

EPOXY RESINS REINFORCED WITH BORON NITRIDE AND ALUMINUM OXIDE PARTICLES: A NUMERICAL THERMAL CONDUCTIVITY ANALYSIS

A Thesis Submitted

In partial fulfillment for the award of the degree of

Master of technology

In

Production Engineering



SUBMITTED BY

**Taha Shees
(2K20/PIE/09)**

UNDER THE GUIDANCE OF

Dr. Sanjay Kumar and Prof. Qasim Murtaza

**DEPARTMENT OF MECHANICAL, PRODUCTION & INDUSTRIAL
AND
AUTOMOBILE ENGINEERING
DELHI TECHNOLOGICAL UNIVERSITY
BAWANA ROAD, DELHI-110042**

CANDIDATE'S DECLARATION

I, TAHA SHEES, hereby certify that the work which is being presented in this thesis entitled "EPOXY RESINS REINFORCED WITH BORON NITRIDE AND ALUMINUM OXIDE PARTICLES: A NUMERICAL THERMAL CONDUCTIVITY ANALYSIS " being submitted by me is an authentic record of my own work carried out under the supervision of Dr. Sanjay Kumar and Prof. Qasim Murataza, Department of Mechanical Engineering, Delhi Technological University, Delhi.

The matter presented in this thesis has not been submitted in any other University/Institute for the award of M.Tech Degree.

TAHA SHEES
(2K20/PIE/09)

CERTIFICATE

I, TAHA SHEES, hereby certify that the work which is being presented in this thesis entitled “EPOXY RESINS REINFORCED WITH BORON NITRIDE AND ALUMINUM OXIDE PARTICLES: A NUMERICAL THERMAL CONDUCTIVITY ANALYSIS” in the partial fulfillment of requirement for the award of degree of Masters of Technology in Production Engineering submitted in the Department of Mechanical Engineering, Delhi Technological University, Delhi is an authentic record of my own work carried out during a period from July 2020 to June 2021, under the supervision of Dr. Sanjay Kumar and Prof. Qasim Murtaza, Department of Mechanical Engineering, Delhi Technological University, Delhi.

The matter presented in this thesis has not been submitted in any other University/Institute for the award of M.Tech Degree.

Dr. Sanjay Kumar
Supervisor
Department of Mechanical Engineering
Delhi Technological University, Delhi

Prof. Qasim Murtaza
Supervisor
Department of Mechanical Engineering
Delhi Technological University, Delhi

ACKNOWLEDGEMENT

It is a matter of great pleasure for me to present my dissertation report on “EPOXY RESINS REINFORCED WITH BORON NITRIDE AND ALUMINUM OXIDE PARTICLES: A NUMERICAL THERMAL CONDUCTIVITY ANALYSIS”. First and foremost, I am profoundly grateful to my guide Dr. Sanjay Kumar and Prof. Qasim Murtaza, Mechanical Engineering Department for their expert guidance and continuous encouragement during all stages of thesis. I feel lucky to get an opportunity to work with them. Not only understanding the subject, but also interpreting the results drawn thereon from the graphs was very thought provoking. I am thankful to the kindness and generosity shown by them towards me, as it helped me morally complete the project before actually starting it.

I would like to extend my gratitude to Prof. S. K. Garg, Head, Mechanical Engineering Department for providing this opportunity to carry out the present work.

Finally, and most important, I would like to thank my family members for their help, encouragement and prayers through all these months. I dedicate my work to them.

DATE:

Taha Shees

PLACE:

(2K20/PIE/09)

Table of Contents

Content	Page No.
Abstract	2
Objective of this Research	3
Chapter 1 INTRODUCTION	4 - 17
1.1 History of Composites	4
1.2 Composites in Brief	4
1.3 Definition of Composite	7
1.4 Types of Composite Materials	7
1.4.1 Metal (MMC)	8
1.4.2 Ceramic (CMC)	8
1.4.3 Polymer (PMC)	8
1.5 Classification of Polymer Composites	9
1.5.1 Fibre (FRP)	9
1.5.2 Particle (PRP)	11
1.5.3 Structural (SRP)	12
1.6 Composite vs Conventional material	12
1.7 Advantages of Composites	14
1.8 Application of Composites in various fields	14
1.8.1 Aircraft	16
1.8.2 Space	16
1.8.3 Sporting goods	16
1.8.4 Medical devices	16
1.8.5 Chemical industry	17
1.8.6 Marine	17
1.8.7 Commercial	17
Chapter 2 LITERATURE SURVEY	18 - 34
2.1 Particulate filled polymer composites	18
2.2 Thermal Conductivity of Polymer composites	19
2.3 Material properties of epoxy resins. BN and Al ₂ O ₃ as reinforcements	20
2.4 Thermal and dielectric behavior of BN and Al ₂ O ₃ reinforced with epoxy resin ...	23
2.5 Thermal Conductivity Models	27
2.6 Knowledge gap in earlier investigations	33
2.7 Chapter Summary	34
Chapter 3 METHODOLOGY	35 - 41
3.1 Mathematical Models used for Thermal conductivity estimation	35

3.2	Concept of ANSYS	36
3.3	General Steps in FEM	38
3.4	Benefits of FEM over other Counterparts	39
3.5	Simulation Method	40
Chapter 4	RESULTS AND DISCUSSION	47 - 52
CONCLUSIONS	53
SCOPE FOR FUTURE WORK	54
REFERENCES	55 – 61

**EPOXY RESINS REINFORCED WITH BORON
NITRIDE AND ALUMINUM OXIDE PARTICLES: A
NUMERICAL THERMAL CONDUCTIVITY
ANALYSIS**

ABSTRACT

An epoxy composite containing boron nitride (BN) and Al₂O₃ micro-fillers implanted was tested for heat conductivity in this thesis. The thermal conductivities of these composites, which had BN-Al₂O₃ contents varying from 0% to 50% volume were numerically derived from simulation using the CAE programme ANSYS modeled using representative volume elements, which explains heat transmission inside epoxy matrix filled with micro-BNs and Al₂O₃. There is an increase in effective thermal conductivity of almost as high as 7-8 times for 50% volume percent BN-Al₂O₃ in epoxy matrix compared to plain epoxy resin. The experimental data on similar filler type and concentrations exhibit similar trends.

Keywords: h-BN, Al₂O₃, Composites, Epoxy resins, FEM, Simulation, RVEs

OBJECTIVES OF THIS RESEARCH

- Formulation of geometrical model to mimic the real-world behavior of BN-Al₂O₃ filled in Epoxy composites.
- Analysis of thermal behavior using finite element (FEM) of the particulate-polymer composite.
- The presence and effect of BN and Al₂O₃ particles on the thermal behavior of these reinforced epoxy composites.

Chapter 1

INTRODUCTION

1.1 History of Composites

A major breakthrough in the history of materials was the creation of composite materials and its accompanying design and production processes. To satisfy the specific needs of an application, composite materials have unique mechanical and physical qualities that cannot be matched by any other material. Many composites are also resistant to corrosion, oxidation, and wear at high temperatures. Because of their unique properties, mechanical engineers have a wide range of design options unavailable to them when working with traditional monolithic materials. Because of the high strength dispersion and poor mechanical and thermal shock resistance of monolithic versions, composite technology allows the use of a whole class of solid materials in these applications. Components may be consolidated to reduce production costs since several composites manufacturing techniques are well-suited to fabricating big, complicated structures. A new product must be developed as a result of this mandate. In order to find homogenous structural materials with the appropriate properties for a specific application, composite materials were created. Tomb paintings at the art museums still show the brick-making process. Spacecraft are frequently using the most sophisticated instances of this technology. Pavements made of steel or RCC are the most readily noticeable. Their near proximity to our personal hygiene makes them an ideal choice for bathroom fixtures. Sinks and counter tops made of solid surface, imitation granite, and cultured marble are common in homes nowadays. Constituent materials are the distinct components that make up composites. A composite is made up of two types of materials: matrix and the filler reinforcement.

1.2 Composites in Brief

These days there is an overwhelming interest in the composites in the practical as well as research world. Composites comprise of reinforcement fibers, particles, in a matrix of flakes and/or fillers in the form of metals, or ceramics or polymer. The

reinforcement is held in place by the matrix and helps the matrix achieve the required shape while also improving the matrix's overall mechanical qualities. So the newly combined materials are stronger than the components as a whole. This substance is termed the reinforcing phase and it consists of fibres or particles that are incorporated into another material known as the "matrix phase." Composites are typically categorized by the matrix material. There are a variety of composites on the market, each with a specific set of uses. There are two types of reinforcing materials: fibrous and non-fibrous (particulates). For structural design applications, composite materials offer a significant advantage over traditional materials because of their greater specific qualities such as strengths be it impact or tensile, fatigue characteristics. Epoxy resins in specific are poly-ether resins with multiple epoxy groups that may be transformed into thermoset resins. Despite there being a solvent which can evaporate, the resins, when formed aren't volatile as such upon curing. One way to refer to epoxies is to call them epo-oxides

Adhesives, packaging, building materials be it flooring, pavement, and aggregates, laminates, covers, molding, and garments are just some of the many applications of epoxy resin. In recent years, they've found use in the aerospace and air transportation industries.

Various electronic components are often encapsulated using epoxy or polyester resin systems because to their.

Despite its early nineteenth-century discovery, boron nitride was not used in industry until the second part of the twentieth century. In the modern periodic table, both nitrogen and boron have the same atomic radii as carbon, and their paired electrons in the exterior shell also happen to be similar. The crystal structure of boron nitride and carbon is also not a surprise. It is possible to synthesize the hexagonal and cubic boron nitride shapes, unlike charcoal, graphite, and stone, which are naturally occurring. H-BN (h-BN) is the name given to the structure grafted upon it (see Figure.1). In the same way that graphite is a plate with a microstructure having layers, it also can lubricate. h-BN prevents sintering and is normally made by pressing the material with a gentle force.

In terms of both shape and characteristics, cubic boron nitride is identical to diamond. C-BN also stands second hardest substance after diamond. Happens to be that only few years ago C-BN got developed industrially, despite the fact that its synthesis was originally performed in 1957.

Hexagonal Boron Nitride (h-BN)

HDPE BN particles, that is, HDPE-enhanced BN particles, were examined by Wenying Zhao et al [55] to determine the thermal conductivity of HDPE-BN particles (HDPE). Composites with poor heat conductivity should have a greater HDPE content.

One that's a little more substantial. Yet another escalation in magnitude. Boron nitride (BN) composites were split using the conduit, which was tested with a variety of carbon and ceramic fibers. The mechanical strength and hardening of composites were determined by the fiber and fiber/matrix interface interfaces. The mechanical properties of C / BN were predicted to be similar to those of C / C due to the structural similarities between BN and biomass. Carbon fiber and a compact matrix make up the two composites. It was also found that in the matrix significantly thermally driven aluminum (AlN) and Boron nitride fillers were utilized to evaluate the influence of particle size and relative structure on the thermal conductivities of Honget.al Jung-Pyo composites by Gofer and colleagues [56]. To enhance particle packing, it features a bimodal distribution of particle sizes. Due to its ability to create conduction networks, the filler matrix structure is exceptionally temperature-conductive and provides low thermal resistance throughout the path. To increase the heat conductivity of polymer encapsulates or substrates, Hatsuo Ishid et al. utilize solid thermal ceramic materials in polymers. According to Jens Eichler et al., BN's nuclear structure is mostly controlled by its physical qualities. H-BN is also known as white graphite because of its hexagonal BN isolator layer's weak van der waals forces, which enable layers to glide smoothly across one other.

1.3 Definition of Composite

Two or more independent components (phases or phase combinations) fuse together on the compound interface to form these, all of them come from different component in the composite.

