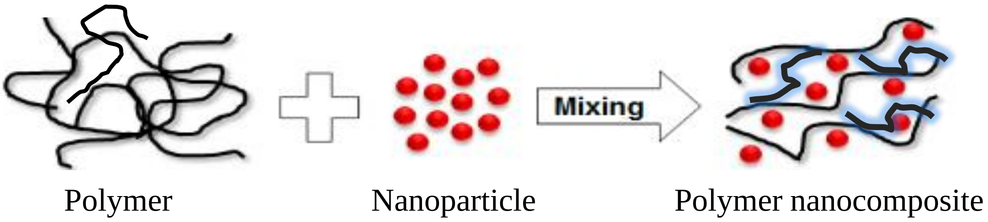

Figure 1 Esxfoliated nanocomposites [5].

The polymer nanocomposite materials are extensively used in many applications ranging from nanoelectronics to the aerospace industries due to their lightweight, high stiffness and strength, and corrosive resistance properties [6]. Besides, the thermally conductive polymer nanocomposite materials are used in electric motor and generator, heat exchanger, and power electronics to enhances heat dispassion performance [7]. Therefore, many study works have been done to improve the effective property of the composite materials and their results depicts the dependency of thermal or mechanical property of polymer nanocomposite material on nanoscopic filler volume fraction [8]–[13], type [4], [11], [14], property like thermal conductivity [15]–[17], geometry [8], [10], [13], [18]–[20], particle/matrix adhesion [9], interface thermal resistance (ITR), [17], [21], and aspect ratio [22], [23]. As per my knowledge, there is no numerical study regarding the combined effect of filler volume fraction, geometry, and operating temperature by considering the effect of interphase on the thermal and mechanical properties of polymer nanocomposites.

1.2. Statement of the problem

Polymer materials are widely used for electronic packaging, and insulating systems for X-ray tubes and high voltage applications, like cable termination, transformer, generator, and motors. [24]–[27]. However, they fail due to the mechanical and thermal loading and the electrical field stress during application [27]. Therefore, it is very important to enhance their thermal and mechanical performance by incorporating them with nanofiller at effective inclusion volume fraction, right inclusion geometry, and accepted operating temperature. Then, this systematic study helps to understand the combined effect of fillers to use the correct composite material for the desired specific application.

1.3. The objective of the research

1.3.1. General objective

The general objective of the research is to numerically determine the effect of filler volume fraction, geometry, and temperature on the thermal and mechanical properties of polymer nanocomposite materials.

1.3.2. Specific objective

The research has the following listed specific objectives to be achieved.

- Study the effect of nanofiller volume Fraction.
- Determine the influence of filler geometry.
- Study the effect of working temperature.

1.4. Scope of the research

The delimitation of the research is from review the literature up to validate the result of the combined effect of filler volume fraction, geometry, and temperature on the thermal and mechanical property of polymer nanocomposite materials to previous experimental or analytical research results.

1.5. Significance of the study

The polymer nanocomposite materials are used in different applications including microelectronics to the aerospace and automotive structural parts. This implies it is very significant to emphasize the production of improved composite material. Therefore, understand the role of nanofiller content, geometry, and operating temperature on the property of polymer nanocomposite material is one of the very crucial things. Then, this study is very significant to understand the effective combination of nanofiller volume fraction, geometry, and temperature to enhance the thermal and mechanical property of polymer nanocomposite materials, to able to select the correct material for the desired specific application.

1.6. Methodology

1.6.1. Data collection method

The important data used as an input for this research is gathered from the literature of previous research works available on the Internet or libraries.

1.6.2. Methodology for analysis

Many researchers use different methodologies for the analysis of nanocomposites materials. The analytical method, molecular dynamics method, multi-scale modeling method, mean-field homogenization method, and finite element method are the most commonly used methodology. In this research, the analytical method, mean-field homogenization (MFH) method, and finite element method (FEM) will be implemented for the analysis of polymer nanocomposite material using the analysis software of Digimat and ANSYS.

The main procedure of the methodology for analysis can be summarized in the following three parts.

Part I: Analytical Method

The analytical method is one of the micromechanics analyses for the determination of the effective elastic modulus and thermal conductivity of the polymer nanocomposite materials. The Three-Phase Lewis-Nielson (LN) and Three-Phase L.E. Nielson analytical model are suitable for the analysis of thermal conductivity and young modules respectively. Those analytical models permit to consider the nanoscopic effect and include different analysis parameters that designate the condition of the polymer matrix and the nanoscopic inclusions [28]-[29].

Part II: Mean Field Homogenization (MFH) method

Digimat – MF software is used to simulate and predict the effective thermal and mechanical properties based on the defined material properties, analysis type, mean-field homogenization scheme, loading type, suitable boundary condition, and nanostructure definitions. Finally, the result is extracting in the post-processor and interpret as well as validate with analytical and experimental results.

Part III: Finite Element Method (FEM)

The 3D representative volume element (RVE) is modeled using Digimat-FE with all the essential user-defined parameters. Then the generated microstructure geometry is imported to CAD Exchanger software to calibrate, assemble and save in Parasolid file type which is later imported in ANSYS workbench software for further analysis.

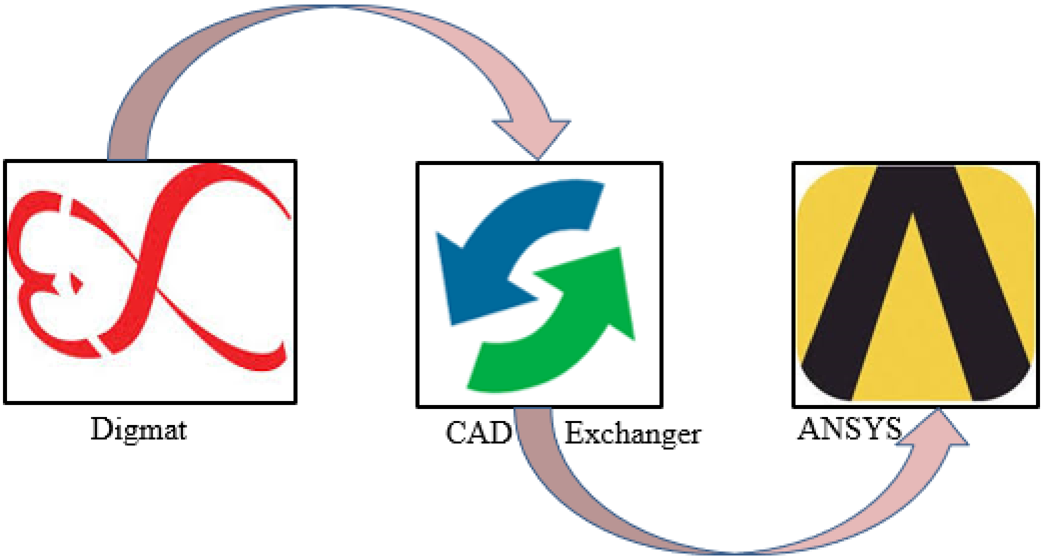

Figure 2 Methodology for Finite Element Analysis.

Generally, all the contextual frame for analysis is summarized in the following chart.

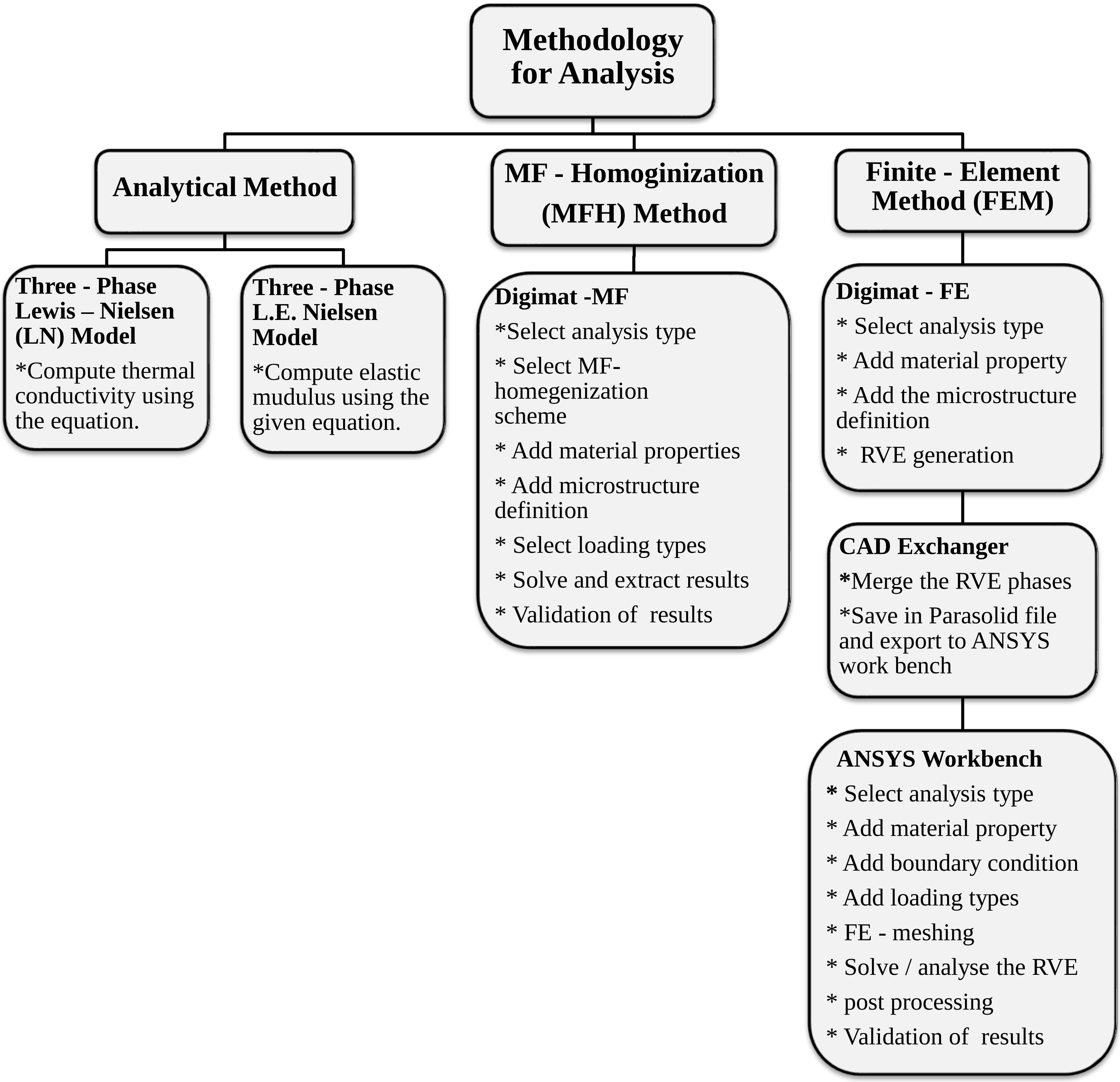

Figure 3 Methodology for Analysis.

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CHAPTER TWO

2. LITERATURE REVIEW

A. Tessema et al. have studied the effect of filler loading, geometry, dispersion, and operating temperature on the thermal conductivity of polymer nanocomposite material. The polymer nanocomposite material sample is prepared from silica nanoparticle reinforced epoxy and carbon nanotube (CNT) reinforced epoxy. The linear unidirectional heat transfer device is used to measure the specimen's thermal conductivity (k). The result of silica nanoparticle reinforced epoxy shows that the thermal conductivity(k) quickly increases for both lower particle loading (< 2wt%) and higher particle loading (> 6wt %). But, the slop of thermal conductivity (k) between the aforementioned percentage weight ratio is reduced by some percentage due to the clustering effect of the particle. The thermal conductivity (k) of carbon nanotube (CNT) reinforced epoxy increases for lower loading (< 4wt %) and decreases beyond the stated percentage weight ratio due to the clustering/agglomeration of particles. The paper also depicts, the state of dispersion of fillers and operating temperature have a direct relation with the thermal conductivity (k) of polymer nanocomposite material [8].

Z. Z. Wang et al. have determined the effect of inclusion volume fraction on the mechanical property of the polymer nanocomposite material. The sample material is prepared from silica of 20 nm average size and epoxy resin by the sol-gel technique. The nano-indentation test with the 1nN load resolution and 0.0002 nm displacement resolution is conducted to determine the elastic modulus of the composite material. The indentation result depicts, the addition of 15 percent of silica particle volume fraction at a well-dispersed state is contributed to enhancing the elastic modulus of composite material from 2.5134 GPa to 3.5117 GPa or by 40 %. The resulted local mechanical property of the sample material is extracted by using high-quality resolution scanning probe microscopy (SPM) [30].

T. Evgin et al. have experimentally investigated the effect of both aspect ratio and percentage weight ratio on thermal conductivity of high-density polyethylene /multi-walled carbon nanotube (MWCNT) nanocomposite. They have used two types of carbon nanotube (MWCNT) filler with the aspect ratio lie between 200-300 and 500-3000. The modulated photothermal radiometer (PTR) is used to measure the thermal diffusivity, density, and specific heat capacity of the sample prepared by melt mixing and then compression molding. The value of thermal diffusivity, density, and specific heat capacity are used to determine effective thermal conductivity. The experimental result of the two specimens with higher and lower aspect ratio shows that the effective thermal conductivity increases with the increment of the percentage of weight ratio of carbon nanotube (MWCNT). However, the thermal conductivity of polymer nanocomposite with a higher aspect ratio of filler is higher than that of polymer nanocomposite with a lower aspect ratio of filler which is enhanced three to four times [23].

S.Y. Fu et al. have reviewed the effect of particle size, particle-matrix interphase adhesion, and particle loading on the mechanical property of particulate-reinforced polymer composite. The paper reviewed and conclude by comparing and evaluating the different experimental results and theoretical models. It's result shows that the particle-matrix adhesion greatly affects the strength and toughness of composite material than particle size and loading. This is because the adhesion controls the toughness or brittleness property and also determines the effective stress transfer. However, the particle loading has more influence on the stiffness of polymer nanocomposite material than that of the particle-matrix adhesion. This is due to, the modulus of nanoscopic filler material is much larger than the polymer matrix. Besides, the stiffness greatly enhanced for nanoscale particle size reinforced composite [9].

Kutvonen et al. have studied the influence of nanoparticle size, loading, and shape on the mechanical property of polymer nanocomposite using molecular dynamic simulations. The result shows that the composite material of small-size nanoparticles is toughest than the composite material of medium and large-sized nanoparticles. This is because of the greater particle-matrix adhesion for a large surface-to-volume ratio. When the weight ratio of filler increases, it enhances the number of particle-monomer interactions which improves the strength of the matrix. However, the further increment of filler loading increases the formation of weak particle-particle interaction which reduces the strength of polymer nanocomposite material. Finally, the elastic modulus of polymer material reinforced with a nanoscopic filler of three different geometry is determined at both 15% and 27% of loading. the result depicts that the polymer material reinforced with rod-liked nanoscale filler has the highest elastic modulus than the polymer material filled with the spherical and triangular shape of nanoscopic filler. Meanwhile, the polymer material reinforced with the triangular shape of the nanoparticle shows the best performance [10].

T. Imai et al. have conducted experimental research to explore the effect of temperature on the mechanical property of layered silicate reinforced nanocomposite. The morphology of nanoparticles in the polymer matrix is determined by using a transmission electron microscope (TEM) and the result shows that the specimen the polymer nanocomposite has an intercalated type in which the polymer chain has distributed between the filler layers. The result of dynamic mechanical analysis (DMA) from the temperature of 25 C^0 and 250 C^0 shows that the polymer (base epoxy resin) has lower thermal resistance than the nanocomposite. Consequently, the layered silicate reinforced epoxy nanocomposite has a 32.5 MPa higher storage modulus at 200 C^0 [31].

