

International Journal of Engineering Sciences & Research Technology

(A Peer Reviewed Online Journal)
Impact Factor: 5.164



Chief Editor
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ABSTRACT

In this paper, an attempt to determine the mechanical properties of particulate filled polymer composites using finite element method (FEM) a powerful computational technique is made. A commercially available designing and analysis software package CATIA is used for modelling and –numerical analysis. Three-dimensional spheres-in-cube lattice array models are constructed to simulate the microstructures of particulate filled polymer composites with filler content ranging from 10 to 40 wt. %. Composites with similar filler contents are than fabricated using simple hand lay-up technique by reinforcing micro-sized hexagonal boron nitride (hBN) in epoxy resin. Important mechanical properties such as tensile strength, compressive strength and flexural strength of these composite samples are measured using computerized Tinius Olsen universal testing machine. The experimentally measured mechanical properties values are compared with the numerical values. This comparison reveals that the FEM simulated values are found to be in reasonable good agreement with the experimental data for tensile, compressive and flexural strength. Further, this study shows that there is gradual enhancement in the tensile, compressive and flexural strength of epoxy resin with increase in filler percentage. This study validates the proposed numerical model for epoxy/hBN composite system for various strengths and proves that finite element analysis can be an excellent methodology for such investigations.

KEYWORD: Polymer matrix composite, epoxy, hexagonal boron nitride, numerical analysis, mechanical properties.

1. INTRODUCTION

With the continued inclination towards electronic device miniaturization, the necessity for reliable, higher performance packaging material is also growing. Selection of packaging material is decisive for signal and power transmission, heat dissipation and guard from moisture and contaminants [1]. To date, increasing attention is being given to conducting polymer composites containing conducting inorganic filler particles. These materials combine properties of each component and often acquire new properties [2]. Polymer matrix composites, combining the benefits of matrix and filler component, are increasingly employed for thermal management and microelectronic packaging because of their superior performances, outstanding processability and most notably low cost [3]. Extensive research has been conducted on the thermal conductivity enhancement of composite materials by incorporation of inorganic fillers such as carbon nanotubes and graphene [4, 5], ceramic oxides [6, 7] and nitrides [8, 9].

Carbon nanotubes and graphene increases the thermal conductivity of the polymer exceptionally but also make the composites electrically conductive which is not required in packaging application as such application required thermally conductive and electrically insulative path and thus obsolete the usage of such filler. The common ceramic filler with good electrical resistivity such as alumina and silica possess low value of intrinsic thermal conductivity. So for improving the thermal conductivity to a high value, high filler loading is required which ultimately reduces the mechanical properties of the material. Nitride filler shows high thermal conductivity at low filler loading because of it high intrinsic thermal conductivity value.

Hexagonal boron nitride (h-BN) known as white graphite was considered to be an ideal candidate due to its relative high thermal conductivity, low coefficient of thermal expansion, stable crystal structure, low dielectric constant and non-toxic [10]. But because of high surface energy and amphiphobic nature, its homogeneous

[Ramat 2020]
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dispersion in polymer is difficult which causes high thermal resistance at the interfaces. Surface modification, therefore, is necessary to improve the BN particles wett ability and adhesion to the matrix. Silane coupling agent has been widely used to modify the surface of inorganic fillers. It is well known that the use of silane coupling agent benefits by improving the phase interfacial bonding strength between the matrix and filler, which enhances the thermal conductivity and electrical insulation. Though, mechanical properties of such composites were always ignored. But, detailed study of mechanical properties of such inorganic particle filled polymer composites is required.

In view of this, the present work consists of development of numerical model using well-known modelling and analysis software CATIA for evaluating the various mechanical properties i.e. tensile strength, compressive strength and flexural strength of the composite material. Later, all the mentioned properties were evaluated experimentally by fabricating the composite using simple hand lay-up technique. Epoxy resin is used as a matrix material whereas hexagonal boron nitride is filler material for the present investigation. Here, the effect of h-BN content in epoxy matrix on different mechanical properties of the composites is reported numerically and experimentally. Also, the comparison between the values obtained by two different methods was presented in the work.