- Devices of electronics comprised of layers of materials is not a composite, but rather some complete structure comprising of many components forming bonds together, and as far as uses are concerned, composites find their usage in the fabrication of several variously shaped components (although one of the materials in the packaging could be considered a composite).
- The reinforcing phase, which is made of fibers or particles, is incorporated into the matrix phase, which is the other material. particles within composites increase their mechanical qualities, be it strength to energy, whereas the matrix's major job is to stress transfer from fiber to fiber or particle to particle in order to save them from any failure.

The goal is to maximize the benefits of both materials' strengths while minimizing the drawbacks of either. Many lightweight and high-strength applications have been effectively replaced by composite materials. As a result of their light weight, great strength, especially tensile, at elevated temperatures and excellent resistance to creep, composites often find themselves being used in these kinds of applications.

1.4 Types of Composite Materials

Composites are generally grouped by the virtue of the composite usage, broadly three of them metal (MMC), ceramic (CMC), and polymer (PMC).

1.4.1 Metal (MMC)

This kind of composite is made up of metal alloys that are reinforced by longitudinal fibers, threads or particles (finite flakes, rather than fibers) that are thin fibers in the form of crystals. They can withstand higher temperatures than PMCs and employ metals as a matrix, but they tend to be more robust in construction. Strength and rigidity, better creep and fatigue tolerance, improved stiffness, wear and abrasion, and the ability to work higher than unreinforced metals are the primary qualities of metals reinforced with strong ceramics or fiber.

1.4.2 Ceramic (CMC)

Carbon, silicon, and carbide fibers, as well as aluminum-calcium alumina silicone, support a ceramic matrix in ceramic composites (CMCs). Heavy ceramic and chemical inert operating temperature restrictions enable CMCs to operate at high power densities while maintaining toughness, low density, and chemical inertness. Because of this, ceramics have a low toughness to fracture. The final material's power is one of the most important objectives in the production of ceramic matrix composites. Several times, for example, associative changes are predicted and not. The strength and stiffness of ceramic items may make them a product engineer's dream in many respects.

1.4.3 Polymer (PMC)

Corrosion-resistant, easy-to-form, and low-density polymeric matrix composites are all advantages of polymeric matrix composites. They're becoming more and more common in a variety of business settings, including the automobile and aerospace industries. Polymers' mechanical qualities, in general, are insufficient for many structural applications, notably in terms of strength and stiffness. The manufacturing of PMCs doesn't need high temperature pressure. Making polymer matrix composites also necessitates the use of more basic machinery. Structural applications became popular for polymer composites because of this.

1.5 Classification of Polymer Composites

Based on their reinforcing materials, we generally classify polymer composites into three groups: Fiber (FRP), Particle (PRP) and Structural (SPC).

Compared to their cross-sectional dimensions, the reinforcing fibers used in fiber reinforced composites have a substantially longer length. If the qualities of such a composite are affected by fiber length, it is referred to as a discontinuous fiber or short fiber composite. Fibers and matrix make up the majority of a fiber reinforced composite's common phase. Composites rely heavily on fibers for their structural integrity. Reinforcement is the primary function of fibers; nevertheless, the matrix acts as a glue and transmits stresses (load) between fibers. Filler is sometimes used to smooth out the production process, giving the composites unique features and lowering the cost of the final product. Polyurethane, polyester, vinyl ester, phenolic resin, epoxy, and other polymers are frequent matrices as well. Epoxy and polyester resins are the most often utilized resin materials. Second place goes to epoxy resin because of its superior adherence and less shrinkage compared to polyester resin.

1.5.1 PARTICLE REINFORCED POLYMERS

They are grouped in two categories, being cheap and extensively used.

- When the matrix is properly bound, large-particle composites operate as a restraint on the mobility of the matrix.
- Composites with 10-100 nm particles that are dispersion-strengthened. Applied loads are borne primarily by the matrix, which is hindered in its ability to bend plastically by the tiny particles.

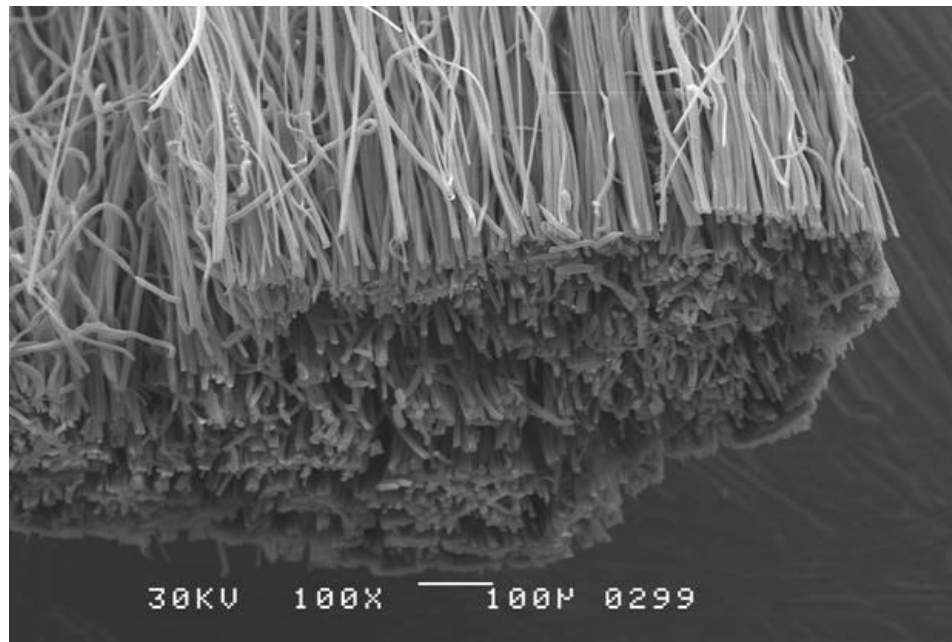


Fig. 1.1: Microscopic image of fiber tow.

Most often, they're employed to increase ductility and reduce the overall weight of the composite. Construction costs may be reduced by using parts. These things may be made at little cost and with minimal effort. High melting point, low density, stiffness, wear and corrosion resistance are some of the beneficial qualities of ceramics or glasses. Thermal and electrical insulators may be made from a wide range of ceramics. Low-temperature ceramics with magnetic, piezoelectric, and superconducting properties are available. These features are included into the final product. The fact that glassware and ceramics are often broken is a major drawback. A tyre vehicle with black carbon particles within an elastomeric polymer poly-isobutylene matrix is an example of a composite strengthened by particles.

1.5.2 Structural Polymer Composites

Matrix-based layers of materials make up the laminar composites' structure. Sandwich constructions are also included in this category. Several old metals and materials have been replaced by polymers in a variety of applications since their introduction. There are several reasons for this, including the benefits of polymers over conventional goods, such as their speed of production and cost reductions when used in composites.

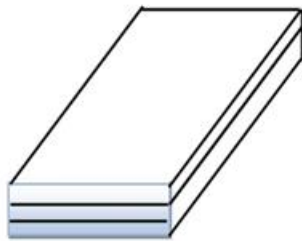


Fig 1.2 Laminate composite

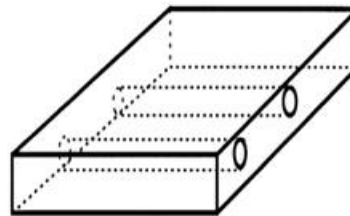


Fig. 1.3 Fiber composite

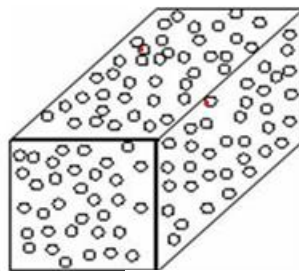


Fig. 1.4 Particulate Reinforced Composites

They've taken an interest in a broad range of technical disciplines, with a special focus on aerospace applications. Modern composites are produced quickly and may be used in a range of working settings with various fillers and fibers. Fillers and fibers alter polymer characteristics to meet high strength or assembly requirements. Fiber-reinforced polymers, in contrast to conventional synthetic textiles, have benefits. Such composites are employed in a variety of fields, from computers to spacecraft, because of their versatility.

1.5.3 Laminate Definition

A single smooth, matrix-shaped sheet of unidirectional fibers or tissue fibers is known as a lamina (also known as a ply or sheet). A laminate is a single piece of plywood that is bonded together. Each sheet may be positioned in a variety of ways and contains a variety of different materials. Average features of composites are determined by the unique characteristics of each individual component. “Stiffness, strength, moisture expansion, and temperature all fall under this category. By assuming the ply is homogeneous, average characteristics are derived. At this stage, we need to account for the lamina's stiffness and strength. This is the term given to the micromechanics of a lamina. Laminated ones in there are bounded by matrices and are made up of multiple fiber layers. Typically, these layers are meant to enhance the matrix-reinforcement bond. Depending on the final use of the material, the orientation of the fiber reinforcement might be either unidirectional or bidirectional. Plastic laminates may be classified as either symmetric or unidirectional cross-plying. Resistance and stability are often required for composites. This is accomplished by aligning the long fibers in a paper-like sheet or lamina. Having said that, these show anisotropic nature and tend to be slow in cross-direction motion (with poor rigidity). It is common for stability and strong strength to be required for multiple different directions in a planar form. Laminates essentially happen to be stacks of fibers arranged in multiple orientations and fused together to form a barrier.

1.6 Composite vs Conventional Material

- When compared to properly manufactured structural components, the toughness resistance of aramid epoxies with reinforced carbon fiber may be as much as 60% more than that of steel and aluminum.
- Degradation-tolerance fiber composites tend to be less expensive across their whole life cycle. It is more flexible than metals and may be fitted for difficult construction demands like aero-elastic wing fitting and the vertical and horizontal aircraft stabilizers, which need a high degree of rigidity and flexibility. Composite materials have a far shorter history of service and

dependability than metals. When compared to Aerospace Aluminum and Carbon Alloy, Aramid-epoxy material has somewhat greater Effect Energy levels.

- Plastic fibers may be made to have superior structural damping qualities, making them less jarring and more resonant than metallic materials.

1.7 Advantage of Composites

The high efficient development of the many composite materials and types of structural fibers now accessible to designers is evidence of their many benefits.

- Towards increased rigidity of the torsion.
- The atmosphere has been changed.
- Towards a strong degree of stability.
- Potential progress in the effects of wear and friction.
- The heat conductivity increased or decreased.
- Downward surplus products.
- Towards strong tolerance to corrosion.
- Good tolerance to impact and injury.
- Carbon rigidity and resilience are stronger than traditional metals.

1.8 Various Applications of Composites

We employ metal matrix and ceramic matrix composites when we need a high-temperature application, such as in a nuclear reactor. Polymer composites may be used in a wide range of industries. Epoxy, phenolic, acrylic, urethane, and polyamide are just a few of the polymers often found in polymer composites. Because each polymer class has unique properties and advantages over the others, its use is dictated by the circumstances. Suitable fillers and reinforcements are added to polyester resin for use in road transportation. Low cost, simplicity of design, and scalability were factors in the decision.

The system and other applications have continued to benefit from the usage of polyester reinforcements. Depending on the application, different amounts of thermoplastics and reinforcing fibers are used. Several automotive components are made from thermoplastics. In addition to cost-effectiveness and mechanical strength, volume is taken into consideration when selecting a material. For typical paint finishing, thermosetting resins are employed, although thermoplastics are more often used for molding. It is possible to make huge pieces in a small amount using press-molded reinforced polyester. From tennis racquets to the space shuttle, polymer matrix composites come handy in many places. A few real-world examples from each sector were chosen rather than just listing the many applications for polymer-based composites. The importance of using a composite material has been emphasized.