M.F. Omar et al. have conducted experimental and numerical predictions of the effect of loading rate and particle geometry on the compressive property of polymer nanocomposite material. The two specimens were prepared in different shapes for static and dynamic compression tests. However, the specimen was examined using a field emission scanning electron microscope to check for any initial surface fracture or flaws. Finally, coated with gold-palladium to remove the effect of the electron charge. The conventional universal testing machine is used for static compression tests whereas the split Hopkinson pressure bar (SHPB) is used for dynamic compression tests. The finding shows that the loading rate affects the compressive property. The drum and rod shape of the nanofiller (Zinc Oxide) helps to smoothly transfer between nanoparticle and polymer which enhances the strength and stiffness of the polymer nanocomposite material. But there is no smooth transfer of applied stress for both flake and needle-shaped nanoscopic filler. Consequently, the strength and stiffness of the polymer nanocomposite material are reduced [12].

Many experimental, analytical, empirical, and numerical research works have been done in the last decades regarding polymer nanocomposites. Consequently, they have explored the influence of nanofiller volume fraction, geometry, state of dispersion, type, and particle-matrix adhesion on the thermal or mechanical property of polymer nanocomposite material. Some of the studies consider the effect of thermal boundary resistance (TBR) to investigate the effect of filler on the thermal property of the improved composite material. However, there are no research works on the determination of the combined effect of nanofiller volume fraction, geometry, and operating temperature on the thermal and mechanical properties of polymer nanocomposites material.

CHAPTER THREE

3. MATERIALS AND ANALYTICAL METHODS

3.1. Materials

Composite materials are a combination of two or more engineering materials that imparts a common property under a specific engineering application. Therefore, its main purpose is to have a new engineering material with enhanced macroscopic or effective material properties. The composite material can be particle reinforced or fiber-reinforced of the given type of matrix. The matrix material that is required to improve its property can be polymer, ceramic, and metal. The polymer matrix composites are particle-reinforced materials that are attractive for an engineering application due to their enhanced effective property with a lighter weight compared to their base material, conventional metals, and ceramics [32]-[33].

3.1.1. Epoxy Resin (Polymer Matrix)

Epoxy resin is the most common type of thermoset polymer that is used as a matrix to produce a polymer matrix composite material due to its excellent mechanical property, thermal stability, and electrical insulation. Unless otherwise, reinforced with other constituent material, epoxy is an intrinsically brittle material [34]-[35]. The epichlorohydrin and bisphenol - A are the basic component of epoxy resin [36]. According to C. P. Wong and R. S. Bollampally [37], the epoxy resin has excellent interfacial adhesion with the silica filler that gives higher elastic modulus and an acceptable increment on the thermal conductivity of the composite material.

3.1.2. Silica (Nanoscopic Filler)

Silica is an inorganic ceramic material that is used as filler material for the polymer matrix to enhance the effective property of the polymer composite material. Inorganic filler reinforced polymer nanocomposite materials are essential for a high voltage insulation system that improves the performance of the equipment [38]. The performance of the high voltage electrical equipment is enhanced by increasing the thermal and mechanical properties of the insulating material. The insulating material is usually subjected to high shear stress and vibration under high thermal loading. These mechanical stresses cause crack instigation and propagation with electric discharge and disastrous failure [39]. Not only the mechanical strength but the heat management of the stator slot is also another problem that requires insulating material with improved thermal conductivity [7]. Therefore, using the polymer nanocomposite materials for an insulating system is one of the undoubted methods of achieving the requirement. For instance, P. Gropper et al. [40] showed that using nanoscopic spherical Silica reinforced epoxy for the stator winding insulation system of large hydro generators and turbines outcomes good enhancement of the effective thermal and mechanical properties with high resistance to electrical stress.

Many experimental research works have been done on the determination of the thermal and mechanical properties of the inorganic nanoscopic filler reinforced polymer matrix composite materials. A. Tessema et al. [8] and R. Kochetov et al. [41] have studied the nano-effect on thermal conductivity of the silica-reinforced epoxy that gives an excellent improvement in the effective property of the composite material for lower filler loading. Moreover, C. P. Wong and R. S. Bollampally [37] and Z. Z. Wang et al. [30] also studied its elastic modulus and conclude that, the material experiences excellent enhancement in its effective young's modulus due to the strong interfacial adhesion between the constituents. Accordingly, these materials are selected to use for this research work to study the effect of particle volume fraction, geometry, and temperature on the thermal and mechanical properties of the composite material. Meanwhile, the nanoscopic silica particle with an average size of 15 and 20 nm is analyzed at different aspect ratios and volume fraction to comprehend the effects on the effective properties of the composite material.

3.2. Analytical Model

The effective thermal conductivity and elastic modulus of the three-phase composite material is a complex function of different parameters and the result vary based on the geometry/aspect ratio of the constituent, the thermal and mechanical property of the filler and matrix phases, the dispersion state of the filler within the matrix, the interphase between particle and matrix [42], the interaction between particles, and the volume fraction [43]–[46]. Since it is very crucial to estimate the property of the composite material for the given property of fillers and matrices. Therefore, the micromechanics models are normally developed to analyze the composite material on the level of individual constituents.

3.2.1. Thermal Conductivity Model

The research work on the estimation of the effective property of the composite material has been some difficult until Maxwell proposed the analytical model for the estimation of effective thermal conductivity (K_{cm}). Thereafter, several studies have been conducted to estimate the effective property of the composite material reinforced with inclusions dispersed within the matrix of base material and find out the analytical expression for prediction of its thermal conductivity. They mainly relate the effective thermal conductivity (K_{cm}) with the geometry of the particle, percentage weight fraction, the state of dispersion, and the physical property of fillers. One of the most prominent and important thermal conductivity models is the three-phase Lewis-Nelsen model [47].

3.2.1.1. Three - Phase Lewis – Nielsen (LN) Model

Many previous studies depict that the effective thermal conductivity of a polymer nanocomposite material was enhanced by reinforced the polymer with a different type of fillers and then the thermal conductivity model of two-phase material was suggested. One of the prominent thermal conductivity models is the Two-Phase Lewis – Nielsen (LN) Model. This model for effective thermal conductivity is adopted from the Halpin – Tsai (HT) mechanical model [48]. It is simple and applicable to different filler shapes and sizes. It is also considering the highest amount of inclusion volume fraction for a different type of packing. According to Lewis – Nielsen's theory for the composites, the effective thermal conductivity is given by [49].

$$K_{cm} = K_m \left(\frac{1 + CD\phi_f}{1 - D\psi\phi_f}\right) \tag{1}$$

$$\text{Where } D = \frac{K_f - K_m}{K_f - CK_m}$$

$$\psi = 1 + \left(\frac{1 - \phi_{max}}{(\phi_{max})^2}\right)\phi_f$$

E_{cm} is the thermal conductivity, ψ is a factor that determines the maximum possible amount of particle, ϕ is a volume fraction, C is a shape factor of particle or constants that depends on the shape, orientation or aspect ratio, ϕ_{max} is a maximum packing fraction, and the subscript f, and m are for filler and matrix respectively.

The above two-phase model does not include the effect of interphase thermal resistance (ITR) caused by the mismatch in thermal expansion and weak chemical adhesion of the base material to the filler surface in polymer nanocomposite material. Consequently, there is ineffective phonon transportation via the interphase layer which is known as kapitza resistance of an interphase boundary. This resistance causes discontinuity of temperature at the particle-matrix interphase. Assume, the effective particle and the interphase layer around it together to be a composite particle (CP) in figure 4. Therefore, it has the size of the effective particle and the thickness of the interphase around it. Mathematically, given by, [41].

$$r_{cp} = r_p + t$$

$$\mathrm{r_{cp}} = \mathrm{r_{ep}} + \mathrm{t_i} \tag{2}$$

Where, $\mathrm{r_{cp}}$ is composite particle radius, $\mathrm{r_{ep}}$ is effective silicate particle radius and $\mathrm{t_i}$ is the thickness of the interphase.

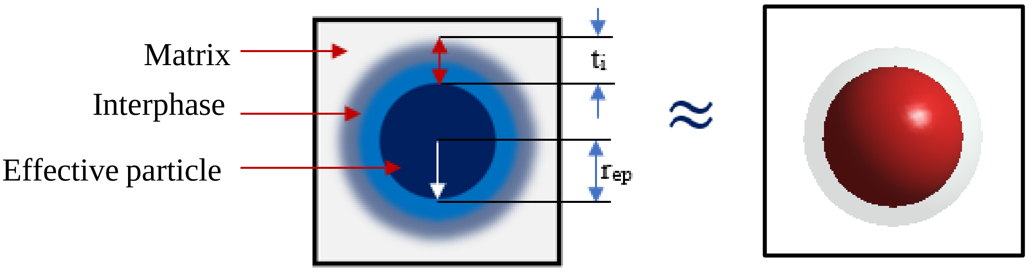


Figure 4 Composite particle embedded in the epoxy matrix.

The thermal conductivity of the composite particle ($\mathrm{K_{cp}}$) is computed according to the series model for a composite material in which the interphase thermal resistance is in series with effective particle thermal resistance and the relation is given by [8], [41].

$$\mathrm{K_{cp}} = \left(\frac{1}{\frac{\phi_{ep}}{\mathrm{K_p}(\phi_{ep} + \phi_i)} + \frac{\phi_i}{\mathrm{K_i}(\phi_{ep} + \phi_i)}} \right) \tag{3}$$

Where, $\mathrm{K_p}$ is the thermal conductivity of the particle, $\mathrm{K_i}$ is the thermal conductivity of the interphase, ϕ_{ep} is the volume fraction of effective silicate particle, and ϕ_i is the volume fraction of the interphase layer around the effective silicate particle within the composite particle.

The volume of a composite particle ($\mathrm{V_{cp}}$) with spherical nanofiller is given by,

$$\mathrm{V_{cp}} = \frac{4}{3}\pi(\mathrm{r_{cp}})^3$$

$$\mathrm{V_{cp}} = \frac{4}{3}\pi(\mathrm{r_{ep}} + \mathrm{t_i})^3$$

$$\mathrm{V_{cp}} = \frac{4}{3}\pi(\mathrm{r_{ep}})^3 \left(1 + \frac{\mathrm{t_i}}{\mathrm{r_{ep}}}\right)^3$$

$$\mathrm{V_{cp}} = \mathrm{V_{ep}} \left(1 + \frac{\mathrm{t_i}}{\mathrm{r_{ep}}}\right)^3 \tag{4}$$

Therefore, the volume fraction of the composite particle (ϕ_{cp}) is given by,

$$\phi_{cp} = \phi_{ep} \left(1 + \frac{\mathrm{t_i}}{\mathrm{r_{ep}}}\right)^3$$

$$\phi_{cp} = \phi_{ep}\delta \tag{5}$$

where ϕ_{ep} is the volume fraction of the effective particle.

$$\Rightarrow \ \delta = \left(1 + \frac{t_i}{r_{ep}}\right)^3$$

The volume fraction of the composite particle can be also written as, [50].

$$\left.\begin{array}{l} \phi_{cp} = \phi_{ep} + \phi_i \\ \phi_{cp} = \phi_{ep}\delta \end{array}\right\} \Rightarrow \phi_i = \phi_{ep}\delta - \phi_{ep}$$

$$\phi_i = \phi_{ep}(\delta - 1)$$

$$\phi_i = \phi_{ep}\left(\left(1 + \frac{t_i}{r_{ep}}\right)^3 - 1\right) \tag{6}$$

Since the chemical reaction between the silicate particle and epoxy interfaces causes the particle surface to decompose to some depth and mix with polymer material (matrix) to form the interface layer around the effective particle as shown in figure 4. Then the volume of the effective particle is smaller than the initial volume of the particle and computed as,

$$V_{ep} = \frac{4}{3}\pi\left(r_{ep}\right)^3$$

$$V_{ep} = \frac{4}{3}\pi\left(r_p - t\right)^3$$

$$V_{ep} = \frac{4}{3}\pi\left(r_p\right)^3\left(1 - \frac{t}{r_p}\right)^3$$

$$V_{ep} = V_p\left(1 - \frac{t}{r_p}\right)^3$$

The volume fraction of the effective particle is then given by,

$$\phi_{ep} = \phi_p\left(1 - \frac{t}{r_p}\right)^3 \tag{7}$$

The effective thermal conductivity of three-phase nanocomposite material is given by [28].

$$K_{cm} = K_m\left(\frac{1 + CD\phi_{cp}}{1 - D\psi\phi_{cp}}\right) \tag{8}$$

Where $D = \frac{K_{cp} - K_m}{K_{cp} - CK_m}$

$$\psi = 1 + \left(\frac{1 - \phi_{max}}{(\phi_{max})^2}\right)\phi_{cp}$$

K_{cm} is the effective thermal conductivity, ψ is a factor that determines the maximum possible amount of particle, ϕ is a volume fraction, C is a shape factor of particle or constants that depends on the shape, orientation or aspect ratio, ϕ_{max} is for maximum packing fraction and the subscript cp, and m denotes the composite particle and matrix, respectively.

3.2.2. Elastic Modulus Models

Similar to thermal conductivity, the young modulus is also a bulk property and it has been represented by an equivalent equation. Among the most notable equations for determining the young modulus of a polymer composite material are those developed by Guth, Einstein, Mooney, Thomas, Quemada, Frankle and Acrivos, Kerner, and Nielsen [51].

3.2.2.1. Three-Phase L.E. Nielsen Model

Halpin and Tsai found a well-known composite theory for determining the elastic modulus of particulate polymer composite material using the semi-empirical relationship that considers the particle geometry/aspect ratio and the matrix Poisson ratio. However, this general equation omits the important parameter that should be encompassed in the theory of elastic modules of particulate polymer composite systems. Nielsen modifies Kerner`s and Halpin – Tsai equation to take in the maximum packing fraction of the particle and suggested the following most general equation [29].

$$\mathrm{E_{cm}} = \mathrm{E_m}\left(\frac{1 + \mathrm{AB}\phi_{\mathrm{cp}}}{1 - \mathrm{B}\psi\phi_{\mathrm{cp}}}\right) \tag{9}$$

$$\text{Where } \mathrm{B} = \frac{\mathrm{E_{cp}} - \mathrm{E_m}}{\mathrm{E_{cp}} + \mathrm{A}}$$

$$\mathrm{A} = \mathrm{k_e} - 1$$

$$\psi = 1 + \left(\frac{1 - \phi_{\max}}{(\phi_{\max})^2}\right)\phi_{\mathrm{cp}}$$

The elastic modulus of the composite particle ($\mathrm{E_{cp}}$) is given by,

$$\mathrm{E_{cp}} = \left(\frac{1}{\frac{\phi_{\mathrm{ep}}}{\mathrm{E_p}(\phi_{\mathrm{ep}} + \phi_{\mathrm{i}})} + \frac{\phi_{\mathrm{i}}}{\mathrm{E_i}(\phi_{\mathrm{ep}} + \phi_{\mathrm{i}})}}\right) \tag{10}$$

$\mathrm{E_{cm}}$ is the overall elastic modulus, $\mathrm{E_i}$ is the elastic modulus of the interphase, ψ is a factor that determines the maximum possible amount of particle, ϕ_{ep} is a volume fraction of effective silicate particle, ϕ_{i} is a volume fraction of the interphase, and B is a constant take into account the relative elastic modulus of the composite particle and the base material, $\phi_{\max}$ is maximum packing fraction, A is shape factor, and $\mathrm{k_e}$ is Einstein`s coefficient.

The young’s modulus and volume fraction of interphase, and the volume fraction of effective particle as well as the composite particle, are computed by the analog relation given in the thermal conductivity analysis.

CHAPTER FOUR

4. MODELING AND SIMULATION APPROACHES

The finite element method and the mean-field homogenization techniques are the most common approaches applied for the simulation and determination of the effective property of a polymer nanocomposite material of different nanoparticle volume fractions, geometry/aspect ratio, and operating temperature. The aforementioned two simulation approaches are implemented in this research work using the ANSYS workbench and Digimat – MF, respectively.

4.1. Mean Field Homogenization Method

Micromechanics is a scientific discipline that is used to study the effective property of a multiphase (inhomogeneous) material and is determined as the average value of the corresponding micro field (RVE). Different homogenization method is implemented to determine the average property of the composite material [52]. Some of the most prominent analytical methods are Voigt, Reuss, Hashin- Shtrikman Bounds, Eshelby's, Self - Consistent, and Mori -Tanaka [53]. Moreover, the finite element analysis (FEA), generalized method of cells (GMC), and mechanics of structure genome (MSG) [54] are also some of the notable numerical approaches.