2. MATERIALS

Thermoset resin Lapox L12 is a liquid, unmodified epoxy resin of medium viscosity is used as the matrix material in present investigation. It is used with its corresponding hardener which is a low viscosity room temperature curing liquid. Hardener K6 is commonly employed with Lapox L12 for hand lay-up applications. Being rather reactive, it gives a short pot life and rapid cure at normal ambient temperatures. The matrix material system selected is supplied by ATUL India Ltd., Gujarat, India. Epoxy used in present investigation possesses density of 1.16 g/cc, tensile strength of 40.5 MPa, flexural strength of 52 MPa and compressive strength of 85 MPa. Boron nitride in its hexagonal crystal structure of size 5 microns used in present investigation is supplied by Souvenir Chemicals, Mumbai. It is of ultra-pure grade with purity level of 99 %. It has density of 2.3 g/cc.

3. SAMPLE PREPARATION

In the present investigation, particulate filled polymer composite is fabricated using simple hand lay-up technique which involves following steps:

1. The room temperature curing epoxy resin epoxy resin (L-12) and corresponding hardener (K-6) are mixed in a ratio 10:1 by weight as recommended.
2. Hexagonal boron nitride will then added in epoxy-hardener combination and mixed thoroughly by hand stirring.
3. Before pouring the epoxy/filler mixture in the mould, a silicon spray is done over the mold so that it will easy to remove the composite after curing. The uniformly mixed dough is then slowly poured into the mould so as to get specimens of size as per ASTM standard.
4. The cast is than cured for 12 hours before it was removed from the mould.

Composites were fabricated with different weight fraction of filler ranging from 0 to 40 wt. % for each set. The list of fabricated composite is presented in table 1 and given name as set A.

Table 1 List of fabricated composites

Set	Composition
Set A1	Epoxy + 10 wt. % hBN
Set A2	Epoxy + 20 wt. % of hBN
Set A3	Epoxy + 30 wt % of hBN
Set A4	Epoxy + 40 wt. % of hBN

4. CHARACTERIZATION

Experimental analysis

The tensile strength, compressive strength and flexural strength of the composites are measured with a computerized Tinius Olsen universal testing machine in accordance with ASTM D638, ASTM D695 and ASTM D790 respectively. The specimens used in present investigation to perform all the tensile tests are of dog-bone shape (length 115 mm, end width 19 mm, mid width 6 mm and thickness 3.2 mm) having both the surface flat. The typical cylinder blocks used for these tests are 12.7 mm in diameter and 25.4 mm in length. The flexural test is performed on rectangular strip 115 mm length, 12 mm in width and 3 mm in thickness.

Numerical Analysis

FEM has become an essential step in the design or modeling of a physical phenomenon in various engineering disciplines. The basis of FEM relies on the decomposition of the domain into a finite number of sub-domains (elements) for which the systematic approximate solution is constructed by applying the variation or weighted residual methods. In effect, FEM reduces the problem to that of a finite number of unknowns by dividing the domain into elements and by expressing the unknown field variable in terms of the assumed approximating functions within each element. CATIA V5 is general-purpose finite-element modeling package for numerically solving a variety of mechanical problems that include static/dynamic, structural analysis (both linear and nonlinear), heat transfer, and fluid problems. Using the finite-element program CATIA V5, Strength analysis is carried out for the composite body. In order to make a Strength analysis, three-dimensional physical models with spheres-in-cuboid in a lattice array have been used to simulate the microstructure of composite materials for different filler concentrations. Furthermore, the effective strength of these composites filled with micro sized boron nitride particle up to about 40 % by volume are numerically determined using CATIA V5.

In present work polymer filled composite material is tested under numerical approach, with different weight % i.e. 10%, 20%, 30%, 40% of epoxy. In this analysis, it is assumed that the composites are macroscopically homogeneous, locally both the matrix and filler are homogeneous and isotropic, the strength contact resistance between the filler and the matrix is negligible and the composite lamina is free from voids. The problem is based on spheres-in-cuboid which is distributed uniformly. The composite modelled and analyzed under numerical analysis is given name as set B.

5. RESULTS AND DISCUSSION

Tensile strength of particle-filled polymer composites depends on the efficiency of stress transfer across the interface between the matrix and the filler. The dependence of tensile strength of epoxy composites filled with hBN with different content is indicated in table 2.