1.8.1 Aircraft

Commercial airplane manufacturers mostly use PMCs. A Composite must not be used in conjunction with secondary components such as graphite / epoxy rubbers and lifts in the Boeing767 and Kevlar-type landing gear door panels and aircraft floorings. When compared to plastics, the life expectancy of rotor blades is increased by more than 100% with the use of graphite/epoxy and glass/epoxy materials, but even the peak speeds are enhanced.

1.8.2 Space

Composites are largely characterized by elements such as weight, high-specific modules, and dimensional flexibility as one of the most important mechanical properties necessary to meet the intended demand during substantial temperature variations in the room.

1.8.3 Sporting goods

A variety of disciplines must be included into the design of sporting equipment in order to maximize performance while also minimizing the risk of damage to those who use it. The diverse properties of materials must be taken into account while constructing sporting equipment. Durability, toughness, and various other mechanical properties and very critical of these properties are all included.

1.8.4 Medical devices

Glass-Kevlar/epoxy lightweight masks are called for in the standard for patients with epilepsy. To guarantee the patient's comfort, portable prosthetic lungs are made of graphite glass and epoxy.

1.8.5 Chemical Industry

Composites have been popular in the chemical industry because to their low weight, moldability, and fire resistant qualities. Engineered plastics were employed for a variety of applications, including storage containers, scrubbers, ducts, exhausts, motors and tubes, blowers, frames, reactors, and more.

1.8.6 Marine

This is in addition to the advantages of lightweight composites, moldability and the chemical industry's sensitivity to fire-resistant qualities. For a wide range of applications, engineered plastics were employed. These included storage containers as well as cleaning equipment as well as ductwork and exhaust systems.

1.8.7 Commercial

Fiber-reinforced polymers are used in a wide variety of commercial applications. Handles without joints or lines are common on pharmaceutical factory brooms.

Chapter 2

LITERATURE SURVEY

It is the goal of this literature review to offer context for this thesis and to stress the importance of this research. The thermal behaviors of the composites are the focus of this book's discussion of related topics. A quick review of the material is covered.

2.1 Particulate filled Polymer Composites

Thermosetting and thermoplastics are the major subgroups of polymers. It is widely used nowadays to significantly enhance the mechanical qualities of PTFE, be it resistance to wear, by metal/ceramic made hard particulate fillers. Polymers and polymer matrix composites with a broad variety of industrial uses, such as electrodes and heaters, may be reinforced with metal particles. Polymer thermal stability is critical, and high-temperature-resistant composites have been studied in [3] and elsewhere. Cheap density, excellent chemical and corrosion resistance, simplicity of manufacture, and being easy to the pocket are all advantages of these engineered polymer composites [4-6]. Research on ceramic-filled polymer composites has been place during the last two decades. Research by R. N. Rotheron [7, 8] found thermoplastics having mineral fillers: production and characterization of fillers. Increasing the stiffness and reducing the cost of polymers are the primary reasons inorganic fillers are used in commercial applications.

The combination of particle reinforced composites and fiber-reinforced composites worked effectively in a variety of real-world applications, including thermal and mechanical sectors. ' The chemical, mechanical, and thermal characteristics of polymer composites are significantly improved when silica particles are included into the matrix of the polymer. Several investigations investigating the influence of particle size on mechanical properties [11- 17] are leading to smaller and smaller particles. To a large extent, mechanical behavior of composites is determined by virtue of such as particle size, shape, vol. fractions, and surface area. With regard

to the mechanical properties of silica particles, Yamamoto et al. [18] focused on fatigue tolerance, tensile properties, and fracture characteristics. Impacts on fracturing properties of silica particle sizes and shapes based on Nakamura et al. Enhanced flexural and tensile strength due to increased particle surface area.

2.2 Thermal Conductivity of Polymer Composites

Thermosetting polyesters (UP) resins are extensively utilized because of their strength, dimensional durability and low weight. They also have good corrosion characteristics and are inexpensive. Thermal and mechanical behavior of ceramic-filled epoxy have been successfully shown by Wong et al. [24]. Thermal conductivity may be approximated using Agari's model. This is a good result. In the field of polymer heat conductivity, researchers like Hansen et al and others have made significant contributions by finding that thermal transfer increases significantly in the direction of orientation and decreases marginally in the direction of orientation. Nevertheless, the majority of these studies focus only on the thermal activities of smooth polymers and ignore all other mechanisms. Some filled polymer composites have been tested for heat conductivity [29-41] in the present literature.

Among the most often utilized fillers are copper and silver, black-burning crystals, short fiber carbon pellets and iron, graphite, magnetite, and coffee nitrides. Progelhoft examined the concepts and techniques for determining the thermal conductivity of composite structures in great detail. Polymers filled with a variety of fillers may be tested for thermal conductivity using Nielsen's Procter and Solc [43] model. As an updated Bruggeman model for the Al₂O₃ / epoxy and AlN / epoxy systems, Nagai and Lai [44] discover that both hypotheses are significant predictors of thermal conductivity. From 0.35 W/mK anisotropy to 50 W/mK orientation ratio, Griesinger et al. found that the thermal characteristics of low-density poly-ethylene (LDPE) improved with increasing orientation ratio. It was discovered by Tavman [46] that polyethylene composites filled with copper powder have mechanical and thermal properties, while it was discovered experimentally by Sofian et al. [47] that metal powder filled HDPE composites (copper, zinc, iron, and bronze) have thermal conductivity, thermal diffusivity, and

specific heat [48]. The thermal conductivity of the metal powder filling content was greatly enhanced to up to 16%. Polymer composites with poor thermal and electrical conductivity were described by Mamunya et al. as an improvement in the hypothesis of the properties of metal-filled polymers. Filler particle interconnectivity and thermal conductivity were also examined by Weidenfeller et al. Polypropylene was extruded and injection molded using commercially available fillers, and the density or heat transport properties of these polymer composites may vary from one sample to another. For the prepared polypropylene, they found a range of 0.27W/mK to 2.5W/mK at 30 volts of thermal conductivity (PP). Although copper conductivity is roughly 40 times greater than that of talc, the (PP) matrix had a talc content of 1.25 percent even though copper conductivity is around 40 times more than that of talc. Thermal conductivity of plastics was significantly influenced by filler type factor studies. According to Kumlutas and Tavman [52], thermal conductivity of polymer composites filled with particulate matter rises by 8 percent and 16 percent from 0.554W/mK-0.681W/mK and 1.116W/mK respectively, which represents a volume filler content of 23 percent and 101 percent, respectively, from the 0.554W/mK value for pure HDPE samples. HDPE matrices filled up with small particles up to 16 percent by volume had its thermal conductivity calculated using various methodologies, and the results were compared. Patnaik et al. concluded that there may be an association between the thermal conductivity of the filled particles and their wear resistance. to the [53]; A Monte-Carlo approach developed by Intelligences was used in the MacroPac project by Sanada et al. [54] to generate a unit cell of randomly distributed micro fillers and investigate their microstructure and thermal conductivity

2.3 Material properties of Epoxy resins, and BN and Al₂O₃ as fillers

Matrix Material: There are several types of epoxy resins. The matrix material is Epoxy LY 556 resin, a chemical member of the epoxide family. The suggested weight ratio for the low temperature curing epoxy resin (Araldite LY 556) and hardener (HY 951) is 10:1. They are organic liquids with epoxide groups in them. Due to its low density (1.1 gm/cc), epoxy is the most often utilized polymer in the industry. The ring of epoxide has three atoms: one oxygen and two carbons. Most epoxies are the result

of the epichlorohydrin reaction with phenols or aromatic amines. Epoxy has a thermal conductivity of just (0.363W/m.K) at its lowest value.

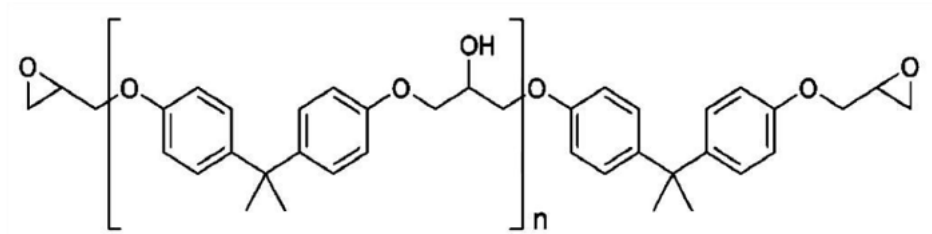


Fig 3.1: Unmodified epoxy pre polymer resin chain.
(‘n’ denotes number of polymerized unit)



Reinforcements: -Hot-pressed Boron Nitride exhibits whitish color and is solid. Because of its low porosity, it can be readily shaped with ordinary carbide tools into complicated designs. Because of the orientation of the platy hexagonal crystals during the hot press consolidation, the composites have anisotropic electrical and mechanical characteristics. Heat transfer is 220W/m.K and density is 2.34 gm/cc correspondingly.

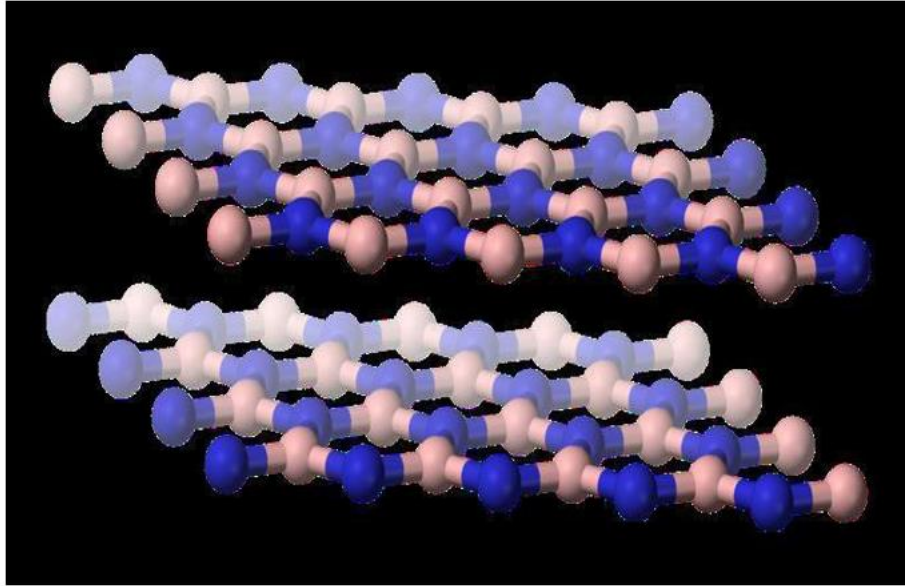


Fig 3.3: Hexagonal crystalline form of Boron Nitride (h-BN or α -BN)

"White graphite" is the name given to boronic acid because of its similar platy hexagonal structure to carbon graphite. Electrical insulator BN, which has great thermal conductivity and strong resistance to thermal shocks, is a suitable choice for high-temperature applications. At temperatures up to 2800 degrees Celsius, BN is stable and inert, although it is reactive at temperatures up to 850 degrees Celsius. These include a pure diffusion bond grade, calcium boron binder system, and boric oxide binder system. Moisture is absorbed by the boric oxide-containing substance (Grade BO) causing swelling and property loss. Grade CA calcium borate-based material is water-resistant.

Similarly, Al_2O_3 also exhibits great mechanical and thermal properties when used as filler.