Digimat-MF is the composite material simulating tool based on the Mori-Tanaka or Interpolative Double Inclusion mean-field homogenization theories and it is very successful for determining the effective property of the polymer nanocomposite material depending on the user-defined pre-phase constituent material properties and the nano-effects like the interphase between inclusion and matrix, the interaction between fillers, and the clustering of the nanoparticle as well as its size distribution. It has a lower simulating time and gives approximate volume average values for the corresponding applied type of loads and boundary conditions [53],[55].

This research work is emphasized only in determining the effect of filler content, geometry, and temperature on the thermal and mechanical properties of polymer nanocomposites. To do these, only the mechanical and thermal type of analysis is considered for the given material properties. The pre-phase material property like density, thermal conductivity, and specific heat capacity are very essential to determine the effective thermal conductivity whereas the elastic parameter is used for calculating the effective young's modulus of the heterogeneous material.

Besides, the microstructure definition such as the phase-type, volume fraction, inclusion size, and shape also considered for both thermal and mechanical analysis.

4.1.1. Mori – Tanaka homogenization scheme

The mean-field homogenization (MFH) is a mean-field theory in which the effective or macroscopic property of the heterogeneous material is determined as the average value of the corresponding micro field (RVE). Therefore, the average stress and the average strain are given by the relation below.

$$\bar{\sigma} = \langle\sigma\rangle_{\omega} = \frac{1}{V}\int_{\omega} \sigma \, dV \tag{11}$$

$$\bar{\varepsilon} = \langle\varepsilon\rangle_{\omega} = \frac{1}{V}\int_{\omega} \varepsilon \, dV \tag{12}$$

Where ⟨ ⟩ denotes average stress or strain field of the RVE with volume V, and domain ω.

Since the volume is the inhomogeneous volume that should be taken into account the property of all the constituent phases. Then, equation 11 and 12 does not solve the problem due to the inhomogeneity. Although, Mori-Tanaka introduces the phase concentration tensor to relate the constituent's average field properties and is based on the approximation of Eshelby's solution for a single filler problem [55]. The model approximates the behavior of the composite material through the dilute inhomogeneities which are subject to an effective matrix field rather than the macroscopic field [56]. Y. Benveniste [57] expressed the Mori -Tanaka method for elastic composite as,

$$\langle\varepsilon\rangle^{(p)} = \bar{A}_{dil}^{(p)}\langle\varepsilon\rangle^{(m)} = \bar{A}_{dil}^{(p)}\bar{A}_{MT}^{(m)}\langle\varepsilon\rangle \tag{13}$$

$$\langle\sigma\rangle^{(p)} = \bar{B}_{dil}^{(p)}\langle\sigma\rangle^{(m)} = \bar{B}_{dil}^{(p)}\bar{B}_{MT}^{(m)}\langle\sigma\rangle \tag{14}$$

Where $\langle\varepsilon\rangle^{(m)}, \langle\varepsilon\rangle^{(p)}, \langle\sigma\rangle^{(m)}$ and $\langle\sigma\rangle^{(p)}$ are average strain and stress tensors of matrix and particle phases respectively. $\langle\varepsilon\rangle$ and $\langle\sigma\rangle$ are macroscopic second-order strain and stress tensor respectively. $\bar{A}_{MT}^{(m)}$ and $\bar{B}_{MT}^{(m)}$ are Mori -Tanaka matrix fourth-order strain and stress concentration tensor respectively. $\bar{A}_{dil}^{(p)}$ and $\bar{B}_{dil}^{(p)}$ are dilute fourth-order strain and stress concentration tensor. The Mori – Tanaka analog form for thermal conductivity of composite material is expressed as, [58].

$$\langle\nabla T\rangle^{(p)} = \bar{A}_{dil}^{(p)}\langle\nabla T\rangle^{(m)} = \bar{A}_{dil}^{(p)}\bar{A}_{MT}^{(m)}\langle\nabla T\rangle \tag{15}$$

$$\langle q\rangle^{(p)} = \bar{B}_{dil}^{(p)}\langle q\rangle^{(m)} = \bar{B}_{dil}^{(p)}\bar{B}_{MT}^{(m)}\langle q\rangle \tag{16}$$

where ∇T and q are the thermal gradients and heat flux vectors, $\bar{A}$ and $\bar{\mathrm{B}}$ are thermal gradient and heat flux second-order concentration tensor.

The Mori -Tanaka matrix fourth-order strain concentration tensor can be expressed in terms of the dilute fourth-order strain concentration tensor as follow

$$\bar{A}_{MT}^{(m)} = \left[(1-\phi)I + \phi \bar{A}_{dil}^{(p)}\right]^{-1} \tag{17}$$

$$\bar{A}_{MT}^{(p)} = \bar{A}_{dil}^{(p)}\left[(1-\phi)I + \phi \bar{A}_{dil}^{(p)}\right]^{-1} \tag{18}$$

Where ϕ is the filler volume fraction and I is the fourth-order identity tensor. The dilute concentration tensor expressed analog to Hill's [59] expression as

$$\bar{A}_{dil}^{(p)} = \left[I + SE_m^{-1}(E_p - E_m)\right]^{-1} \tag{19}$$

Where E_p and E_m are the elastic modulus tensor of particle and matrix and S is Eshelby's fourth-order stiffness tensor [60]. The effective elastic modulus tensor ($\mathrm{E_{CM}}$) of the composite material is given by [58].

$$E_{CM} = \left[E_m + \phi\,(E_p - E_m)\,\bar{A}_{MT}^{(p)}\right]$$

$$E_{CM} = \left[E_m + \phi\,(E_p - E_m)\,\bar{A}_{dil}^{(p)}\left[(1-\phi)I + \phi \bar{A}_{dil}^{(p)}\right]^{-1}\right]$$

$$E_{CM} = \left[E_m + \phi\,(E_p - E_m)\,\left[I + SE_m^{-1}(E_p - E_m)\right]^{-1}\left[(1-\phi)I + \phi\left[I + SE_m^{-1}(E_p - E_m)\right]^{-1}\right]^{-1}\right] \tag{20}$$

Similarly, the Mori -Tanaka matrix and particle second-order gradient can be expressed by the following relation [57].

$$\bar{A}_{MT}^{(m)} = \left[(1-\phi)I + \phi \bar{A}_{dil}^{(p)}\right]^{-1} \tag{21}$$

$$\bar{A}_{MT}^{(p)} = \bar{A}_{dil}^{(p)}\left[(1-\phi)I + \phi \bar{A}_{dil}^{(p)}\right]^{-1} \tag{22}$$

Where ϕ is the filler volume fraction and I is the second-order identity tensor. The dilute particle gradient concentration tensor expressed analog to the Hill's [59] expression as

$$\bar{A}_{dil}^{(p)} = \left[I + SR_m(K_p - K_m)\right]^{-1}$$

Where, K_p and K_m are the thermal conductivity tensor of particle and matrix, R_m or (K_m^{-1}) is the resistivity tensor and S is Eshelby's second-order thermal conductivity tensor for diffusion problem [61]. The effective thermal conductivity tensor ($\mathrm{K_{CM}}$) of the composite material (CM) is given by, [58].

$$\mathrm{K_{CM}} = \left[K_m + \phi\,(K_p - K_m)\,\bar{A}_{MT}^{(p)}\right]$$

$$\mathrm{K_{CM}} = \left[K_m + \phi\,(K_p - K_m)\,\bar{A}_{dil}^{(p)}\left[(1-\phi)I + \phi\bar{A}_{dil}^{(p)}\right]^{-1}\right]$$

$$\mathrm{K_{CM}} = \left[K_m + \phi\,(K_p - K_m)\,\left[I + SK_m^{-1}(K_p - K_m)\right]^{-1}\left[(1-\phi)I + \phi\left[I + SK_m^{-1}(K_p - K_m)\right]^{-1}\right]^{-1}\right] \quad (23)$$

The temperature has a significant effect on the effective property of the composite materials. Consequently, a significant elastic strain results from the expansion of the material with the increase in temperature. Therefore, the overall stress of homogeneous material is given by, [62]

$$\sigma(\mathrm{x}) = \mathrm{E}(\varepsilon(\mathrm{x}) - \alpha\Delta\mathrm{T}) \quad (24)$$

$$\sigma(\mathrm{x}) = \mathrm{E}\,\varepsilon(\mathrm{x}) + \beta\Delta\mathrm{T}; \qquad \beta = -\mathrm{E}\alpha$$

Where E is the modulus of elasticity, α is the coefficient of thermal expansion, $\varepsilon(\mathrm{x})$ is a total strain, and $\Delta\mathrm{T}$ is temperature change.

Since the polymer nanocomposite, RVE boundary displaced corresponding to the macroscopic strain, and change in temperature results from the applied uniaxial loads and uniform change in temperatures. Therefore, the macroscopic average stress $\langle\sigma\rangle$ of the composite is given by,

$$\langle\sigma\rangle = \mathrm{E_{CM}}(\langle\varepsilon\rangle - \bar{\alpha}\Delta\mathrm{T})$$

$$\langle\sigma\rangle = \mathrm{E_{CM}}\langle\varepsilon\rangle + \bar{\beta}\Delta\mathrm{T} \quad (25)$$

Where $\mathrm{E_{CM}}$ is effective elastic modulus tensor, $\bar{\alpha}$ is the coefficient of thermal expansion tensor, and $\langle\varepsilon\rangle$ is a macroscopic average strain.

The volume average strain of the fillers is related to the volume average of strain over the entire composite RVE by the strain concentration tensor as below.

$$\langle\varepsilon\rangle^{(\mathrm{p})} = \bar{\mathrm{A}}_{\mathrm{MT}}^{(\mathrm{p})}\langle\varepsilon\rangle + \varphi^{\varepsilon}\Delta\mathrm{T} \quad (26)$$

Using the Mori -Tanaka homogenization scheme [55], [62].

$$\varphi^{\varepsilon} = \left(\bar{\mathrm{A}}_{\mathrm{MT}}^{(\mathrm{p})} - \mathrm{I}\right)\left(\mathrm{E_p} - \mathrm{E_m}\right)^{-1}(\beta_{\mathrm{P}} - \beta_{\mathrm{m}}) \quad (27)$$

The total macroscopic average strain $\langle\varepsilon\rangle$ is also determined from the volume average property of the composite material by using bellow relation,

$$\langle\varepsilon\rangle = \phi\,\langle\varepsilon\rangle_{\omega_1} + (1-\phi)\langle\varepsilon\rangle_{\omega_0} \quad (28)$$

The composite effective thermo-elastic stiffness is determined using equation 25 with the given elastic stiffness tensor given by equations 20 and the relation given by equation 29 [55], [62].

$$\bar{\beta} = (1-\phi)\beta_{\mathrm{m}} + \phi\beta_{\mathrm{P}} + \phi\left(\mathrm{E_p} - \mathrm{E_p}\right)\varphi^{\varepsilon} \quad (29)$$

4.1.2. Homogenization Scheme of Three-Phase Composites

The multi-phase nanocomposites are materials with more than two phases. It has the matrix phase, the inclusion phase, and the interphase between the matrix and the inclusions with different volume fractions and material properties [55],[63]-[64]

The property of the interphase between the particle and the polymer matrix is one of the important nano factors that should be considered during the modeling of the composite material. However, knowing the specific thickness and the property of the interphases is yet remains a challenge. In addition to this, the nanofiller can be agglomerate into one due to the chemical agent or the stereoscopic effect, electrostatic and intermolecular Van der Waals forces. Consequently, this affects the dispersion state of the particles on the polymer matrix and in return affects the effective thermal and mechanical properties of the polymer nanocomposite materials [52], [55], [65]–[68]. This paper is based on the assumption of uniform distribution of the particle on the matrix and there is no interaction between particles. According to [55] with under considering the aforementioned nano effects, the particle is homogenized first with the interphase and then yields an effective particle. This effective particle is then homogenized with the matrix material based on the Mori-Tanaka homogenization method. Figure 5 illustrates the homogenization technique of multi-phase composite material.

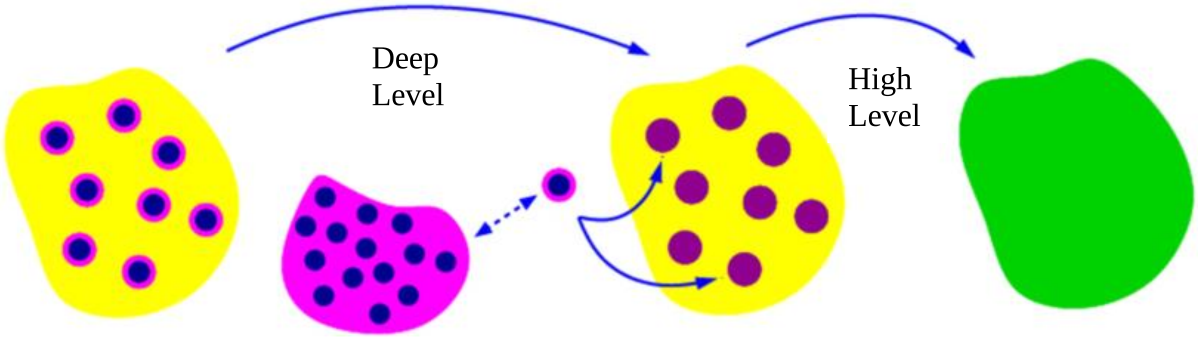


Figure 5 Multi-Level homogenization principle [55].

4.1.3. Microscopic Boundary Condition

The choice of suitable microscopic boundary conditions (B.C) is a crucial step in the numerical homogenization method. These boundary conditions (B.C) are applied to the representative volume element (RVE) to determine the effective thermal and mechanical properties of the polymer nanocomposite material from its average response and it can be the guarantee for achieving accurate results. Meanwhile, the type of analysis can be thermal, mechanical, or thermo-mechanical analysis. The most common way of applying the local field magnitudes, like temperature and displacement that represents macroscopic boundary conditions into representative volume element boundaries, are Dirichlet (linear displacement), Neumann (constant traction), Mixed, and Periodic boundary conditions [55], [69]. Since the Dirichlet condition overestimates the macroscopic field results whereas the Neumann condition underestimates.[70]-[71] Then the periodic boundary condition (PBC) is applied in the simulation by the MFH method of this research work.

4.1.3.1. Periodic Boundary Condition

The periodic boundary condition (PBC) is a set of boundary conditions that is important to define the boundary value problem on the representative volume element (RVE) to estimate the effective property of the composite material by finite element analysis approach. This approach requires imposing the Periodic boundary condition (PBC) on all outside faces of the representative volume element (RVE) in which the field variables are periodic with the corresponding surfaces. This requires a set of the equation that relates the degree of freedom of the nodes lying on opposite faces with an identical mesh [55], [72]. Compared with the other type of boundary condition, the Periodic boundary condition has not only the highest convergence rate of the average property of the composite material with increasing representative volume element (RVE) size and it is the most important boundary condition to estimate accurate effective property [55], [70], [71], [73]-[74]. Figure 6 shows the periodic boundary condition of the 2D with pressure loads.

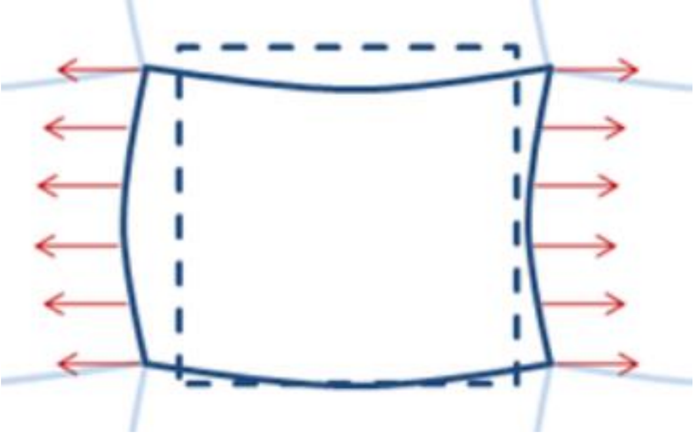


Figure 6 Periodic Boundary Condition [55].

Figure 7 shows the 3D- RVE subjected to the uniaxial temperature gradient and also a uniaxial tensile displacement loading with pressure load at given zero initial displacements.

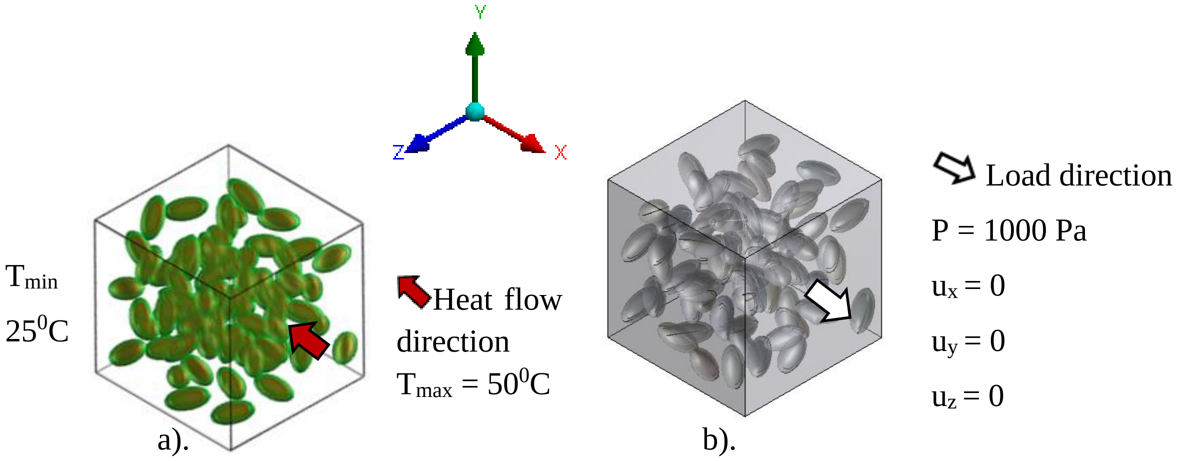


Figure 7. a). B.C of thermal analysis. b). B.C of mechanical analysis.

4.2. Finite Element Method

The finite element method (FEM) is a general numerical method for computing and obtaining an approximate solution to any engineering problem in which the dependent variable satisfies the representative equation within the boundary of the domain. It employs meshing in preprocessed, which allows us to characterize the model with finite elements and to fully capture the spatial discontinuity of the inhomogeneous material. The finite element method has been incorporated into some commercial software packages and it is very significant for the determination of the mechanical and thermal property of polymer nanocomposite materials [2],[75].

Nowadays, the FEM is one of the most prominent tools for solving engineering or mathematical physics problems with complex geometry and loading by modeling and solving the representative volume element (RVE) of the composite material [76].

R.D. Peng et al. [77] have modeled a unit cell with a 2D uniform arrangement of nanoparticles and determines the effect of the interphase layer, particle shape, and degree of clustering on the mechanical property of PNCMs. N. Sheng et al. [3]. have studied the overall young modulus and its dependency on the matrix and clay property as well as the internal clay structure parameter by modeling the effective particle that represents the nanoclay dispersed in a polymer matrix with intercalated structure type. B. Mortazavi et al. [78] have developed 3D finite element modeling for the determination of the effect of interphase on thermal conductivity and stiffness of the PNCM reinforced with randomly oriented and unidirectional particles. The result shows, the interphase thickness has a significant effect on a spherical particle but its effect decreases for other geometry of particles. R.S. Fertig et al. [79] have developed the local orthotropic finite element model and then the number of flak group with varied orientations were embedded to estimate the elastic modulus.

W. Ogierman and G. Kokot [80] have studied the effect of particle geometry on the elastic modulus of particle reinforced composite using the homogenization technique and the results show that the cylindrical particle provides the highest stiffness over spherical and prismatic shaped particles. L. Adam et al. [81] have modeled the nanocomposite using MFH and FE approaches to determine the influence of filler clustering and size distribution on the stiffness. R. Kothari et al. [21] have modeled the axisymmetric model for silica particle unit cells and studied the thermal conductivity with consideration of the effect of kapitza resistance. H.W. Wang et al.[82] have developed the 3D multiparticle unit cells and studied the effect of interphase with two layers of different stiffness, particle size and shape, clustering, and volume fraction on mechanical property. The result depicts, the young modulus decreases with the degree of clustering and it is high for fillers with a cylindrical shape. A. Hamada et al.[83] have studied the thermal and mechanical property of metal matrix composite using both finite elements (FE) and mean-field homogenization (MFH) approaches. Trzepieciński et al.[84] have studied the mechanical property using the homogenization technique by modeling the 3D representative volume element embedded with a prism and icosahedron-shaped solid inclusion.

4.2.1. Representative Volume Element (RVE)

The modeling complexity of a system with the maximum number of elements and computational limitation of FEM for a composite material limited to the modeling of representative volume element (RVE) which is the smallest volume of the composite material in which the measurements can be made that yields the required value representative of the whole material. Meanwhile, it is a heterogeneous material with known inclusion and matrix property [85]–[88].

The size of the representative volume element (RVE) is a crucial thing for creating finite element modeling. W.J Drugan and J.R. Willis [88] drive the quantitative estimates of the minimum size of representative volume element (RVE) and they have shown that the minimum size of the RVE for any reinforcement volume fraction level is at most twice the reinforcement diameter. However, the macroscopic array of the polymer nanocomposite material is assumed to be a square array composed of square representative volume elements with randomly distributed particles of different geometry. The RVE is generated using Digimat -FE which is a multiscale simulating tool for estimating the effective properties of PNCM based on the finite element method (FEM).

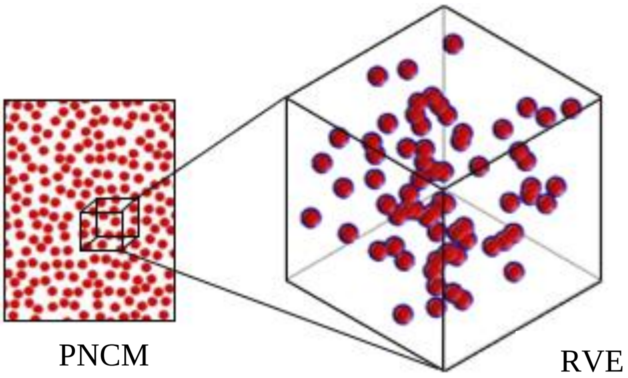


Figure 8 Constructing of RVE of the polymer nanocomposite material structure.

The physical properties of the silicate particles and epoxy are also important to model and analyze the RVE of the composite material. Then the Characteristic material property of the silica and epoxy is summarized in table 2. Besides, the study is conducted in the temperature range of 25-50 ^{0}C to include the glass transition temperature of the material and obtain the maximum value of the effective thermal conductive. Only for the validating purpose, the different set of volume fraction is considered for each thermal and mechanical analysis as shown in tables 3 and 4, respectively.

Table 1 Characteristic property of the materials [8], [30].

Physical Property	**Epoxy**	**Silica (SiO_2) (99.5%)**
Elastic Modulus (GPa)	2.5134	68.9
Poisons ratio	0.35	0.17
Density (kg/m^3)	1220	$(\frac{2200+2600}{2}) = 2400$
Thermal conductivity (W/m. K)	0.15	1.5
Specific Heat Capacity (J/kg. K)	1046	745
Coefficient of Thermal Expansion (10^{-6}/K)	$(\frac{45+65}{2}) = 55$	0.56
Average Particle Size (nm)	$(\frac{10+20}{2}) = 15$	
Temperature Limits (°C)	25 - 50	

Since the filler content is given by the particle weight fraction in percent, then the relation below is applied to change it to volume fraction and the obtained result is given in table 2.

$$\phi_p = \left(\frac{W}{W + (1 - W)\frac{\rho_p}{\rho_m}} \right) \tag{30}$$

Table 2 Phase fraction in % weight ratio and volume fraction for thermal analysis.

PNCM	Weight Ratio (%)	Volume Fraction
Neat ER	0	0
ER-SiO_2	2	0.0101
ER-SiO_2	4	0.0204
ER-SiO_2	6	0.0309
ER-SiO_2	8	0.042

Table 3 Particle volume fraction for mechanical analysis.

PNCM	Volume Fraction
Neat ER	0
ER-SiO_2	0.03
ER-SiO_2	0.06
ER-SiO_2	0.08
ER-SiO_2	0.10
ER-SiO_2	0.15

4.2.2. Interphase

The size and property of the interphase are a very significant thing in generating the RVE for the analysis. Interphase is a boundary region in which the volume of material is affected by the chemical interaction of the constituent materials in the interface. The term interphase was originally introduced by L. H. Sharpe [89] to distinguish from and substituted the 2D boundary surface called an interface. According to L. T. Drzal et al. [90], the interphase has altered property from those of bulk materials. The mixing technique, a chemical agent that is added to the nanofiller to improve its surface or to enhance the dispersion state, and the density change due to the alignment of the polymer chain are the main factors that determine the property and the size of the interphase.

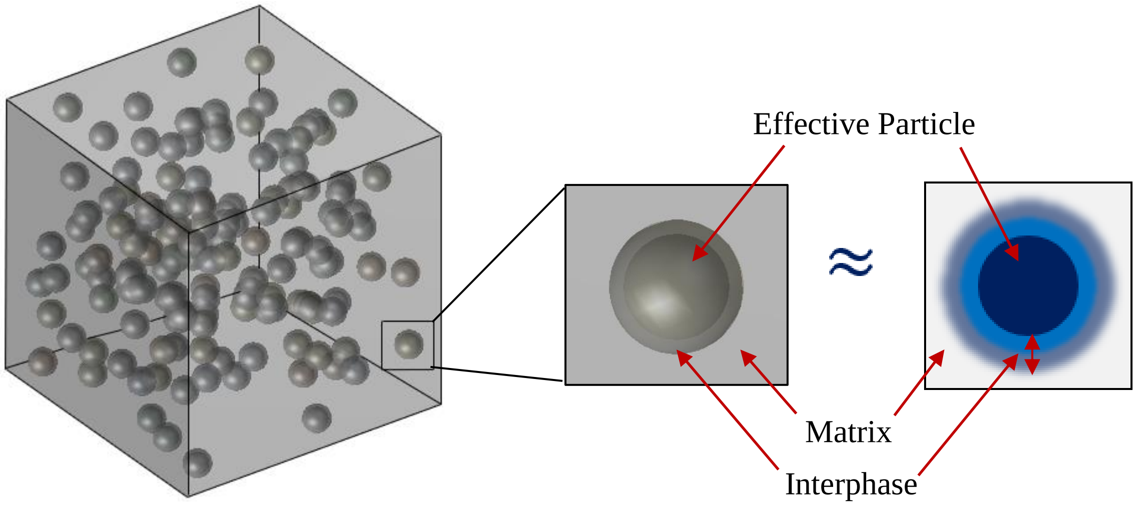


Figure 9 Interphase of silicate particle reinforced epoxy matrix composite material.

The variation in the composition state of constituents makes it difficult to quantify and put the interphase property in a specific value. This means, the composition of silicate is higher on the surface of effective particles and decreases toward the matrix. In the same manner, the composition of the matrix is higher around the interface between matrix and interphase but decreases toward the surface of the effective particle. The experimental result of J. M. Torralba et al. [91] confirms these facts. Although, some literature suggested different indirect methods for its estimation. R. Kochetov et al. [41] determine the size of the interphase by comparing the analytical and experimental results and suggested that the interphase size between nanoscopic silicate particle and the epoxy matrix is between the range of 1.6 nm and 2.5 nm. Then, the average interphase size (2.05 nm) of the given size is taken to model the RVE of this research work. Therefore, the volume of the single silicate particle embedded in an epoxy matrix is determined using the relations given by.

$$V_P = \frac{4}{3}\pi\left(r_p\right)^3$$

$$V_P = \frac{4}{3}\pi(7.5\mathrm{nm})^3$$

$$V_P = 1{,}767\ \mathrm{nm}^3$$

The volume of the composite particle (effective silicate particle and interphase) is given by,

$$V_{cp} = \frac{4}{3}\pi\left(r_{cp}\right)^3$$

$$V_{cp} = \frac{4}{3}\pi\left(r_p + t\right)^3$$

$$V_{cp} = \frac{4}{3}\pi(7.5\mathrm{nm} + 1.025\mathrm{nm})^3$$

$$V_{cp} = 2{,}595\ \mathrm{nm}^3$$

Therefore, the volume fraction of the single nano silicate particle within the composite particle is also determined by,

$$\phi_p = \frac{V_P}{V_P + V_{cp}}$$

$$\phi_p = \frac{1{,}767}{(1{,}767 + 2{,}595)}$$

$$\phi_p = 0.405$$

$$\phi_p = 40.5\%$$

The volume of the affected silicate layer (V_{as}) on the surface of effective silicate particle is given by,

$$V_{as} = \frac{4}{3}\pi\left(r_p\right)^3 - \frac{4}{3}\pi\left(r_{ep}\right)^3$$

$$V_{as} = \frac{4}{3}\pi(r_p)^3 - \frac{4}{3}\pi(r_p - t)^3$$

$$V_{as} = \frac{4}{3}\pi(r_p)^3\left(1 - \left(1 - \frac{t}{r_p}\right)^3\right)$$

$$V_{as} = V_P\left(1 - \left(1 - \frac{t}{r_p}\right)^3\right)$$

Therefore, the volume fraction (ϕ_{as}) of affected silicate layer is written as,

$$\phi_{as} = \phi_P\left(1 - \left(1 - \frac{t}{r_p}\right)^3\right)$$

$$\phi_{as} = 0.405\left(1 - \left(1 - \frac{1.025}{7.5}\right)^3\right)$$

$$\phi_{as} = 0.144$$

$$\phi_{as} = 14.4\%$$

Since the nature of the interphase is a composite material. Therefore, the property of the composite material is the volume-weighted average of the phases or determined based on the properties of the particle and matrix. Consequently, the thermal conductivity (K_i) and elastic modulus (E_i) of the interphase are given by the rule of the mixture as below [2].

$$K_i = \phi_{as}K_p + (1 - \phi_{as})K_m \tag{31}$$

$$E_i = \phi_{as}E_p + (1 - \phi_{as})E_m \tag{32}$$

The other physical properties of the constituents that are required to model the interphase are also calculated using the above equation and the obtained value is given in table 4.

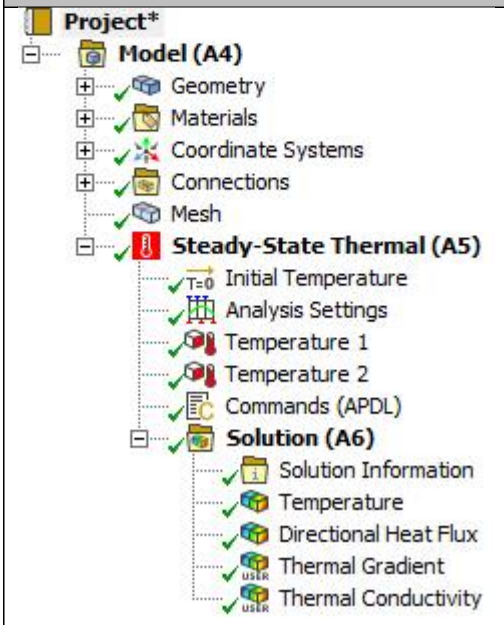
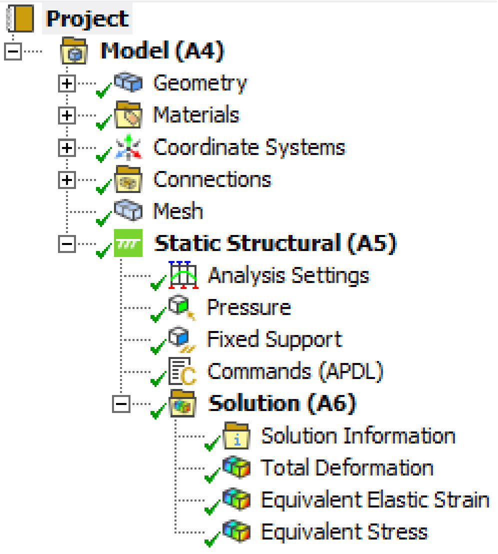
Table 4 Interphase physical properties.