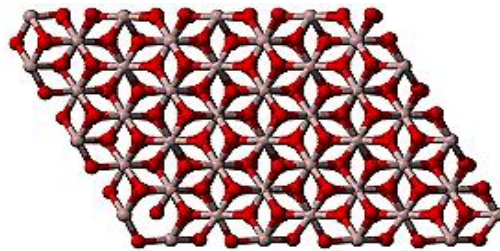


Fig. The molecular crystalline form of Al_2O_3

The important individual properties are shown in the table below

Material	Mean Particle Size (μm)	Thermal Conductivity ($\text{W m}^{-1}\text{K}^{-1}$)	Density (g/cm^3)
BN	2.5	220	2.1
Micro Al_2O_3	5	29	3.89
Nano Al_2O_3	0.19	27	
Epoxy		0.22	1.17

2.4 Thermal and Dielectric Behavior of BN And Al_2O_3 Reinforced in Epoxy Resin.

BN HDPE composites have been researched for their heat conductivity, for example, by dispersing BN HDPE particles with HDPE particles surrounded by BN particles. Composites with bigger HDPE sizes have a greater thermal conductivity than those with smaller HDPEs. As the filler content rises, so does the heat conductivity. Thermal conductivity of composites may be improved by using both BN particles and alumina short fiber [55]. BN particles alone can't do this. It has been studied the fracture behavior of boron nitride (BN) composites reinforced with a variety of carbon and ceramic fibers. The mechanical strength and toughness of the composites were discovered to be controlled by the properties of the fibers and the fiber-matrix interface.

Based on the structural similarities between BN and biomass, C / BN was anticipated to have a mechanical activity comparable to C / C. Carbon fiber and a tiny matrix frame make up the two composites. Fillers of aluminum nitride (AlN) and boron nitride (BN) are included into the epoxy matrix in order to identify the impact of particle size and relative structure on the thermal conductivity of composites. The incorporation of micro-electronic devices at high capacities and frequencies, such as light emitting diodes (LEDs), memory chips, and other electronic devices, results in vast amounts of heat being generated and easily distributed by PCBs and/or electronic devices, e.g.

The thermal stability limit of the system might be exceeded as a result of the generated heat.

In the A-stage, the viscosity of bisphenol-A polybenzoxazin is very low, making it possible to dampen and combine the filler. An increase in particle packing rate may be seen as a result of this bimodal distribution of particle size. This filler matrix technology provides a highly thermally conductive composite due to its ability to form conducting networks with low thermal resistance throughout the route. Heat loss in packaging of microelectronics is becoming more essential as the need for smaller, faster circuits grows. Increasing the conductivity in substrates has long been investigated by applying highly thermally conductive ceramic materials to polymers. The atomic structure of BN has a significant impact on the material's physical properties. As a result, oil and pure graphite, commonly known as h-bn [59], are isoelectronic. The hexa-BN stages are linked by soft Van der Waals forces, making it easy to see each other's layers. Because of this, h-BN may be found in sintered structures (such as side dams) where it serves as a lubricant or release agent or it can be found in a suspension or coating (e.g., extrusion of aluminum or titanium). An aluminum nitride composite (LLDPE) that is conductive to the thermostat (AlN). LLDPE composite with aluminum nitride filler was developed in the form of thermal press molding. Various vapor phase deposition processes may be used to create c-BN films that are bombarded with ions during film formation.

Although SiO₂f / SiO₂ composites lose tensile strength significantly when exposed to high temperatures, the crystal growth in the composites is thought to be to blame. Large amounts of recent experimental information on particle composites' thermal and electrical conductivities are well represented in the Lewis-Nelson model.

The growth of heat conduction in electric power networks has become a major problem. As a result of their isolation qualities, polymers that are both thermoplastic and thermal material exhibit low heat conductivity. Inorganic fillers that are very heat in contrast to the polymer matrix may be used to alleviate this issue.

As with other polymer matrix materials and only slightly smaller than many ceramics, Boron Nitride has a very high electrical resistivity and collapse resistance (both 1015 kV/mm) as well as a relatively high allowable (about 4,0 V/mm). Both the cooling and the heat transmission capacities are great. The Chao Zhang power sector may be able to use boron nitride as an inorganic filler source due to these impressive properties. Epoxy composites are widely used in the oil and micro-electronics industries because of their exceptional electrical, mechanical, and thermal qualities, low cost, and high functional efficiency. There are a number of structural characteristics that differentiate epoxy composites from other materials. As a result, we choose the filler that best meets our expectations.

It is easier to disperse filler because to its production method of mixing liquid phases, which is followed by procedure, than thermoplastic polymers H. There is a twinkle in the sky. Boron Nitride is a popular filler owing to its good thermal conductivity and isolating properties. Electrical isolation and thermostatic properties have been recognized in this material, which is often present in hexagonal or cubic like allotropes of carbons. Toshikatsutanaka et al have lately predicted the use of high-temperature composite dielectrics in the creation of small power appliances and high density and voltage design used in the area of power electronics. With the growth of cubic and hexagonal BN filler material, there is a general trend of lower collapse intensity.

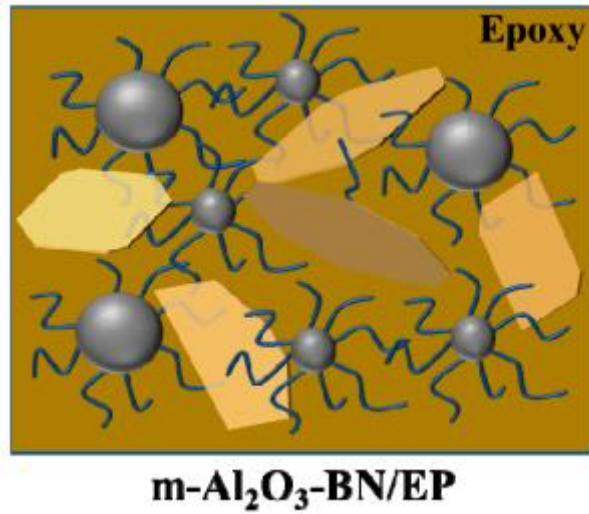


Fig. Al₂O₃-BN Epoxy

Literature is available on the preparation of these reinforced epoxy composites.

The fabrication of Al₂O₃-BN Epoxy composites in brief goes as follows. Starting off with preparation of epoxy, that is mixing with the hardener, at around 150 rpm at ambient temperature. Then comes the filler material which is mixed at around 600+ rpm for more than a couple of hours. This is followed by pouring into mould after which curing and degassing is done at 100+ degree centigrade. This is briefly what goes into our composite manufacture practically.

2.5 Thermal Conductivity Models

Many of these models have been examined in comprehensive review publications [27]. Thermal conductivity may be calculated by placing the materials be it series or parallel in respect to heat flow direction, which in turn yields the maximum and minimum limit of keff.

For the parallel conduction model

$$k_c = (1 - \phi)k_m + \phi k_f$$

Where k_c , k_m , and k_f respectively being THE keff of the composite and the matrix correspondingly, and ϕ is the reinforcement volume percent, respectively.

For the series conduction model:

$$\frac{1}{k_c} = \frac{(1 - \phi)}{k_m} + \frac{\phi}{k_f}$$

According to the Rules of Mixture, equations above show the correlations between variables (ROM). Tsao developed an equation that links the keff of a bi-phased mixture (solid state) to the respective conductivities of its constituent reinforcements and to two factors.

shows the distribution of the two stages in relation to each other. For Cheng and Vachon, the discontinuous phase was assumed to have a parabolic distribution during continuous phase.

An algorithm has been developed that does not need extra parameters to solve Tsao. Agari and Uno suggested a novel model for x-filled polymers that include both parallel and series conduction processes. the formula that determines thermal conductivity of the composite is based on this model

$$\log(k_c) = \phi C_2 \log(k_f) + (1-\phi) \log(C_1 k_m)$$

Experimentally determined unity-order constants, C1, C2. C1 depicts the impact of the particles on the polymer's secondary structure, such as crystal size and the polymer's crystallinity. In addition, C2 may be readily monitored by the particles that form conductive chains.

In order to improve the thermal conductivity of composites, the more readily particles form conductive chains, the greater the thermal conductivity of the particle. Eventually, they took into consideration the form of the particles, and they revised the model. This semi-empirical model seems to suit the experimental data rather well. However, when they wanted to determine the requisite constants for each form of reinforced matrix, significant experimental data is required. The correct equation for the keff of an endlessly diluted reinforced matrix having sphere like fillers is

$$k_{eff} = k_m \frac{k_f + 2k_m + 2\phi (k_f - k_m)}{k_f + 2k_m - \phi (k_f - k_m)}$$

Thermal conductivities of the composite, the matrix, and the dispersed phase are K, Kc, and Kd, respectively. ϕ is the volume fraction of the dispersed phase. When it comes to dilute materials, the well-known Maxwell equation may be used. The electrical analogy was used by Russell to build one of the first model systems. Using a series-parallel network, he developed equation for the composite's thermal conductivity, assuming the discrete phase and isotropic lines are planes scattered in the matrix material (Tavman I.H, 1998).

The Halpin – Tsai Equation was updated by Lewis and Nielsen to provide the results of the particle form and the position or kind of packing for a dual-style method.

$$\frac{k_{eff}}{k_m} = \frac{1+AB\varphi}{1-B\psi\varphi}$$

$$A = k_E - 1$$

$$B = \frac{k_f/k_m - 1}{k_f/k_m + A}$$

$$\psi = 1 + \left(\frac{1 - \varphi_m}{\varphi_m^2} \right) \varphi$$

Type of dispersed phase	Direction of heat flow	A
Cubes	Any	2
Spheres	Any	1.5
Aggregates of spheres	Any	$(2.5/\varphi_m) - 1$
Randomly oriented rods Aspect ratio=2	Any	1.58
Randomly oriented rods Aspect ratio=4	Any	2.08
Randomly oriented rods Aspect ratio=6	Any	2.8
Randomly oriented rods Aspect ratio=10	Any	4.93
Randomly oriented rods Aspect ratio=15	Any	8.38
Uniaxially oriented fibers	Parallel to fibers	2L/D
Uniaxially oriented fibers	Perpendicular to fibers	0.5

Shape of particle	Type of packing	ϕ_m
Spheres	Hexagonal close	0.7405
Spheres	Face centered cubic	0.7405
Spheres	Body centered cubic	0.60
Spheres	Simple cubic	0.524
Spheres	Random close	0.637
Rods and fibers	Uniaxial hexagonal close	0.907
Rods and fibers	Uniaxial simple cubic	0.785
Rods and fibers	Uniaxial random	0.82
Rods and fibers	Three dimensional random	0.52

The values of A and ϕ_m for various systems are given above,

Apart from these, in Equivalent Inclusion methods, be it differential effective medium or mean field approach, the inclusion is taken care of by using the expression:

$$K_i^{eff} = \frac{K_i}{1 + K_i/ha}$$

K_i being the thermal conductivity of the inclusion,

A, the inclusion radius,

and h, the thermal conductance at the interface.

Using Mean Filed Approach, the thermal conductivity of the composite

$$\frac{K_c}{K_m} = \frac{\phi^{eff}(1 + 2V_f) + (2 - 2V_f)}{\phi^{eff}(1 - V_f) + (2 + V_f)}$$

K_m - thermal conductivity of the matrix,

V_f is volume fraction of particles and

$\phi^{eff} = K_i^{eff}/K_m$.

Using differential effective medium:

$$(1 - V_f) = \frac{\varphi^{eff} - \frac{K_c}{K_m}}{\varphi^{eff} - 1} \times \left(\frac{K_c}{K_m} \right)^{-1/3}$$

2.6 The Knowledge Gap in Earlier Investigations

Though many studies have been done on the thermal and dielectric properties of particle composites in the past, there is a substantial knowledge gap that requires a well-planned and systematic investigation in this field of polymer composites. According to a thorough examination of the scientific literature:

- Some research solely tries to improve the polymer's heat conductivity, rather than adjusting its thermal and dielectric characteristics to fit electronic applications.
- The majority of fillers employed in the past have been epoxy or polyimide, and no data is available on epoxy-based composites.
- Computational work in terms of evaluating mechanical and thermal conductivity has been done on adding fillers to epoxy resins but properties using Al₂O₃ with BN as fillers haven't been computed as yet.
- Microstructural characteristics (volume fractions, particle dispersion, particle aggregation, component qualities) do not adequately interact with the heat conductivity of a composite material.