Interphase Physical Property	**Values**
Density (kg/m^3)	1372.8
Thermal conductivity (W/m. K)	0.34
Specific Heat Capacity (J/kg. K)	1002.7
Coefficient of Thermal Expansion (10^{-6}/K)	47.2
Poisons ratio	0.324
Elastic Modulus (GPa)	12.073

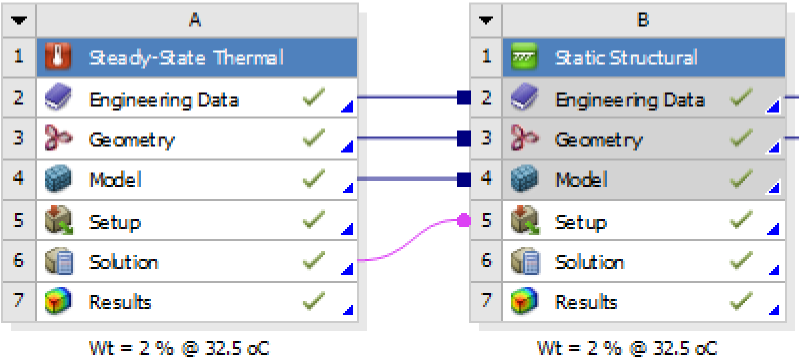
4.2.3. FEA Procedures

The 3D representative volume element (RVE) is imported in ANSYS workbench software for thermal and mechanical analysis. The effective thermal conductivity of the composite material is determined from the steady-state thermal analysis whereas the effective elastic modulus is obtained from the static structural analysis. Table 5 illustrates the main procedure of thermal and mechanical analysis on the ANSYS workbench.

Table 5 Thermal and Mechanical analysis procedure.

Thermal Analysis	Mechanical Analysis
 Project* Model (A4) Geometry Materials Coordinate Systems Connections Mesh Steady-State Thermal (A5) Initial Temperature Analysis Settings Temperature 1 Temperature 2 Commands (APDL) Solution (A6) Solution Information Temperature Directional Heat Flux Thermal Gradient Thermal Conductivity	 Project Model (A4) Geometry Materials Coordinate Systems Connections Mesh Static Structural (A5) Analysis Settings Pressure Fixed Support Commands (APDL) Solution (A6) Solution Information Total Deformation Equivalent Elastic Strain Equivalent Stress

The effect of temperature on the effective thermal conductivity of the composite material is obtained from the steady-state thermal analysis by applying a constant temperature as an entire body temperature of the RVE. Moreover, the temperature effect on the effective modulus of elasticity is determined from the combined thermal and mechanical analysis as shown below.



A
1 Steady-State Thermal
2 Engineering Data
3 Geometry
4 Model
5 Setup
6 Solution
7 Results
Wt = 2 % @ 32.5 oC

B
1 Static Structural
2 Engineering Data
3 Geometry
4 Model
5 Setup
6 Solution
7 Results
Wt = 2 % @ 32.5 oC

Figure 10 Thermo-mechanical analysis.

CHAPTER FIVE

5. RESULT AND DISCUSSION

5.1. Result

The adding of nano silicate particles to the epoxy matrix is contribute to enhance the effective mechanical and thermal properties of the composite material. The shared property of the composite material is determined by using the mean-field homogenization (MFH) and finite element method (FEM) as described in the methodology part of the research. Therefore, this part presents the result of MFH, FEM, and Analytical models that shows the effect of volume fraction, particle geometry, and operating temperature on mechanical and thermal properties of the polymer nanocomposite material.

5.1.1. Result of MFH

The result of MFH for the effect of nanoparticle percentage weight ratio and geometry on the thermal conductivity of the polymer nanocomposite material is given in table 6. The result shows that the effective thermal conductivity of the composite material is increased with the increasing of the content of both spherical ($\alpha = 1$) and ellipsoidal ($\alpha = 2$) nano silicate particles. Moreover, the effect of particle volume fraction and geometry on the elastic modulus of the composite material is determined by the MFH method as well and the result is given in table 7. Despite the difference in the magnitude of enhancement, the effective elastic modulus of the material is increased with the increasing of the particle volume fraction of both geometries.

Table 6 The MFH result of Thermal conductivity.

PNCM	Weight Ratio (%)	Thermal Conductivity ($Wm^{-1}K^{-1}$)	
		$\alpha = 1$	$\alpha = 2$
Neat ER	0	0.15	0.15
ER-SiO_2	2	0.18101	0.20067
ER-SiO_2	4	0.22444	0.26565
ER-SiO_2	6	0.27782	0.34234
ER-SiO_2	8	0.34777	0.43824

Table 7 The MFH result of Elastic modulus.

PNCM	Volume Fraction	Elastic Modulus (GPa)	
		α = 1	α = 2
Neat ER	0	2.5134	2.5134
ER-SiO_2	0.03	2.6645	2.7417
ER-SiO_2	0.06	2.8243	2.9826
ER-SiO_2	0.08	2.9361	3.1513
ER-SiO_2	0.10	3.0523	3.3263
ER-SiO_2	0.15	3.3645	3.7951

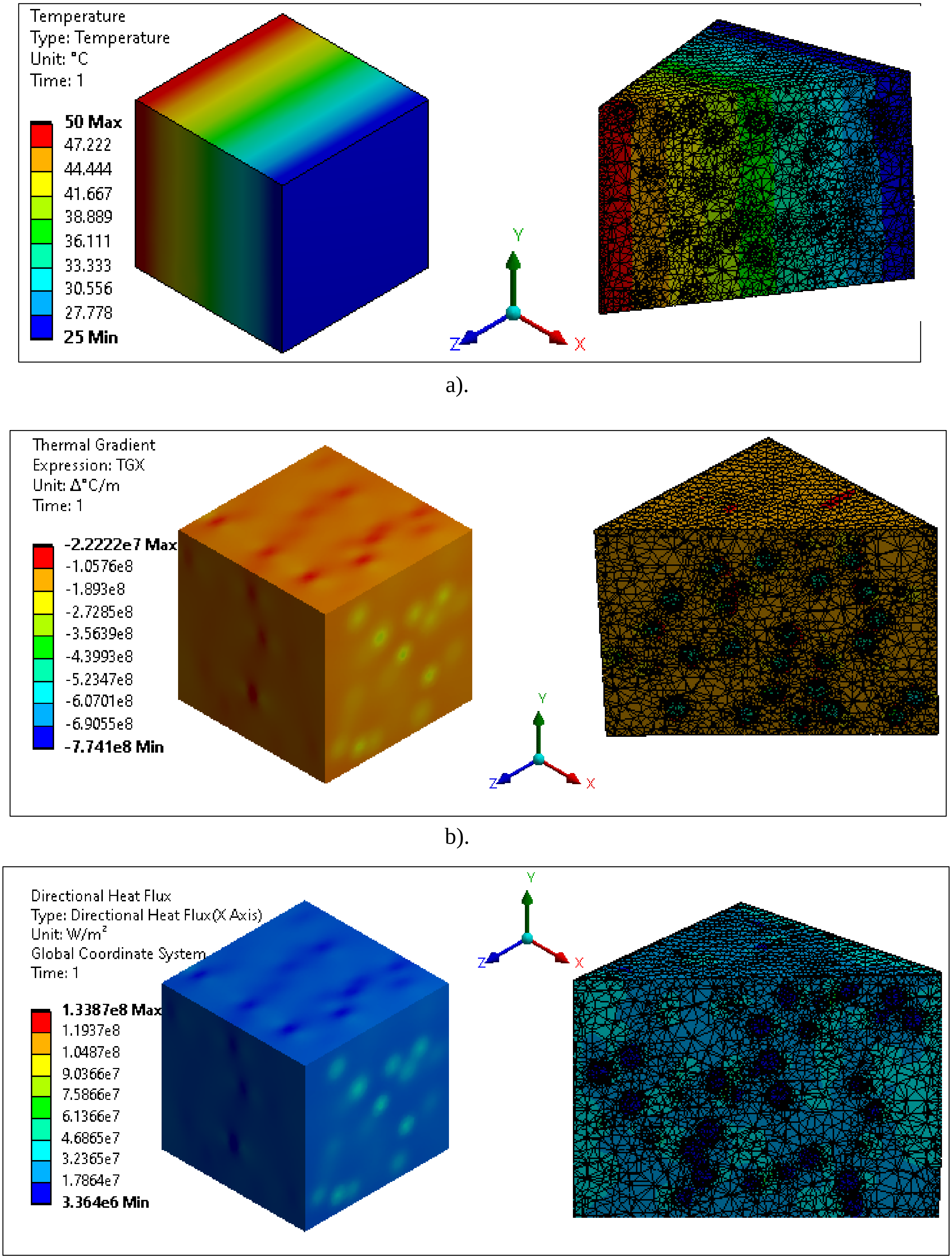
The working temperature also has a significant effect on the effective thermal and mechanical properties of the polymer composite materials. The MFH approach is applied to predict the variation of the elasticity modulus with temperature via the thermomechanical analysis. Table 8 provides the modulus of elastic determined at three different working temperatures and the result implies, the effective young modulus is reduced with increasing the temperatures.

Table 8 The MFH result of Elastic modulus at different temperatures.

	Analysis-1		Analysis-2		Analysis-3	
Wt%	Temprature (^{0}C)	Elastic Modulus (GPa)	Temprature (^{0}C)	Elastic Modulus (GPa)	Temprature (^{0}C)	Elastic Modulus (GPa)
2	32.5	3.004	38.5	2.825	46.5	2.546
4	32.5	3.435	39.2	3.157	47.2	2.761
6	32.5	3.896	39.5	3.642	48.2	3.086

5.1.2. Result of FEM

The RVE that represents the macroscopic composite material is analyzed in the ANSYS workbench to determine the effect of nanoparticle content and geometry/aspect ratio on the overall thermal and mechanical properties of the polymer nanocomposite material. The 25 ^{0}C and 50 ^{0}C temperatures are applied on the opposite surface (Y-Z plane) of the 200 nm 3D RVE. Since the thermal conductivity is the ratio of the negative thermal heat flux (TFX) to the thermal gradient (TGX) along the same direction (X-direction), then they are included in the analysis as the user-defined parameter. Figure 11 shows the temperature profile, thermal gradient, and directional heat flux in the X-direction of the RVE that is modeled for an 8 % weight ratio of spherical nanoscopic silicate particles.



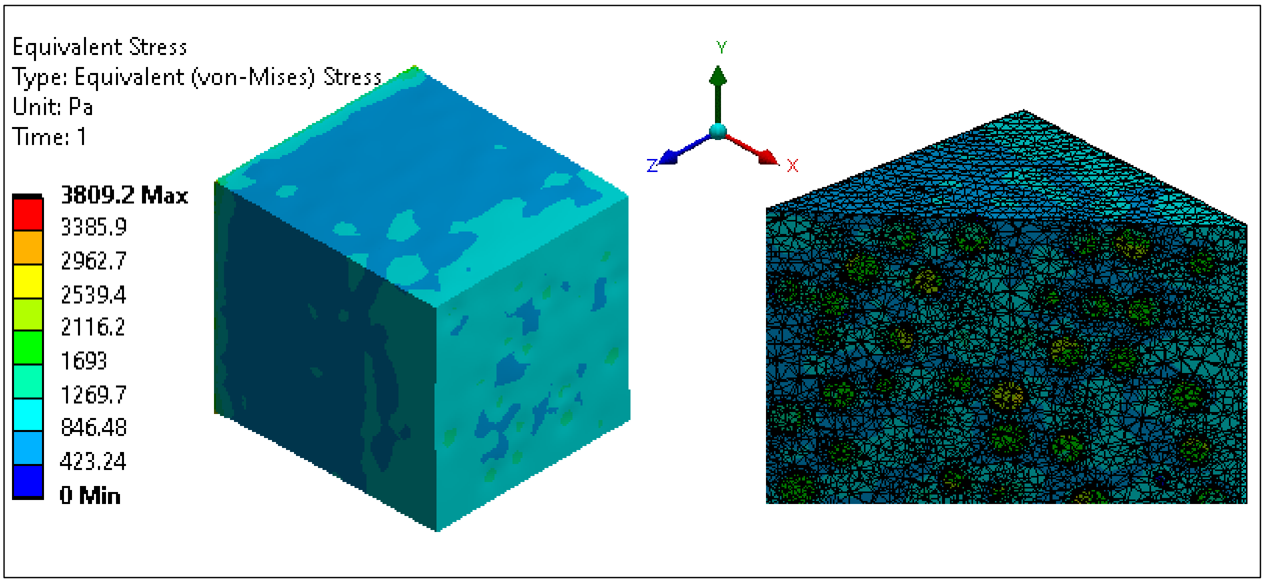
a).

b).

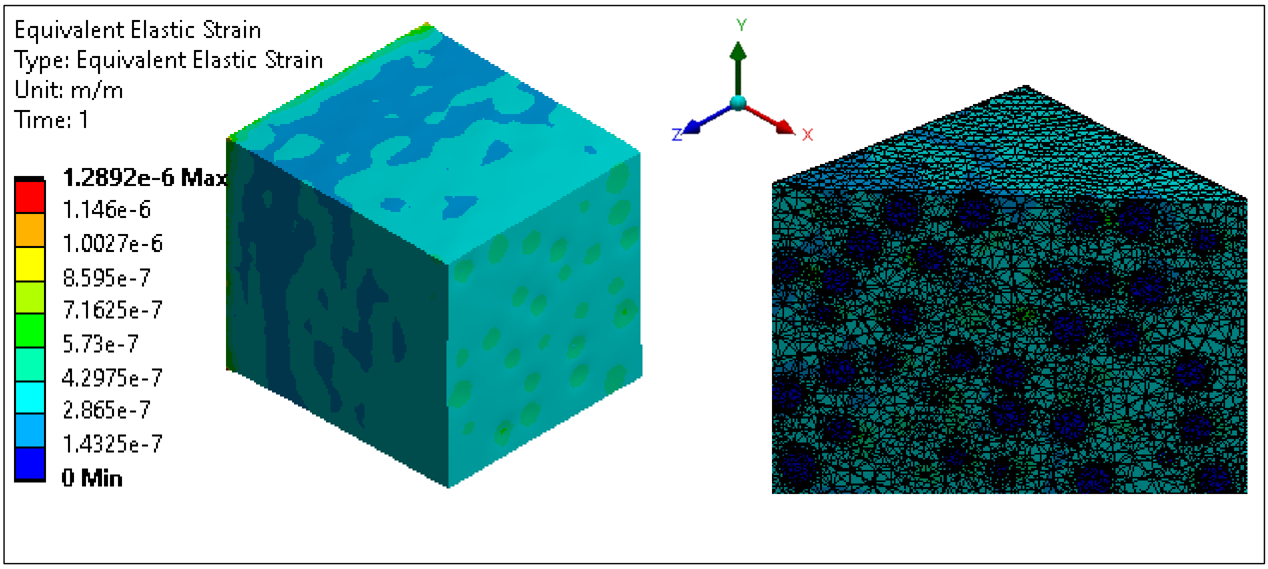
c).

Figure 11. a). Temperature profile. b). Thermal gradient. c). Directional heat flux.

The direct pressure load of 1000 Pa is applied on the surface that is opposite to the fixed surface of 200 nm 3D cubic polymer composite RVE. Figure 12 shows the equivalent (Von-Mises) strain and the equivalent (Von-Mises) stress developed on the RVE modeled with a 15 % volume fraction of silicate particles. Therefore, the effective modulus of elasticity is the ratio of average the equivalent (Von-Mises) stress to the average equivalent strain and the obtained result is given in table 9.



a).



b).

Figure 12 a). Equivalent (von-Mises) stress. b). Equivalent (von-Mises) elastic strain.

The FEA result of effective thermal conductivity is given in table 9 and the result shows the thermal conductivity increases with the increase of the percentage weight ratio of nano silicate particles in the epoxy matrix. Moreover, the result of elastic modulus is also given in table 10 and the result depicts the elastic modulus is increased with increasing of the particle volume fraction of particles in both geometries. The thermal conductivity and elastic modulus of the composite material reinforced with ellipsoidal (α = 2) silicate particle is higher compared to the composite material of the spherical particle.

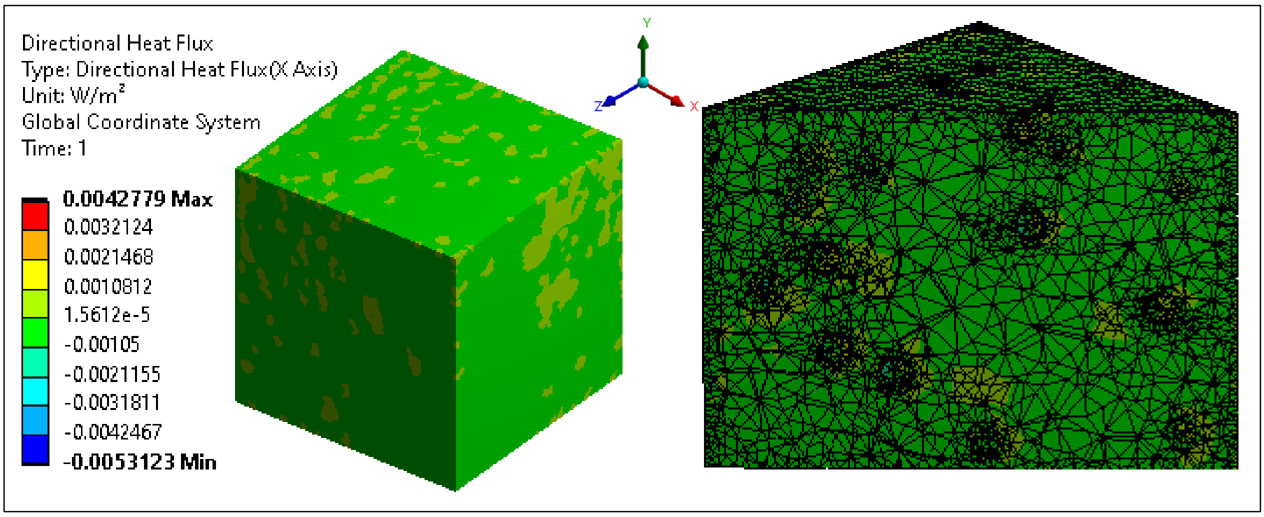
Table 9 The FEM result of Thermal conductivity.

PNCM	Weight Ratio (%)	Thermal Conductivity ($Wm^{-1}K^{-1}$)	
		α = 1	α = 2
Neat ER	0	0.15	0.15
ER-SiO_2	2	0.2005	0.2020
ER-SiO_2	4	0.2186	0.2341
ER-SiO_2	6	0.2394	0.2583
ER-SiO_2	8	0.3107	0.3209

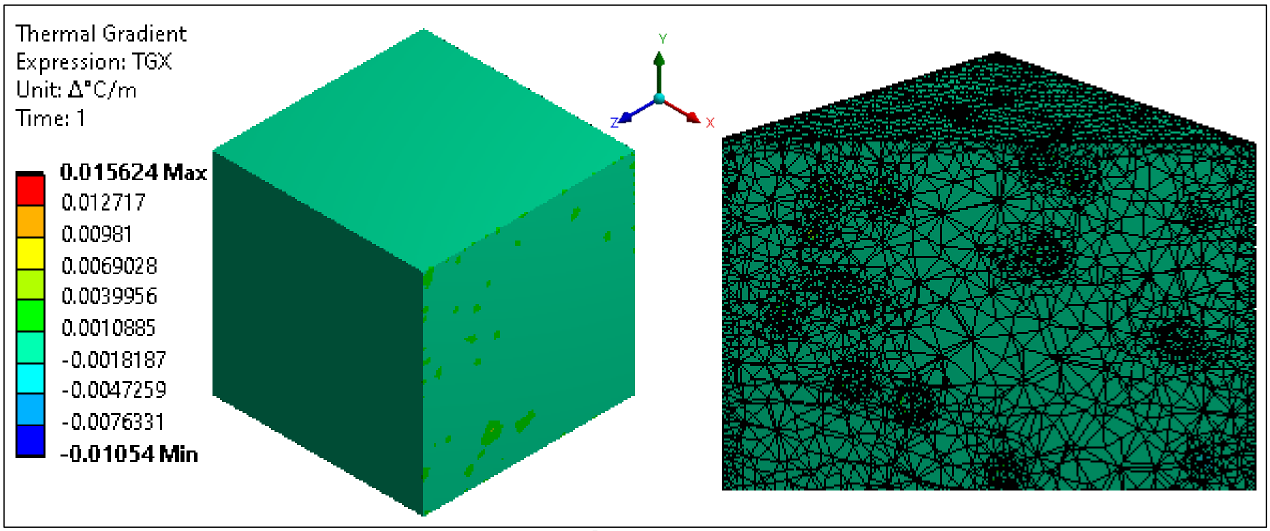
Table 10 The FEM result of Elastic modulus.

PNCM	Volume Fraction	Elastic Modulus (GPa)	
		α = 1	α = 2
Neat ER	0	2.5134	2.5134
ER-SiO_2	0.03	2.7246	2.7841
ER-SiO_2	0.06	2.8574	2.9284
ER-SiO_2	0.08	3.0594	3.1189
ER-SiO_2	0.10	3.1206	3.1858
ER-SiO_2	0.15	3.7567	3.9013

The effect of temperature on the effective thermal conductivity of the polymer composite material is also determined from the thermal analysis on the ANSYS workbench. Figure 13 shows the directional heat flux and thermal gradient with their respective sectional part of the composite RVE of 6 % silicate particle weight ratio at 48.2 ^{o}C temperature. Table 11 presents the result of effective thermal conductivity at three different temperature which is applied to the entire composite RVE and the result is extracted from the obtained directional heat flux and thermal gradient along the single direction.



a.)



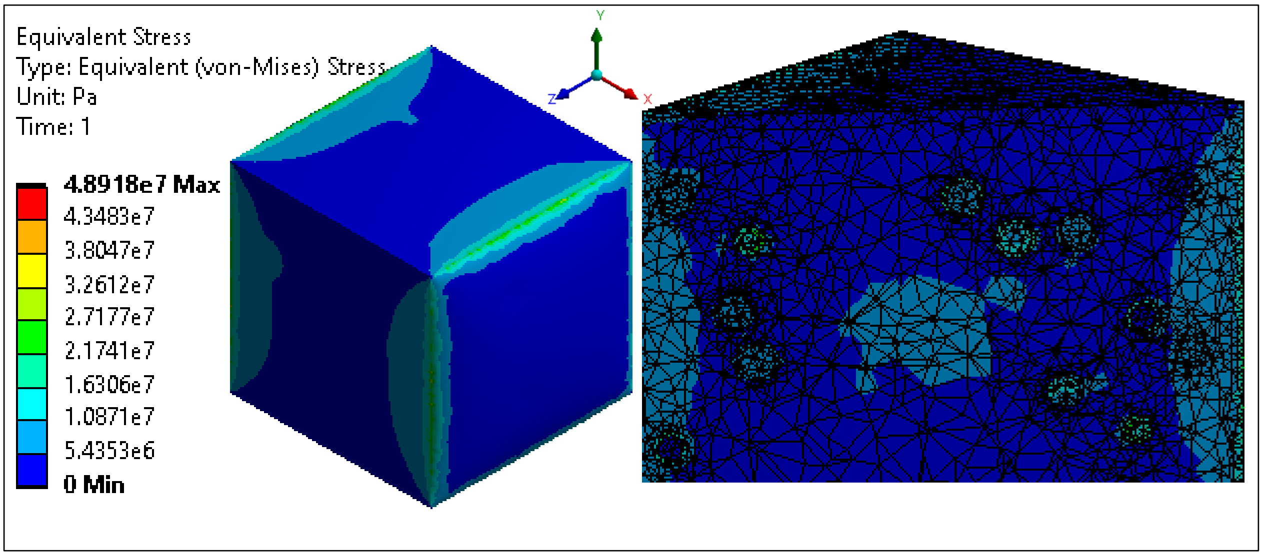
b.)

Figure 13 a). directional heat flux b). thermal gradient

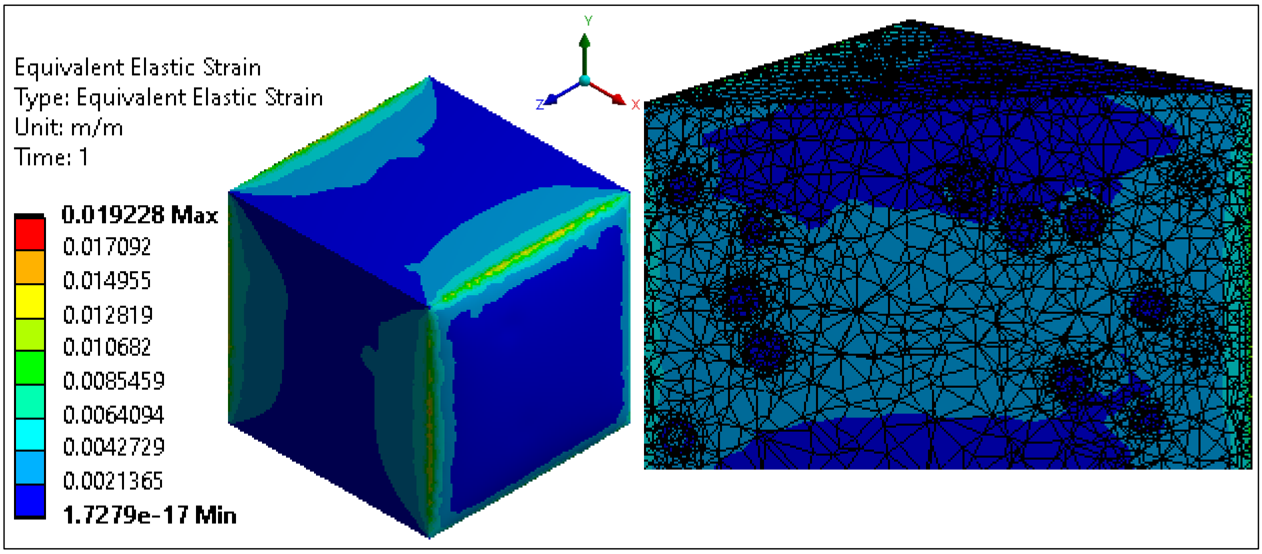
Table 11 The FEM result of Thermal conductivity at different temperatures.

	Analysis-1		Analysis-2		Analysis-3	
Wt. %	Temperature (^{0}C)	Thermal Con. (W/m. K)	Temperature (^{0}C)	Thermal Con. (W/m. K)	Temperature (^{0}C)	Thermal Con. (W/mK)
2	32.5	0.1914	38.5	0.2046	46.5	0.2272
4	32.5	0.2007	39.2	0.2118	47.2	0.2331
6	32.5	0.2119	39.5	0.2292	48.2	0.2420

The effect of temperature on the effective elastic modulus of the polymer composite material is estimated from the thermomechanical analysis on the ANSYS workbench. Since the thermomechanical analysis is the combination of both the thermal and mechanical analysis, then the result of the steady-state thermal analysis type is imported in the static structural analysis type to determine the effect of the temperature on the mechanical properties of the composite RVE. In addition to the imported three different temperature loads, the same direct pressure load is also applied on the RVE surface in the static structural analysis. figure 14 presents the total stress and strain obtained from the thermomechanical analysis of the 6 % silicate particle weight ratio at 48.2 °C temperature.



a).



b).

Figure 14 a). Equivalent (von-Mises) stress b). Equivalent (von-Mises) elastic strain

The effective elastic modulus of the polymer composite material is computed from the average macroscopic stress and strain corresponding to the applied direct pressure load of 1000 Pa and the temperatures on the 200 nm 3D cubic polymer composite RVE by the thermomechanical analysis on ANSYS workbench. Therefore, the obtained result of effective modulus of elasticity is given in table 12.

Table 12 The FEM result of Elastic Modulus at different temperatures.

	Analysis-1		Analysis-2		Analysis-3	
Wt.%	Temperature (^{0}C)	Elastic Modulus (GPa)	Temperature (^{0}C)	Elastic Modulus (GPa)	Temperature (^{0}C)	Elastic Modulus (GPa)
2	32.5	3.020	38.5	2.825	46.5	2.606
4	32.5	3.476	39.2	3.246	47.2	2.872
6	32.5	3.942	39.5	3.748	48.2	3.209

5.1.1. Result of Analytical Models

The analytical result of the effective thermal conductivity and elastic modulus of the polymer nanocomposite is determined using the three-phase Lewis Nielsen (LN) and L.E. Nielsen model, respectively. The shape factor that depends on the distribution and aspect ratios of the inclusion is also considered in the analytical analysis of thermal and mechanical properties of the composite material. The value of the shape factor is given in table I-A and it is 1.5 and 1.58 for the spherical and ellipsoidal inclusions, respectively. Besides, the maximum packing fraction of the spherical filler type is taken to be 0.637 which is given in table II-A.

The result of the analytical model given in tables 13 and 14 shows that the effective property of the composite material is improved with the increase of particle volume fraction of both geometries.

Table 13 The result of three - Phase Lewis – Nielsen (LN) models.

PNCM	Weight Ratio (%)	Thermal Conductivity ($Wm^{-1}K^{-1}$)	
		$\alpha = 1$	$\alpha = 2$
Neat ER	0	0.15	0.15
ER-SiO_2	2	0.1771	0.1928
ER-SiO_2	4	0.2099	0.2487
ER-SiO_2	6	0.2504	0.3258
ER-SiO_2	8	0.3021	0.4397

Table 14 The result of three - Phase L.E. Nielsen model.

PNCM	Volume Fraction	Elastic Modulus (GPa)	
		α = 1	α = 2
Neat ER	0	2.5134	2.5134
ER-SiO_2	0.03	2.6408	2.7401
ER-SiO_2	0.06	2.7983	3.0089
ER-SiO_2	0.08	2.9236	3.2163
ER-SiO_2	0.10	3.0685	3.4506
ER-SiO_2	0.15	3.542604482	4.1873

5.2. Discussions

Different previous research works well thought out the nano effects in their analysis and they conclude that the effective property of the polymer nanocomposite material is highly reliant on the nano effects. In this research work, the effect of the inclusion volume fraction, geometry or aspect ratio, and the operating temperature is determined numerically by the MFH and FEA methods and then the obtained numerical result is discussed in detail and validate with well-known analytical models and the experimental result that is taken from journals [8]

5.2.1. Effect of Particle Volume Fraction

The effective thermal conductivity of the polymer nanocomposite material as a function of the spherical silicate particle percentage weight ratio obtained from the mean-field homogenization (MFH) approach, finite element analysis method (FEM), and the analytical approach is given in figure 15. The result of all these methods depicts the effective thermal conductivity increases with the increasing of the inclusion weight ratios. The experimental result shows that the thermal conductivity initially increases linearly up to the 2 % of particle weight ratio and then the slope of the thermal conductivity declines to some value up to the 6% of particle weight ratio and finally increases linearly with the inclusion percentage weight ratios. Since the cluster or agglomerate of the particle can affect the heat transfer channels between the constituent phases, then the particle dispersion state of the sample material could be the main reason for the nonlinear relation between the thermal conductivity and the particle weight ratio.

Unlike the experimental result taken from literature and the FEM, the result of the Analytical and MFH method indicates the increment of the thermal conductivity is almost linear with the nano silicate particle contents. Moreover, the state of random distribution of the particles within the epoxy matrix and the probabilistic placement of particles in the RVE causes variation in the slope of thermal conductivity. Meanwhile, the result of the FEM is more agree with the experimental result with a maximum deviation of 5.7% at 6 % of particle weight ratio. However, the value of thermal conductivity obtained from the MFH and Analytical approaches are 19.7 % and 10.9 % higher than the experimental result of a similar particle weight ratio, respectively.