2.7 Chapter Summary

Reinforced composites' thermal conductance models, particle enhanced polymer composites, polymer-matrix thermal conductivity composites, and thermal / dielectric structures have all been thoroughly analyzed by various researchers. The research project's objectives have already been laid out in detail. Characterization definitions and finite element analysis are covered in this section.

Chapter 3

METHODOLOGY

This section explains how these composites are made and how they are applied numerically. This chapter also discusses the behavior of composite materials and how thermal conductivity is measured empirically using a Finite Element model.

3.1 Mathematical Models used for Thermal conductivity estimation

The process starts off by discretization of the domain into small elements called finite elements as the illustration shows 6 elements and 7 nodes.

Since we assume a steady thermal behavior, the heat transfer from a high to low temperature would be given by Fourier law:

$$q_x = -kA \frac{\partial T}{\partial X}$$

Where q stands for heat flux and A for Area of cross section, k gives thermal conductivity while the remaining term is the temperature gradient along the direction of heat flow.

Applying energy balance at each of the nodes and separating the known terms from the unknown.

$$A \begin{bmatrix} U_1 + U_2 & -U_2 & 0 & 0 & 0 & 0 \\ -U_2 & U_2 + U_3 & -U_3 & 0 & 0 & 0 \\ 0 & -U_3 & U_3 + U_4 & -U_4 & 0 & 0 \\ 0 & 0 & -U_4 & U_4 + U_5 & -U_5 & 0 \\ 0 & 0 & 0 & -U_5 & U_5 + U_6 & 0 \end{bmatrix} \begin{Bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{Bmatrix} = \begin{Bmatrix} U_1 AT_1 \\ 0 \\ 0 \\ 0 \\ 0 \\ U_6 AT_7 \end{Bmatrix}$$

Where U_i is (k_i/l_i) , k and l being the thermal conductivities and lengths of the elements respectively.

We would not jump deeper into the complete derivation of the matrix.

Like seen above finite element formulations in heat transfer boil down to,

[conductance matrix] [temperature matrix] = [Heat Flow Matrix]

$$[\mathbf{K}]^{(G)} = A \begin{bmatrix} U_1 & -U_1 & 0 & 0 & 0 & 0 & 0 \\ -U_1 & U_1 + U_2 & -U_2 & 0 & 0 & 0 & 0 \\ 0 & -U_2 & U_2 + U_3 & -U_3 & 0 & 0 & 0 \\ 0 & 0 & -U_3 & U_3 + U_4 & -U_4 & 0 & 0 \\ 0 & 0 & 0 & -U_4 & U_4 + U_5 & -U_5 & 0 \\ 0 & 0 & 0 & 0 & -U_5 & U_5 + U_6 & -U_6 \\ 0 & 0 & 0 & 0 & 0 & -U_6 & U_6 \end{bmatrix}$$

This is the typical global conductance matrix for a body divided into 7 nodes.

3.2 The Concept Of ANSYS

The FEM, first described in 1950s, is a powerful computer approach for dealing with a variety of real-world engineering difficulties that are subject to complicated domain circumstances. Engineering disciplines rely heavily on the use of finite element method (FEM) to create or simulate physical phenomena. Most physical phenomena have an impact on a number of different field variables over the whole continuum of matter (solid, liquid, or gas). The vibratory or weighted residual techniques, which are used to build structural system approaches in FEM, can only break down a certain number of domains (components) into subdomains. The FEM is in charge of the whole project and has a slew of ideas for improving it. For each section, FEM decreases the number of unknown function to that by separating the domain into elements and specifying an unknown field component. Field values are used to represent these functions in certain cases, known as nodes. These variables are often referred to as interpolation characteristics or interpolation characteristics. The nodes are frequently located near the organization's borders. For example, the employment of finite elements enables this approach to be used in numerous engineering fields to tackle issues of limit, original, and Eigen interest in a realistic and practical manner. It is possible to solve a broad variety of technical problems using the FEM, which is a computer programmer. A finite element model set like ANSYS may be used to solve multiple issues, including static/dynamic concerns, structural (linear and non-linear) motion and fluids, thermal motion and electromagnetic challenges

3.3 General Steps in FEM

Initially the problem's governing differential equations are converted to an integral form. This is done in essential two ways.

Using the calculus of variance, an integral form that corresponds to the specified differential equation may be obtained. The integral must be lowered in order to solve the issue. For structural mechanics issues, the integral form expresses the system's total potential energy. There are no limits on the weight functions used in this technique, therefore the combined form may be constructed as an integral weighted into the governing difference equation. The divergence theory often modifies this whole procedure in order to lower the solution's accuracy requirement. This crucial feature is set to zero in order to aid in the search for a solution. Structures' virtual work is shown by the integral form if weight is known as virtual displacement in structural mechanics difficulties. This is the second stage, which divides the issue area in many smaller pieces, called elements. One-dimensional (1-D) problems only require line segments with lengths but no underlying structure, which are referred to as components. In order to deal with larger-scale issues, the components are designed with both shape and size in mind. Axisymmetric and two-dimensional (2D) problems with square, rectangular, or quadrilateral components are employed. For a square domain, curved-sided components are the best option. To solve 3-D issues, a tetrahedron with parallel pipes that are either straight or curved is employed. To decompose a domain into its constituent parts, a mesh is used. For a good approximation of the major variable in the issue, this stage employs interpolating functions (sometimes referred to as form functions) and undefined values of the primary variable at specified fixed positions, called nodes.

Polynomials are the most common choice for their structure. For 1-D modules, there are a minimum of two nodes at the ends. Additional nodes have been added to the unit. For 2-Dimensional and 3-Dimensional objects, meshes are present close to the vertices (total of three triangle nodes, minimum of 4 rectangular, tetrahedral

and quadrilateral nodes and a minimum of 8 parallel pipeline formed components nodes). Additional nodes may be found on or within the perimeters of the current network. The primary node variable values are referred to as the liberty degrees. If a full set of polynomials has just a few terms, the number of elements needed to get an accurate solution to the main variable expression will have to be infinite. Polynomials must then be included in the phrase. No matter how many algebraic equations you use, this remains true. To make the issue manageable, just a few parts and an expression are needed, using only a few words. Instead, we'll have to make do with a shaky compromise. (Therefore, an approximation for the major variable chosen is the definition of an approximate solution.) Having said that, the accuracy of the estimation answer may be enhanced by raising the total number of predicted nodes or constituents. At this point, a new approximation method is introduced: the integral form. The algebraic equations of the main variable nodal values are the when the integral representation is in vibrational form. The algebraic equations are set to zero when the combined model happens to be weighted residual type. To acquire the whole domain, the algebraic equations are first formed across all elements using a sensible object known as the element equations (called global equations). We are now including our main variable boundary conditions into our algebraic equations. The calculation values at nodes of the primary variable are found by solving the updated algebraic equations. Last but not the least, step is post-processing of the solution. To put it another way, the solution first evaluates the problem's secondary variables. A graph (for 1D issues) or 2-D-3D contours (if required) are used to build the graphical variety across the domain.

3.4 Benefits of FEM over other Counterparts

- Finite Element Method is unrestricted on product form and may be applied to any part of the body or location.
- The use of FEM to any part of the body or area with any product form is possible since it has no geometric restrictions.

- It is possible to study domains using more than one material (composite).
- Any domain with an irregular form and any set of boundary conditions may benefit from this technique.
- The solution's precision may be enhanced by either fine-tuning the mesh or using higher-degree polynomials as approximations.
- A computer is able to solve these with ease. Moreover a generalized code can be developed for the analysis of many of the problems.
- The geometry and structure in FEM can be greatly similar to the real world prototype
- Mesh refinement can be done and this gives even more accurate results
- Visualization of complex problems can be done conveniently using FEM.

3.5 Simulation Method

This part of the book summarizes modeling done for numerical simulations into the thermal conductivity of the polymer compounds under consideration. The formulation of the same is shown below.

K EFF OF BN-AL₂O₃ FILLED in EPOXY MATRIX COMPOSITES:

Problem Description

Functional design and use of composite materials are dependent on determining composite materials' effective qualities. The microstructure of the composite has a significant impact on the effective characteristics and may be adjusted to a significant degree. Microstructure refers to the distribution of reinforcing inclusions in the matrix as well as their form, size, distribution be it orientation or spatial. Despite the fact that most composites include random distributions, periodic composites may provide a wealth of information on how the microstructure affects the effective qualities of the material. Since these periodic structures are highly inherently symmetric, systems with these structures may be studied more simply. This composite body thermal study is carried out with the aid of the finite-element software ANSYS. For four different filler concentrations, the microstructure of composite materials was simulated using 3D geometrical models having a spheres-in-a-cube lattice. ANSYS is used to evaluate the thermal behavior of these composites reinforced with the duo of Al₂O₃ and BN, each at equal volume percentages up to 50% volume.

Assumptions made:

Ideally, there are some assumptions taken into account for simulation

1. Composites under consideration are evenly filled with the reinforcement

2. Local homogeneity and isotropy is maintained in both the matrix and the filler.
3. The contact resistance is considered negligible at the polymer composite interface.
4. We assume a void free RVE.
5. The fillers are arranged uniformly.

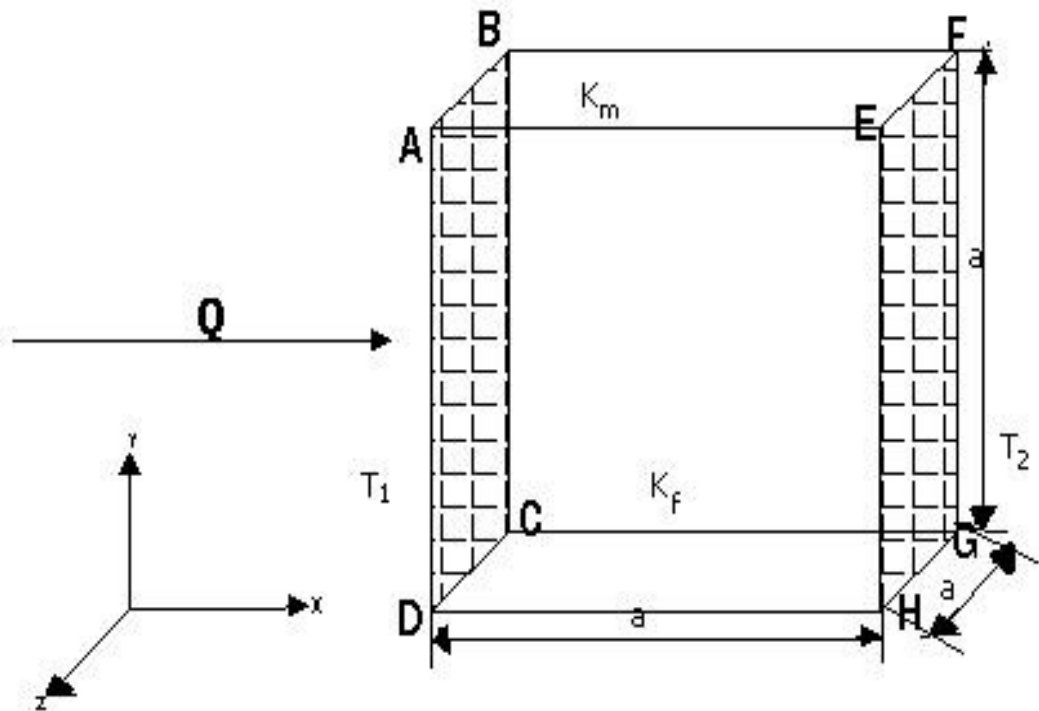


Fig. 3.1

Numerical Analysis

Periodic boundary conditions were used to compute as they have shown better results. They help in maintaining continuity between consecutive representative volume elements. It takes care of the continuity of the representative volume elements. A thermal gradient of temperature, say 100 centigrade is applied between the opposite faces while the other faces are kept at equilibrium. The Heat flux is measured and hence thermal conductivity is evaluated.

There are nodes along the surfaces ABCD where temperatures are specified as T1 and convective heat transfer coefficients at the ends are assumed. Figure depicts the heat flow direction and boundary conditions. Surfaces parallel to the flow of heat may also be considered to be adiabatic for all other surfaces. In the inner area and on the adiabatic bounds, we do not know the temperatures. The heat flux through the nodes is measured. Using the discretized form of Fourier's law, the thermal conductivity is evaluated like any finite element software.

GEOMETRICAL MODELLING

The modeling of microstructures of materials isn't anyways an easy task, more so when the said material is complex like a composite. All of these modeling can go far beyond a basic computing capability. This is when the material designer in ANSYS comes to the fore. The solution it gives is to homogenize the material properties.

As a first step, the material properties of the constituent materials are defined in the engineering data. These properties are then used in the designer as shown. The Representative Volume Element (RVE) is chosen or user defined. In our problem, the RVE used is a random particle composite mimicking the post-mixing structure of Al₂O₃-BN fillers in epoxy.

An RVE Is a cube like a lattice having periodic geometry. It means that the RVE taken multiple times in order in all directions will be the original macroscopic composite.

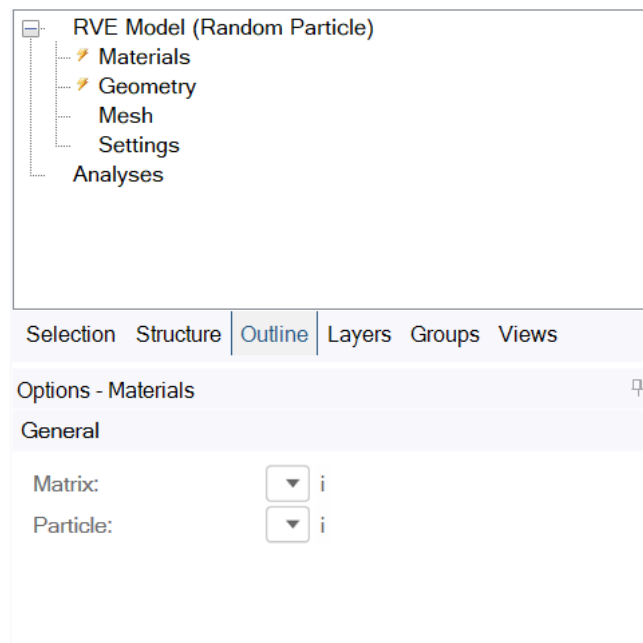


Fig. 3.2

After selecting the predefined materials, comes the geometry modeling. In this step spherical particles are seeded into the matrix. The reinforcement volume fraction is

defined like shown. The particles may be of a constant diameter or uniformly varying within a particular range. We have the particle diameter uniformly varying within a range of 5-10 microns.

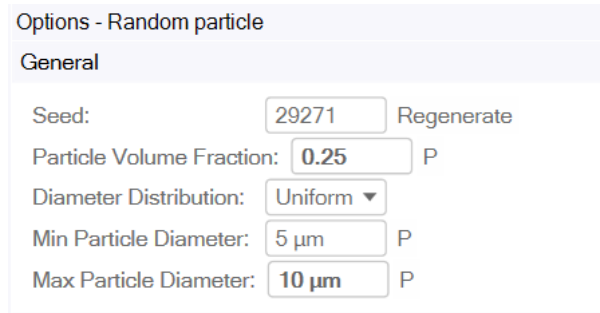
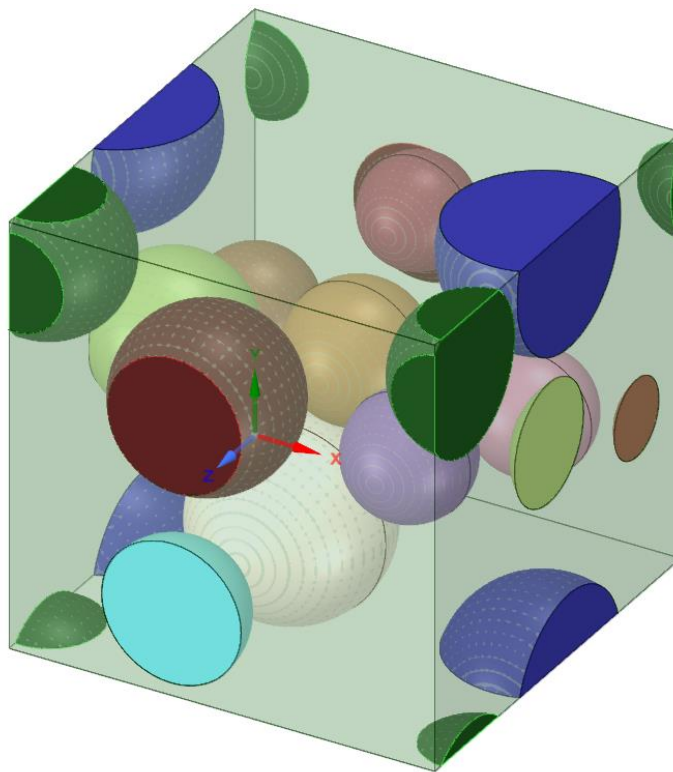


Fig 3.3(a)



ANSYS
2020 R1

Fig. 3.3(b)

The figure 3.3 (a) shows the interface through which particle seeding can be done, the filler volume fraction may be defined and the particle diameter may be set. A

provision is also given for hollow particles. Figure 3.3(b) shows outer surface of the composite formulated, how the fillers in spherical form are arranged in an RVE, and finally a depiction of the outer surface with sphere boundaries inside it. The BN-Al₂O₃ particles are put in order to maintain the homogeneity and mimic the real world mixing of fillers that takes place. It had also been shown from literature that solution using FEM gives the closest result when pitched with experimental results.

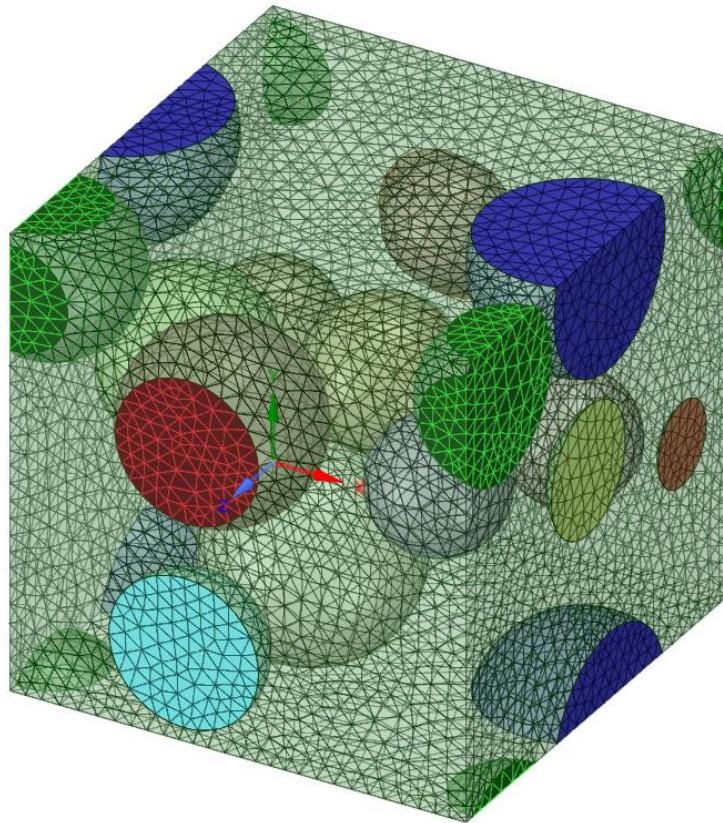


Fig 3.4 A typical meshing done over the geometry.

Meshing is done in order to create nodes so that calculations of the numerical simulation may take place over that particular element. The meshing done over our geometry is shown in the figure. The elements are tetrahedral shaped. The approximate statistics of the meshing was around 1 lakh elements and 1.5 lakh nodes on a geometry having a size of about 20 microns. The mesh consistency test was also done and refinement of the meshes gave the same result. This is followed

by multiple iterations for the differential equations to converge towards desired results.

```
Number of total nodes = 170507
Number of contact elements = 0
Number of spring elements = 0
Number of solid elements = 119740
Number of total elements = 119740
```

Fig. 3.5 Meshing data for the geometry

Boundary Conditions

The last part of the modeling and setup phase is the application of boundary conditions. Periodic boundary conditions were used to compute as they have shown better results. It takes care of the continuity of the representative volume elements. A thermal gradient of temperature, say 100 centigrade is applied between the opposite faces while the other faces are kept at equilibrium. The Heat flux is measured and hence thermal conductivity is evaluated.

```
Options - Settings
 Use Periodic Boundary Conditions
 Use Material Symmetry in XY
 Use Material Symmetry in XZ
 Use Material Symmetry in YZ
```

Fig. 3.6 Boundary condition settings

Chapter 4

RESULTS AND DISCUSSIONS

The simulations were carried out on ANSYS as earlier mentioned, Al₂O₃-BN were taken in equal volume percentages each, and the total volume percentage of this mixture was varied and we obtained the results for six different concentrations starting from 0% and going on to, 50 % of Al₂O₃-BN mixture concentrations.

The fillers were also taken individually, both Al₂O₃ and BN, and their individual concentrations were also varied in the same concentration range, and their results were obtained.

When both the fillers were taken together, their total volume fraction was kept constant and their ratio BN:Al₂O₃ was varied and its effect on the thermal conductivity was observed.

All of the results are tabulated, plotted and discussed below.

A typical temperature contour is shown below, we observe a uniform gradient along the length which depicts macroscopically homogenous mixing.