Generally, the result of all approaches indicates that the addition of an 8% nano silicate particle weight ratio in the epoxy matrix enhances the effective thermal conductivity of the polymer material by more than twice its neat property.

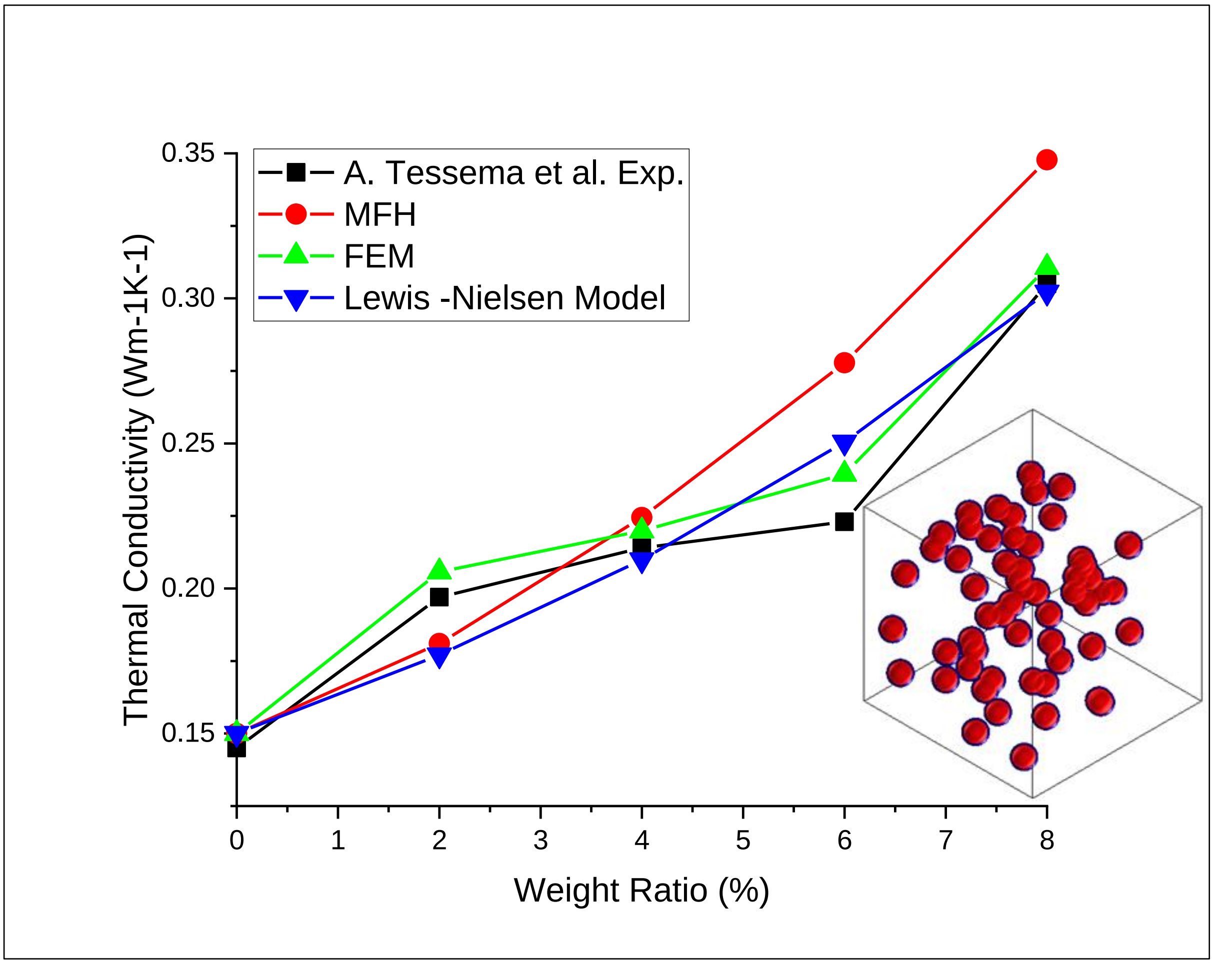


Figure 15 Effect of particle volume fraction on effective thermal conductivity.

The result of the elastic modulus of the polymer nanocomposite material as a function of the spherical nano silicate particle volume fraction obtained from MFH, FEM, and Analytical approaches is also given in figure 16. The result of all approaches depicts the young modulus increases with the increment of particle volume fraction. The agglomeration of the inclusion causes the experimental result of elastic modulus to vary its slope as the particle fraction increases. Meanwhile, the results obtained from MFH and Analytical approach are very close to the experimental result up to the 10 % of particle volume fraction with a very small variation of 3.19 % and 2.29 %, respectively. Although, the difference grew to 4.37 % and decline to less than 1 % at the 15 % silicate volume fraction, respectively. Therefore, the analytical model is more agree with the experimental results taken from the journal.[30]

The addition of 15 % of silicate volume fraction into the epoxy matrix can improve the effective elastic modulus of the polymer nanocomposite material around 40 % of the value for neat polymer materials. Besides, the strong interphase adhesion strength between silicate and epoxy contributes to increasing the young modulus of the composite material. Generally, the result of the Analytical model, FEM, and MFH approaches shows that the effective thermal conductivity and young's modulus of the composite material are highly dependent on the amount of the inclusions mix with the polymer matrix.

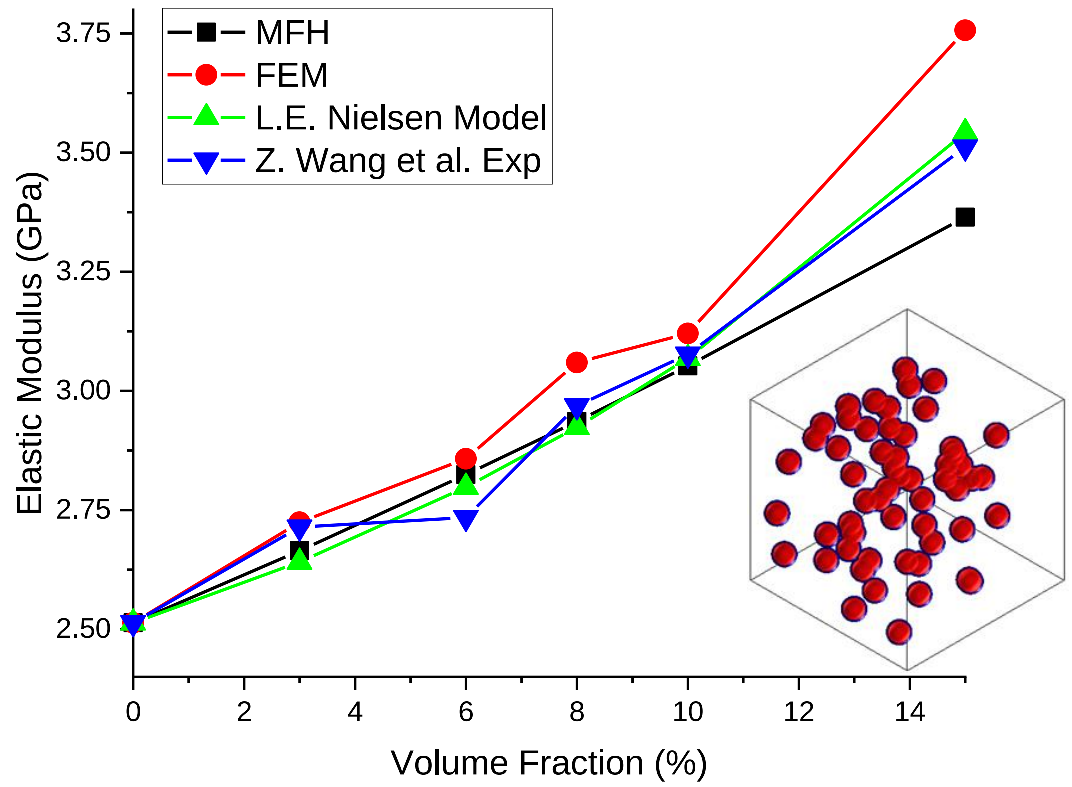


Figure 16 Effect of particle volume fraction on effective elastic modules.

5.2.2. Effect of Particle Geometry

Figure 17 provides the result of thermal conductivity as a function of the spherical ($\alpha = 1$) and ellipsoid ($\alpha = 2$) particle volume fraction obtained from MFH, FEM, and Analytical approaches. The result of the MFH scheme and Analytical model shows the increment of the effective thermal conductivity is almost linear with both spherical and ellipsoid silicate particle contents. According to the Analytical and MFH method results, adding of ellipsoid ($\alpha = 2$) particle of 8 % weight ratio in the epoxy matrix improves the thermal conductivity by 31.3 % and 20.6 % than reinforced with the spherical particle at the same particle weight ratio, respectively.

Unlike the others, the FEM result indicates the aspect ratio has a small effect on the overall thermal conductivity of the composite materials. Meanwhile, the thermal conductivity of polymer composite material reinforced with ellipsoidal silicon dioxide filler is 7 % and 8 % improved than filled with the spherical geometry inclusions at 4 % and 6 % weight ratio, respectively. Generally, the thermal conductivity of the PNCM is increasing with the increase of the particle percentage weight ratio and it is higher for ellipsoid particles than a composite of a spherical particle within equal inclusion contents.

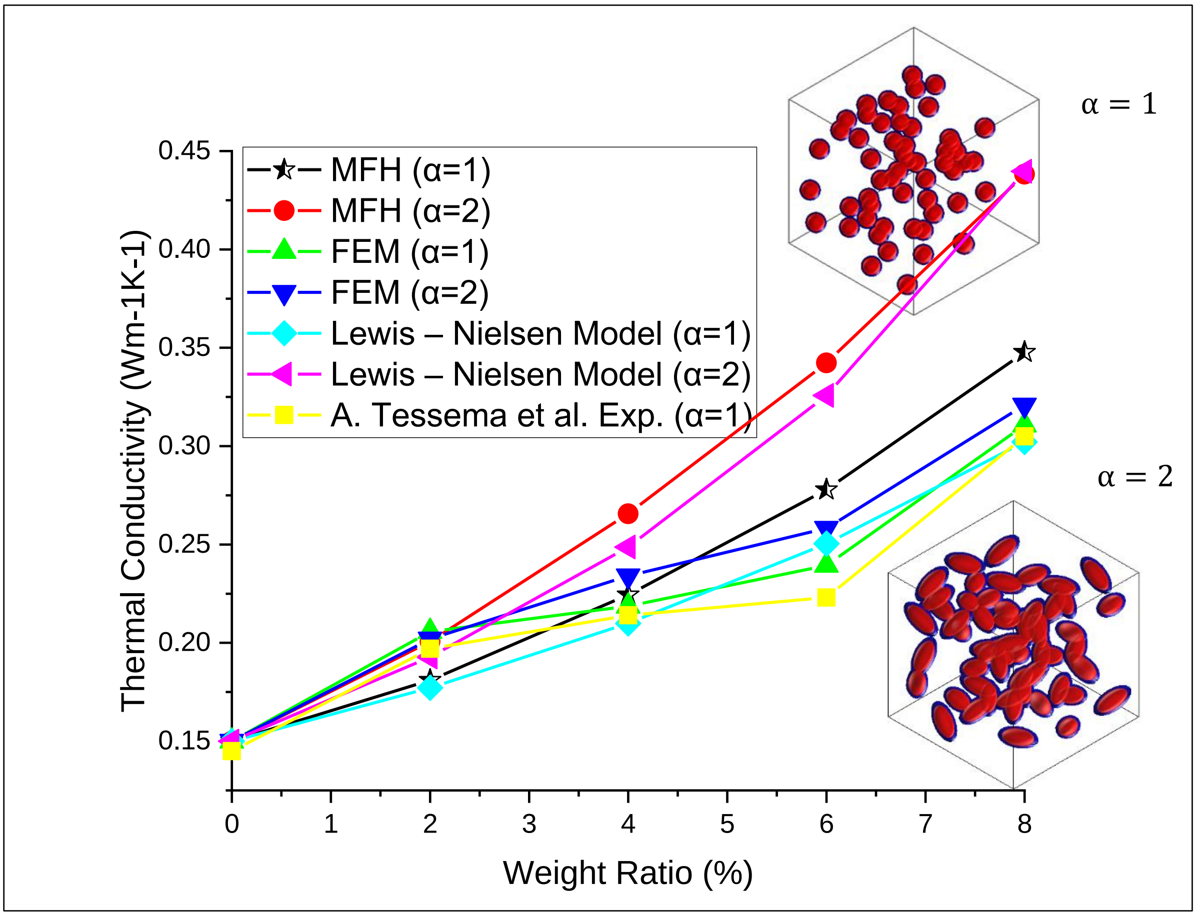


Figure 17 Effect of particle geometry on effective thermal conductivity.

The MFH, FEM, and analytical method are also applied to estimate the effect of inclusion geometry on the young's modulus of the PNCM and the result is given in figure 18. The result of the Analytical and MFH method implies the effective elastic modulus of neat epoxy can be improved by 15.4 % and 11.3 % by the addition of 15 % ellipsoid nano silicate volume fraction instead of fill with a spherical particle of the same volume fraction. The elastic modulus of the PNCM is increasing with the increase of the particle volume fraction and it is higher for ellipsoid particles than a composite of a spherical particle within equal inclusion contents.

Generally, the random distribution and generation of particles within the 3D RVE cause particle-to-particle interactions. Consequently, it stiffening the materials and also creates the particle-particle heat transfer channels which overcome the thermal barriers due to the low thermal conductivity of the constituents. Since this probability is high for the inclusion of higher aspect ratios, then the effective thermal conductivity and young modulus are higher for the polymer material filled with ellipsoidal inclusions than filled with spherical inclusions of equal volume fractions.

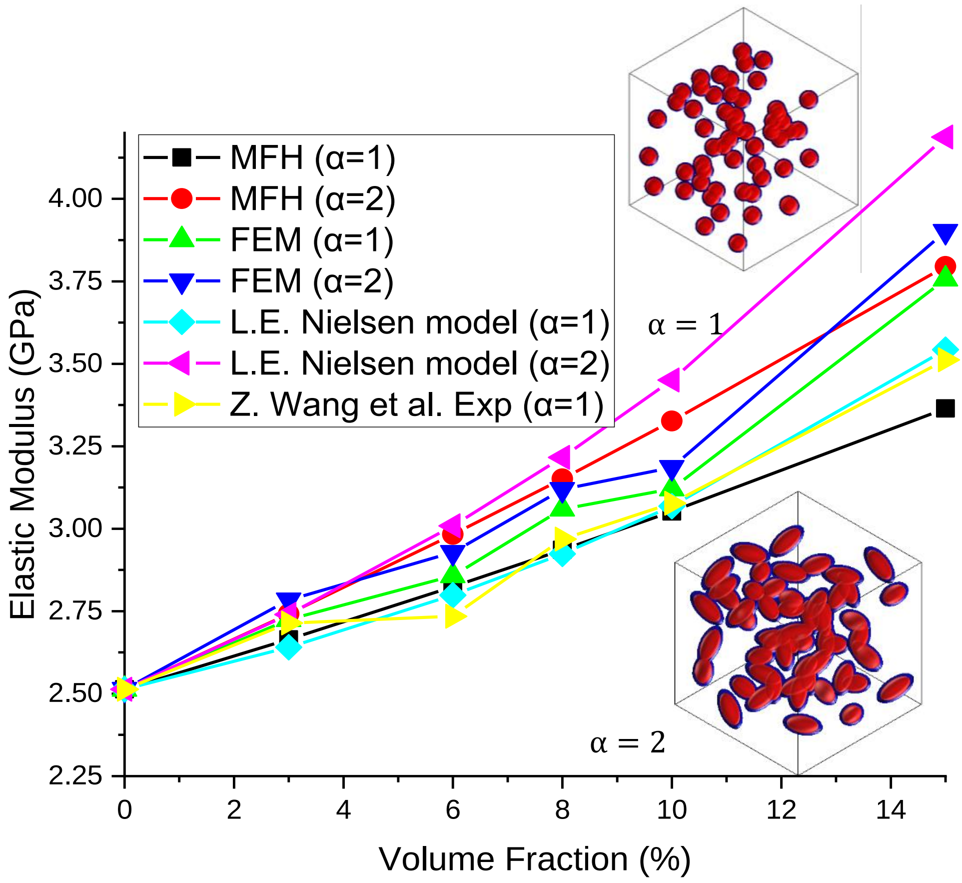


Figure 18 Effect of particle geometry on the effective elastic modulus.