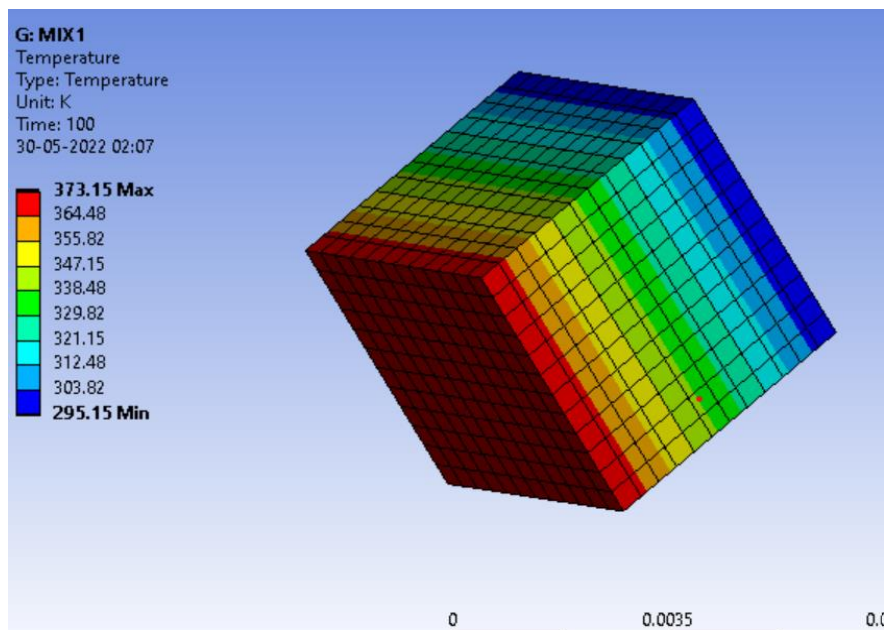


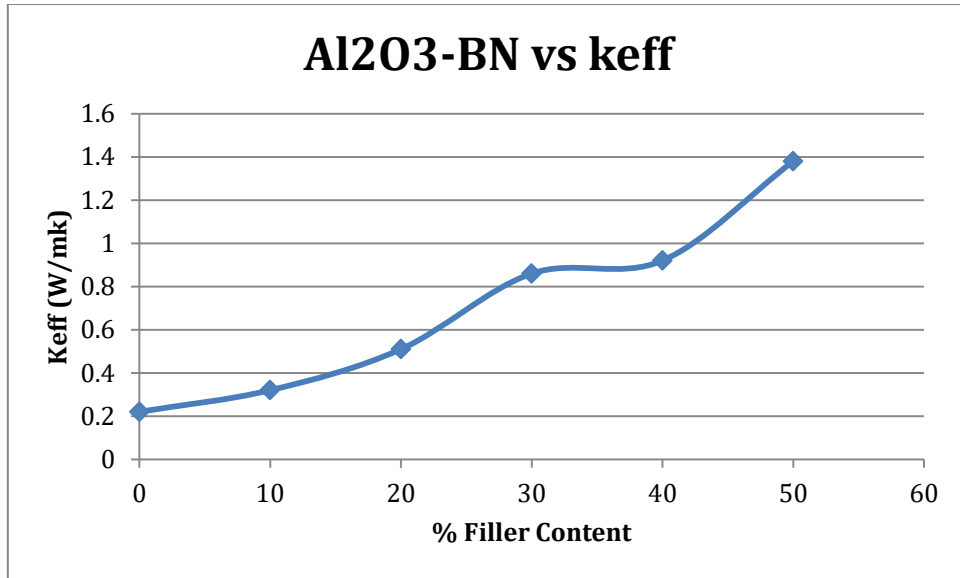
Fig.4.1 Temperature contour of Al₂O₃-BN-epoxy mixture

The effective thermal conductivities were also obtained at all the mixture concentrations. They are tabulated shortly below. Upon increasing the concentration of Al₂O₃-BN filler, the heat flux showed an increasing trend. This shows a direct impact on the effective thermal conductivity since the Temperature-length gradient does not change. We will jump into the numeric and the percentages of increment shortly after we have tabulated the effective thermal conductivities.

Table 4.1 Effective thermal conductivities with increasing filler volume percentages

Mixture no.	Vol% of filler Al ₂ O ₃ -BN	Eff k
I	0	0.22
II	10	0.32
III	20	0.51
IV	30	0.86
V	40	0.92
VI	50	1.38

The thermal conductivities show a considerable increase upon adding filler. This is also in sync with the experimental literature available on this. Even though the filler concentrations and the Al₂O₃ to BN ratio was different, the variation due to which can be estimated, the trend and even the numbers are pretty much matching. The trend is also plotted for easier investigation.



Similarly, for individual fillers like BN or Al₂O₃, the graph once again shows an increasing trend upon increment of reinforcement. The magnitudes of increase in thermal conductivity are less as compared to using both of them as fillers and this vouches for using the combination of Al₂O₃-BN as a filler. The values are once again tabulated below in Table 4.2.

Table 4.2

Mixture No.	Vol % of BN filler	Effective k (W/mk)
I	0	0.22
II	5	0.27
III	10	0.31
IV	15	0.35
V	20	0.48
VI	25	0.65
VII	50	0.88

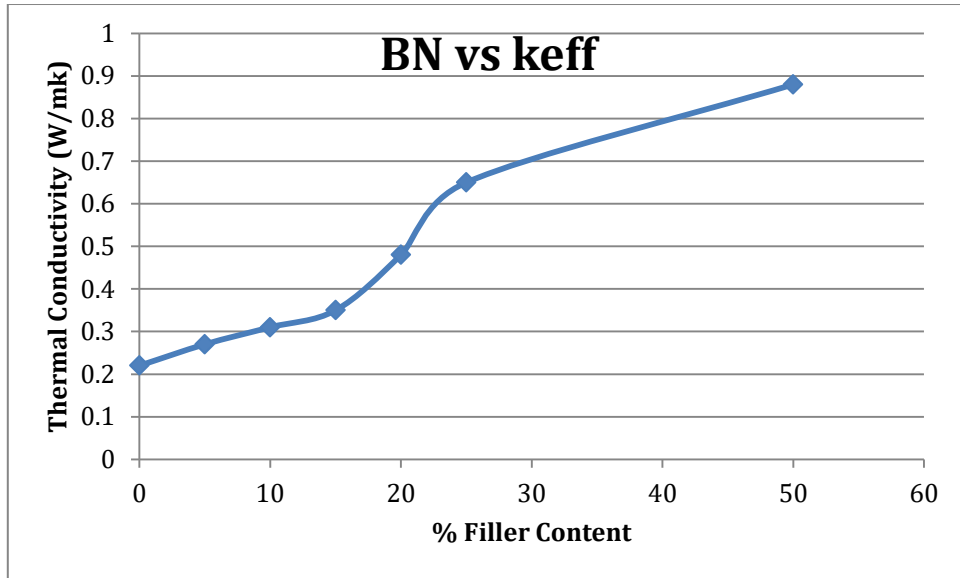


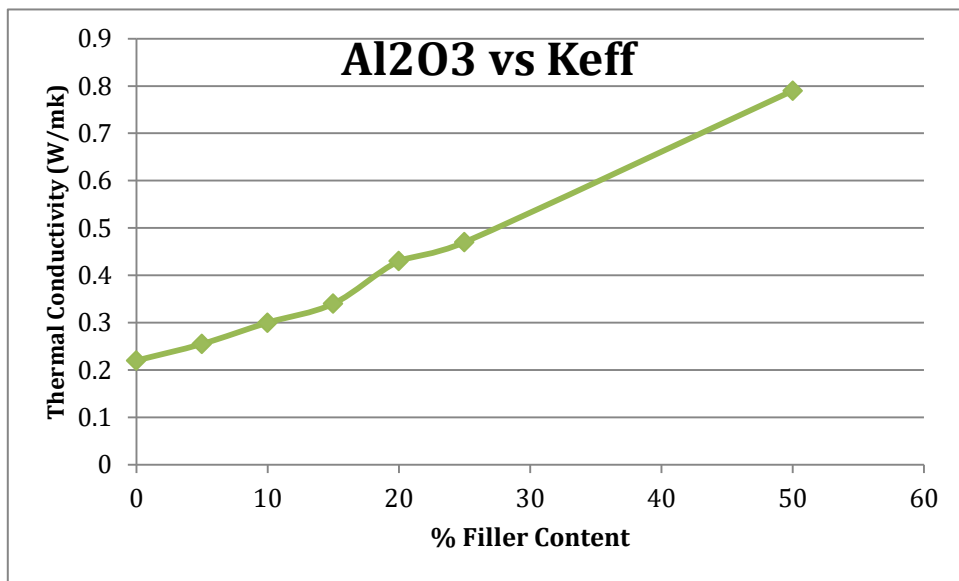
Table 4.3

Mixture No.	Vol % of Al ₂ O ₃ filler	Effective k (W/mk)
I	0	0.22
II	5	0.255
III	10	0.3
IV	15	0.34
V	20	0.43
VI	25	0.47
VII	50	0.79

Table 4.4

Mixture No.	Vol % of Al ₂ O ₃ filler	Effective k (W/mk)
I	0	0.22
II	5	0.255

III	10	0.3
IV	15	0.34
V	20	0.43
VI	25	0.47
VII	50	0.79



Comparing the thermal behavior using AL₂O₃ and BN as fillers with the limited experimental literature that we have, when the weight percentage of the filler was increased to as high as 80%, they observed almost 8 times increment in the thermal conductivity which is a huge boost. In our results also the increment at 50% gives us around 7 times increment in thermal conductivity. This is much more than what could have been achieved using just a single filler say BN. The numerical values testify the same. However, there has to be a cap on how much filler we can add for the simple reason that the advantages of epoxy may not get compromised and that other properties of the material obviously need to be kept in check.

Observations on BN specifically as a filler, the thermal conductivity values show a jump at 30 % volume of reinforcement. This behavior may be attributed to dependence of thermal conductivity on particle size and this is an area where study can be done. Any filler cannot be practically be added beyond a certain limit of because of other factor limitations. For example, for BN after a certain limit the viscosity starts to increase significantly causing difficulty in mixing while preparation.

On equal volume percentage of fillers i.e., 40% volume, the BN: Al₂O₃ filler ratio was changed and thermal conductivities evaluated. The ratio was varied in 5:3 and 3:5 and the results of Keff obtained respectively are 0.86 W/mk and 0.79 W/mk. However, the thermal conductivity for equal volume fractions of BN and Al₂O₃ tops them all at 0.92 W/mk.

CONCLUSIONS

The work presented can be summarized as follows:

- Finite Element Method is used to simulate the thermal behavior enhancement of Epoxy composites having more than one filler particle namely Al_2O_3 and BN.
- The results obtained show that they are in phase with the experimental data that we have.
- Hence FEM may be extensively used owing to its near accurate results.
- As the volume% of filler increases, it impacts the thermal conductivity significantly showing its weightage in this multi-variate problem.

With the increase in demand for the combination of electrically insulating and thermally conducting polymers especially in the area of microelectronics led to the research of many materials and this hybrid filler combination of Al_2O_3 and BN is definitely up there on that parameter. There is considerable enhancement in thermal conductivity. As in the terms of researchers there is good creation of thermal transport pathways in this combination.

So this is definitely going to benefit some certain electronic applications especially places where miniaturization is happening or increment of processing speed is intended, as these have closely placed conductors which need insulation from one another.

SCOPE FOR FUTURE WORK

These findings open up a broad range of possibilities for future study into thermal behavior. The following directions for future study should be considered: significance size, shape and orientation of filler on thermal behavior of these composites. And last and very obvious, newer composites and their combinations need to be researched upon so that we keep getting closer the desired result in terms of all properties in totality.

REFERENCES

- [1] S.W. Gregory, K.D. Freudenberg, P. Bhimaraj and L. S. Schadler, A study on the friction and wear behavior of PTFE filled with alumina nanoparticles, *J. Wear*, 254 (2003) : pp. 573–580.
- [2] K. Jung-il, P.H. Kang and Y.C. Nho, Positive temperature coefficient behavior of polymer composites having a high melting temperature, *J. Appl. Poly Sci.*, 92 (2004) : pp. 394–401.
- [3] S. Nikkeshi, M. Kudo and T. Masuko, Dynamic viscoelastic properties and thermal properties of powder-epoxy resin composites, *J. Appl. Poly. Sci.*,69 (1998): pp. 2593- 2598.
- [4] K. Zhu and S. Schmauder, Prediction of the failure properties of short fiber reinforced composites with metal and polymer matrix, *J. Comput. Mater. Sci.*, 28 (2003): pp. 743– 748.
- [5] Yun sheng Xu, D.D.L. Chung and Cathleen Mroz, Thermally conducting aluminum nitride polymer-matrix composites, *Composites Part A*, 32(2001)1749-1757.
- [6] I. H. Tavman, Thermal and mechanical properties of copper powder filled poly (ethylene) composites, *J. Powder Tech.*, 91 (1997):pp. 63–67.
- [7] R.N. Rethon, Mineral fillers in thermoplastics: filler manufacture, *J. Adhesion*, 64 (1997):pp. 87–109.
- [8] R.N. Rethon, Mineral fillers in thermoplastics: filler manufacture and characterization, *J. Adv. Poly., Sci.*, 139 (1999): pp. 67–107.

- [9] L.E. Nielsen and R.F. Landel, *Mechanical properties of polymers and composites*, Second ed., Marcel Dekker, New York, (1994): pp.377–459.
- [10] S.T. Peters, *Handbook of composites*, second ed., Chapman and Hall, London, (1998): pp. 242–243.
- [11] R.J. Young and P.W.R. Beaumont, Failure of brittle polymers by slow crack growth Part- 3 Effect of composition upon the fracture of silica particle-filled epoxy resin composites, *J. Mater. Sci.*, 12(4) (1977): pp. 684–692.
- [12] A.J. Kinloch, D.L. Maxwell and R.J. Young, The fracture of hybrid particulate composites, *J. Material Sci.*, 20 (1985): pp. 4169–4184.
- [13] R. Young, D.L. Maxwell and A.J. Kinloch, The deformation of hybrid particulate composites. *J. Mater. Sci.*, 21 (1986): pp. 380–388.
- [14] S.W. Koh, J.K. Kim and Y.W. Mai, Fracture toughness and failure mechanisms in silica-filled epoxy resin composites: effects of temperature and loading rate, *J. Polymer*, 34(16) (1993): pp. 3446–3455.
- [15] W.J. Cantwell and A.C. Moloney, *Fractography and failure mechanisms of polymers and composites*, Elsevier, Amsterdam (1994): pp. 233.
- [16] M. Imanaka, Y. Takeuchi, Y. Nakamura, A. Nishimura and T. Lida, Fracture toughness of spherical silica-filled epoxy adhesives. *Int. J. Adhesin Adhesive*, 21 (2001): pp. 389– 396.
- [17] H. Wang, Y. Bai, S. Lui, J. Wu and C.P. Wong, Combined effects of silica filler and its interface in epoxy resin, *J. Acta. Material*, 50 (2002): pp. 4369–4377.

- [18] I. Yamamoto, T. Higashihara and T. Kobayashi, Effect of silica-particle characteristics on impact/usual fatigue properties and evaluation of mechanical characteristics of silica-particle epoxy resins, *Int. J. JSME*, 46 (2) (2003): pp. 145–153.
- [19] Y. Nakamura, M. Yamaguchi, A. Kitayama, M. Okubo and T. Matsumoto, Effect of particle size on fracture toughness of epoxy resin filled with angular shaped silica, *J. Polymer*, 32(12) (1991): pp. 2221–2229.
- [20] Y. Nakamura, M. Yamaguchi, M. Okubo and T. Matsumoto, Effect of particle size on impact properties of epoxy resin filled with angular shaped silica particles, *J. Polymer*, 32(16) (1991): pp. 2976–2979.
- [21] Y. Nakamura, M. Yamaguchi, M. Okubo and T. Matsumoto, Effects of particle size on mechanical and impact properties of epoxy resin filled with spherical silica, *J. Appl. Polym. Sci.*, 45 (1992): pp. 1281–1289.
- [22] R.B. Burs, *Polyester Molding Compounds*, Marcel Decker, New York, 1982.
- [23] G. Lubin (Ed.), *Handbook of Fiber Glass and Advanced Plastics Composites*, Van Nostrand Reinhold, New York, (1969).
- [24] C. P. Wong, Raja S. Bollampally, Thermal Conductivity, Elastic Modulus, and Coefficient of Thermal Expansion of Polymer Composites Filled with Ceramic Particles for Electronic Packaging, *J. of Appl., Polymer Sci.*, (1999): pp.3396–3403.
- [25] D. Hansen and C. Ho, Thermal conductivity of high polymers, *J. of Poly. Sci. Part A*, 3(2) (1965): pp. 659–670.

- [26] S. Peng and R. Landel, Induced anisotropy of thermal conductivity of polymer solids under large strains, *J. Appl. Poly. Sci.*, (1975): pp. 49–68.
- [27] C.L. Choy, and K. Young, Thermal conductivity of semicrystalline polymers– A Model, *J. Polymer*, (1977): pp. 769–776.
- [28] I. Tavman, Thermal anisotropy of polymers as a function of their molecular orientation, experimental heat transfer, fluid mechanics, and thermodynamics, Elsevier (1991): pp. 1562–1568.
- [29] R.C., Progelhof, J.L. Throne and R.R. Ruetsch, Methods of predicting the thermal conductivity of composite systems, *J. Polymer Engineering and Science*, 16(9) (1976):pp. 615–625.
- [30] Geon-Woong Lee, Min Park, Junking Kim, Jae Ik Lee and Ho Gyu Yoon, Enhanced thermal conductivity of polymer composites filled with hybrid filler, *Composites*, (2006) : pp.727–734.
- [31] Wenying Zhou ,Caifeng Wang, Tao Ai , Ke Wu, Fenjuan Zhao and Hang zhou Gu, A novel fiber-reinforced polyethylene composite with added silicon nitride particles for enhanced thermal conductivity, *Composites*, (2009):pp. 830–836.
- [32] Aiping Yu, Xiaobo Sun, Elena Bekyarova, Mikhail E. Itkis, and Robert C Haddon, Enhanced thermal conductivity in hybrid graphite nano platelet carbon nanotube filler for epoxy composites, *Adv. Mater.* (2008):pp.4740–4744.
- [33] Hsiao Yen Ng, Thermal conductivity of boron nitride-filled thermoplastics: effect of filler characteristics and composite processing conditions, *Polym. Composites*, (2005):pp.778-790.
- [34] K. C. Yung and H. Liem, Enhanced thermal conductivity of boron nitride epoxy-matrix composite through multi-modal particle size mixing, *J. App. Polym. Sci.*, (2007):pp. 3587–3591.
- [35] Shoichi Kume, Ikuko Yamada and Koji Watari, High-Thermal-Conductivity AlN Filler for Polymer/Ceramics Composites, *The American Ceramic Society*,(2008): pp.153-156.

- [36] Makoto Imanaka, Yoshihiro Takeuchi, Yoshinobu Nakamura and Atushi Nishimura, Fracture toughness of spherical silica-filled epoxy adhesives, *Int. J. of Adhesion & Adhesives*, (2001):pp.389–396.
- [37] Haiying Wang, Yilong Bai, Sheng Liu and C.P. Wong, Combined effects of silica filler and its interface in epoxy resin, *Acta Mater.*, (2002): pp.4369–4377.
- [38] H. Tavman, Thermal and mechanical properties of aluminum powder-filled high density polyethylene composites, *J. App. Polym. Sci.*, (1996): pp.2161-2167.
- [39] Armin Bunde, Percolation in Composites, *J. of electro ceramics*, (2000):pp.81-92.
- [40] A. P. Vinogradov, A. M. Karimov and A. K. Sarychev, Permittivity of composite percolation materials: similarity law and equations of state, *Sov. Phys.*, (1988):pp.301-308.
- [41] H.S. Tekce, D. Kumlutas and I.H. Tavman, Determination of the thermal properties of polyamide-6 (nylon-6)/copper composite by hot disk method, In: *Proceedings of the 10th Denizli Material Symposium*, (2004): pp. 296–304.
- [42] R.C. Progelhof, J.L. Throne and R.R. Ruetsch, Methods of predicting the thermal conductivity of composite systems, *J. Polymer Engineering and Science*, 16(9) (1976): pp. 615–625.
- [43] M.Tech. Thesis 2013 Mechanical Engineering Department, N. I. T. Rourkela
Page 46
- [44] P. Procter, J. Solc, Improved thermal conductivity in microelectronic encapsulates. *IEEE Trans on Hybrids Manuf. Technol*, (1991): pp. 708–713.
- [45] Y. Nagai, G.C. Lai, Thermal conductivity of epoxy resin filled with particulate
- [46] aluminum nitride powder, *J. Ceram Soc Jpn*, (1997): pp. 197–200.
- [47] A. Griesinger, W. Hurler and M. Pietralla, A photo thermal method with step heating for measuring the thermal diffusivity of anisotropic solids, *Int. J. of Heat and Mass Transfer*, (1997): pp. 3049–3058.

- [48] I. Tavman, Thermal anisotropy of polymers as a function of their molecular orientation, experimental heat transfer, fluid mechanics, and thermodynamics, Elsevier (1991): pp.1562–1568.
- [49] N.M. Sofian, M. Rusu, R. Neagu and E. Neagu, Metal powder-filled polyethylene composites. V. thermal properties, J. Thermoplastic Composite Materials, 14(1) (2001): pp. 20–33.
- [50] Rajlakshmi Nayak, Alok satapathy, A study on thermal conductivity of particulate reinforced epoxy composites, (2010).
- [51] Y.P. Mamunya, V.V. Davydenko, P. Pissis and E.V. Lebedev, Electrical and thermal conductivity of polymers filled with metal powders, J. European Polymer, 38(9) (2002): pp. 1887–1897.
- [52] B. Weidenfeller, M. Hofer and F.R. Schilling, Thermal conductivity, thermal diffusivity, and specific heat capacity of particle filled polypropylene, J. Composites Part A: Applied Science and Manufacturing, 35(4) (2004): pp. 423–429.
- [53] H.S. Tekce, D. Kumlutas, and I.H. Tavman, Determination of the thermal properties of polyamide-6 (nylon-6)/copper composite by hot disk method, In: Proceedings of the 10th Denizli Material Symposium, Denizli, (2004): pp. 296– 304.
- [54] D. Kumlutas, and I.H. Tavman, A numerical and experimental study on thermal conductivity of particle filled polymer composites, J. of Thermoplastic Composite Materials, 19 (2006): pp. 441.
- [55] Patnaik Amar, Md. Abdulla, Satapathy Alok, B. Sandhyarani and K. S. Bhabani, A study on a possible correlation between thermal conductivity and wear resistance of particulate filled polymer composites, J. Materials and Design, (In press) (2009).
- [56] Kazuaki Sanada¹, Motoki Kurachi¹ and Yasuhide Shindo, Microstructure and thermal conductivity of polymer composites with nano and micro fillers.

- [57] Wenying Zhou, Shuhua Qi, Qunli An, Hongzhen Zhao and Nailiang Liu, Thermal conductivity of boron nitride reinforced polyethylene composites, *Materials Research Bulletin* (2007):pp.1863-1873.
- [58] Cameron G. Gofer, James Economy, Youren Xu and Avigdor Zangvil, Edgar Lara-Curzio, Matt K. Ferber & Karren L. Moreb, Characterization of fiber/matrix
- [59] M.Tech. Thesis 2013, Mechanical Engineering Department, N. I. T. Rourkela Page 47, interfaces composites with a boron nitride matrix, *Composites Science and Technology*, (1996):pp. 967-975.

PAPER NAME

Taha Shees Thesis 1.pdf

AUTHOR

Taha

WORD COUNT

10952 Words

CHARACTER COUNT

60600 Characters

PAGE COUNT

57 Pages

FILE SIZE

1.8MB

SUBMISSION DATE

Jun 7, 2022 9:45 AM GMT+5:30

REPORT DATE

Jun 7, 2022 9:46 AM GMT+5:30**● 6% Overall Similarity**

The combined total of all matches, including overlapping sources, for each database.

- 4% Internet database
- 3% Publications database
- Crossref database
- Crossref Posted Content database
- 4% Submitted Works database

● Excluded from Similarity Report

- Bibliographic material
- Quoted material
- Small Matches (Less than 8 words)