5.2.3. Effect of Temperature

Figure 19 presents the effect of working temperature on the effective thermal conductivity of the polymer composite materials. The result of thermal conductivity is determined from the thermomechanical analysis at three different temperatures. The FEM result of the 2 % silicate particle weight ratio implies the effective thermal conductivity increases almost linearly with the temperature increment. Meanwhile, the result is 1.9 % lower than the experimental result at the first temperature test but it is it exceeds by 3.1 % at the final temperature test. Unlike the experimental result taken from the journal [8], the thermal conductivity of the 4 % silica particle weight ratio highly increases with the temperature. A similar condition is observed on the result of the 6 % particle weight ratio.

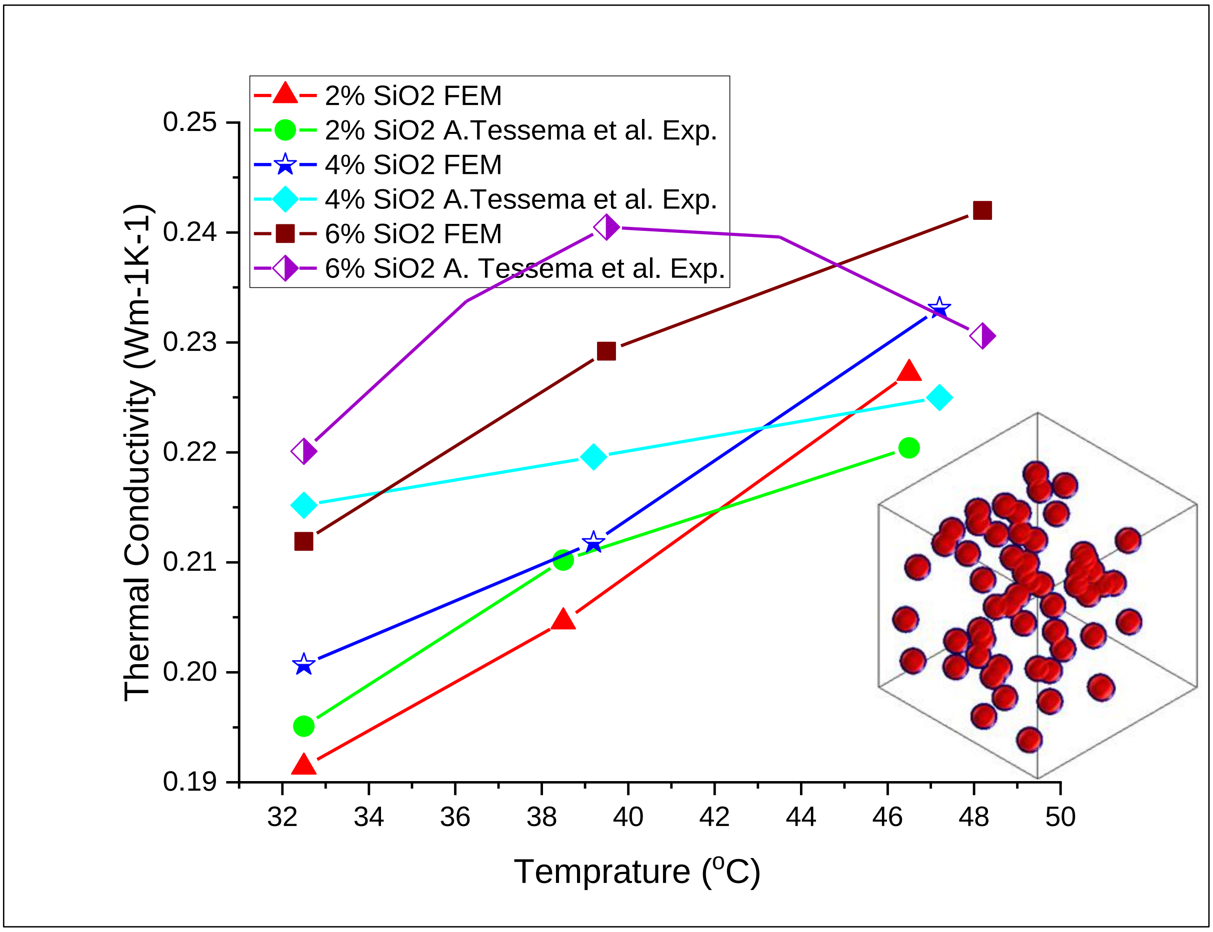


Figure 19 Effect of temperature on the effective thermal conductivity.

Since heat is transferred by the phonon vibrations in the particle reinforced polymer composite material, then the increment in temperature causes the molecular vibration which gives high phonon proliferation. Consequently, the effective thermal conductivity reaches its maximum value and the temperature is the glass transition temperature of the material. However, the phonon scatters beyond this temperature and the effective thermal conductivity reduces with temperature. as far as the random placement of the silica particle in the composite RVE can vary the glass transition of the composite materials than the FEM result given in figure 19 may not exactly match with the experimental results.

The temperature effect on the effective elastic modulus is predicted by FEM and MFH approaches. The macroscopic overall stress and strain corresponding to the uniaxial loads and uniform change in temperature is estimated from the thermomechanical analysis. Figure 20 provides the effective elastic modulus of the polymer nanocomposite material obtained from the numerical analysis of the composite RVE at three different temperatures.

Generally, the FEM and MFH approach result given in figure 20 depicts the elastic modulus decreases with increases the temperature. Specifically, the FEM result indicates the elastic modulus polymer composite material of 2 % and 6 % of silica particle weight ratio reduced by 13.7 % and 18.5 % with the given change in temperature, respectively. Moreover, the MFH approach result indicates the elastic modulus polymer composite material of 2 % and 6 % of silica particle weight ratio reduced by 15.2 % and 20.79 % with the given similar temperature change, respectively. This implies that the temperature has less effect on the polymer composite material of lower particle percentage weight ratios.

The temperature increment can rise the atomic vibrations which reduce the atomic bond or force by increasing the atomic distance within the given composite structure. Consequently, the stiffness of the nanoscopic particle reinforced polymer composite material reduces with increases the temperature.

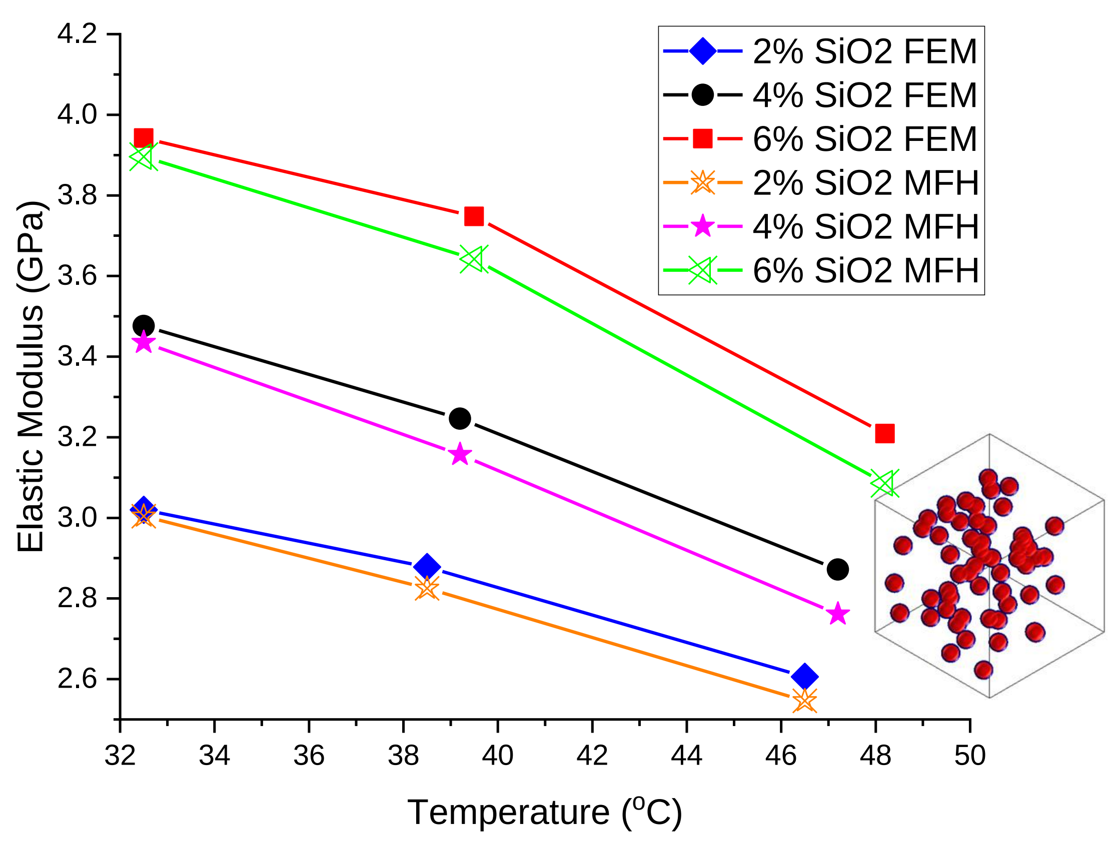


Figure 20 Effect of temperature on the effective elastic modulus.

CHAPTER SIX

6. CONCLUSION AND RECOMMENDATION

6.1. Conclusion

The effect of nano silicate particle volume fraction, geometries, and temperature on the effective thermal conductivity and elastic modulus of polymer nanocomposite material is investigated numerically using finite element method (FEM) and mean-field homogenization (MFH) approaches. For the validation purpose, the result of the Analytical model and the experimental work is also considered in this research. The following conclusions are drawn based on the result of the proposed approaches.

- The nanocomposite's effective thermal conductivity and Young's modulus of the polymer nanocomposite material increase with the increase of the nanoscopic silicate particle volume fraction within the epoxy matrix.
- The addition of ellipsoid ($\alpha = 2$) nano silicate particles improves both elastic modulus and thermal conductivity better than the spherical ($\alpha = 1$) nanoscopic inclusion of the same volume fraction.
- The effective thermal conductivity of the polymer composite material increases with increases in temperature and reaches its maximum value at the glass transition temperature of the composite material. However, beyond that temperature, the phonon disseminates, and the thermal conductivity reduces with temperature. Meanwhile, the random placement of the silica particle in the composite RVE can affect the thermal conductivity by varying the composite's glass transition temperature.
- The temperature increment causes the atomic vibration, which reduces the atomic bond strength within the polymer composite structures. Therefore, the effective modulus of elasticity/stiffness of the polymer nanocomposite decreases as the temperature increases.

6.2. Recommendation and Future Works

In this research work, the role of nanoscopic silica particle content, geometry, and working temperature on the effective thermal conductivity and elastic modulus of the epoxy matrix composite material is determined by the numerical approach and validated with an analytical model and experimental results taken from the journal. However, the particle dispersion state, size, shape (rather than ellipsoid), and the accurate size and properties of the interphase have a significant effect on the thermal and mechanical properties of the polymer nanocomposite materials. I recommend the future researcher consider and determine their role on the overall property of polymer composite materials.

The microstructure composite RVE is generated by Digimat multiscale simulation software and imported to the ANSYS workbench for further analysis. Meanwhile, it is possible to model using random sequential algorism (RSA) prepared in phyton script for more precision and minimize the effect caused by the random probabilistic placement of the particles within the composite representative volume element (RVE).

In the mean-field homogenization (MFH) approach, only the Mori-Tanaka homogenization scheme is considered and used for the analysis. But double inclusion homogenization scheme also gives good results and it is recommended for analysis of higher particle volume fraction.

The glass transition temperature of the polymer nanocomposite materials is not determined in this thermomechanical analysis but it is the important temperature to realize the thermal and mechanical behavior of the composite materials. I recommend the future researchers determine and evaluate the properties around and beyond that temperature.

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APPENDIX - A

Table I-A: Shape factors for several filler types.[51]

Filler Type	Aspect Ratio	C
Spheres	**1**	**1.5**
Cubs	1	2.0
Flakes	-	2.0
Random Fibers	**2**	**1.58**
Random Fibers	5	2.45
Random Fibers	10	4.93

Table II-A: Maximum packing fraction of selected fillers.[51]

Filler Type	Packing Geometry	ϕ_{max}
Spheres	Hexagonal	0.74
Spheres	Face centered cubic	0.74
Spheres	Body-centered cubic	0.60
Spheres	Simple cubic	0.52
Spheres	Random	0.637
Irregular	Random	0.637
Fibers	Random (L/D = 5:1)	0.52
Fibers	Random (L/D = 20:1)	0.20
Fibers	Unidirectional Random	0.637
Flakes	Random (L/t = 56:1)	0.33

Table III-A: Relative Einstein Coefficient for different poison's ratios.[29]

Poison's Ratio (v_1)	k_e at v_1/ (k at v_1= 0.5)
0.5	1.00
0.4	0.90
0.35	0.867
0.30	0.84
0.2	0.80

APPENDIX – B

Appendix I-B: Eshelby's tensor

The Eshelby's tensor component for an ellipsoid particle of aspect ratio ($\alpha = \frac{b}{a}$) embedded in an isotropic elastic matrix with the poisons ratio of V_m are, [1].

$$S_{1111} = \frac{1}{2}\left[\frac{1}{(1-V_m)}\left(\frac{4\alpha^2-2}{\alpha^2-1} - 2V_m - h(\alpha)\left(1-2V_m+\frac{3\alpha^2}{\alpha^2-1}\right)\right)\right]$$

$$S_{2222} = S_{3333} = \frac{1}{4}\left[\frac{1}{(1-V_m)}\left(\frac{3\alpha^2}{2(\alpha^2-1)} + h(\alpha)\left(1-2V_m-\frac{9}{4(\alpha^2-1)}\right)\right)\right]$$

$$S_{1122} = S_{1133} = \frac{1}{2}\left[\frac{1}{(1-V_m)}\left(2V_m - \frac{\alpha^2}{\alpha^2-1} + h(\alpha)\left(1-2V_m+\frac{3}{2(\alpha^2-1)}\right)\right)\right]$$

$$S_{2211} = S_{3311} = \frac{1}{2}\left[\frac{1}{(1-V_m)}\left(\frac{h(\alpha)}{2}\left(\frac{3\alpha^2}{\alpha^2-1} - (1-2V_m)\right) - \frac{\alpha^2}{\alpha^2-1}\right)\right]$$

$$S_{2233} = S_{3322} = \frac{1}{4}\left[\frac{1}{(1-V_m)}\left(\frac{\alpha^2}{2(\alpha^2-1)} - h(\alpha)\left(1-2V_m+\frac{3}{4(\alpha^2-1)}\right)\right)\right]$$

$$S_{1212} = S_{1313} = \frac{1}{4}\left[\frac{1}{(1-V_m)}\left(-2V_m - \frac{2}{\alpha^2-1} - \frac{h(\alpha)}{2}\left(1-2V_m-\frac{3(\alpha^2+1)}{\alpha^2-1}\right)\right)\right]$$

$$S_{2323} = \frac{S_{2222}-S_{2233}}{2}$$

where $h(\alpha)$ is a function is given by,

$$h(\alpha) = \frac{\alpha}{(\alpha^2-1)^{\frac{3}{2}}}\left[\alpha(\alpha^2-1)^{\frac{1}{2}} - \cosh^{-1}\alpha\right]$$

The function $h(\alpha)$ for an ellipsoid particle of $\alpha > 1$ is given by,

$$h(\alpha) = \frac{\alpha}{(1-\alpha^2)^{\frac{3}{2}}}\left[-\alpha(\alpha^2-1)^{\frac{1}{2}} + \cos^{-1}\alpha\right]$$