Table 2 Tensile strength of epoxy/hBN composites

Set	Measured Tensile Stress (MPa)	Set	Simulated Tensile Stress (MPa)
Set A1	41.3	Set B1	43.2
Set A2	43.4	Set B2	45.6
Set A3	44.9	Set B3	47.2
Set A4	46.2	Set B4	49.5

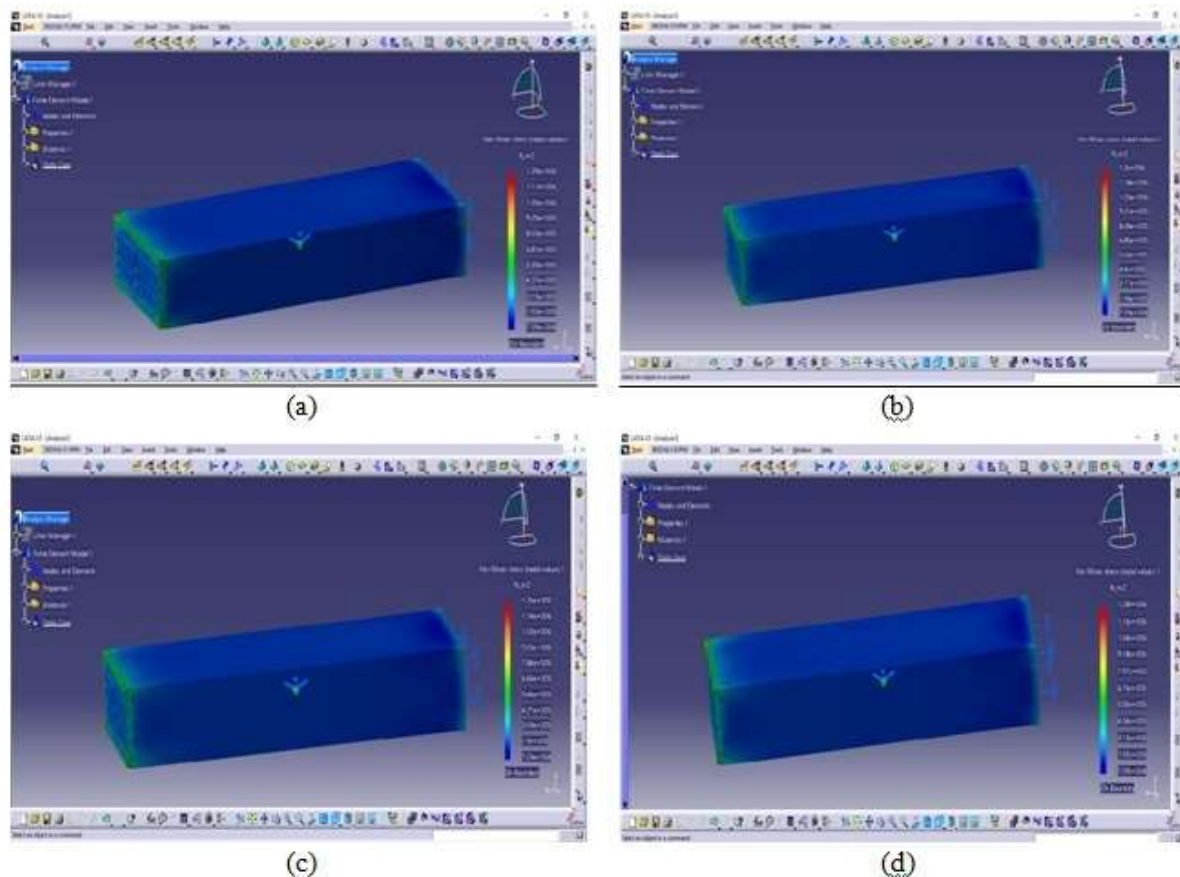


Figure 1: Tensile stress obtained from numerical analysis (a) 10 wt. % filler loading, (b) 20 wt. % filler loading, (c) 30 wt. % filler loading, (d) 40 wt. % filler loading

The measured value and the simulated values are presented. For numerical analysis purpose, the tensile load is kept constant i.e. 500 N. The complete analysis is done with 500 N load and stress value is obtained at different filler loading. For experimental analysis, load is gradually increases from no load condition to breaking point. Various points were obtained which shows the value of stress for different loading condition. From the analysis, stress obtained for 500 N load is taken and compared with the value obtained from numerical analysis.

Table 3 Compressive strength of epoxy/hBN composites

Set	Measured Compressive Stress (MPa)	Set	Simulated Compressive Stress (MPa)
Set A1	93.5	Set B1	95.4
Set A2	95.6	Set B2	98.3
Set A3	98.8	Set B3	101.3
Set A4	100.9	Set B4	104.8

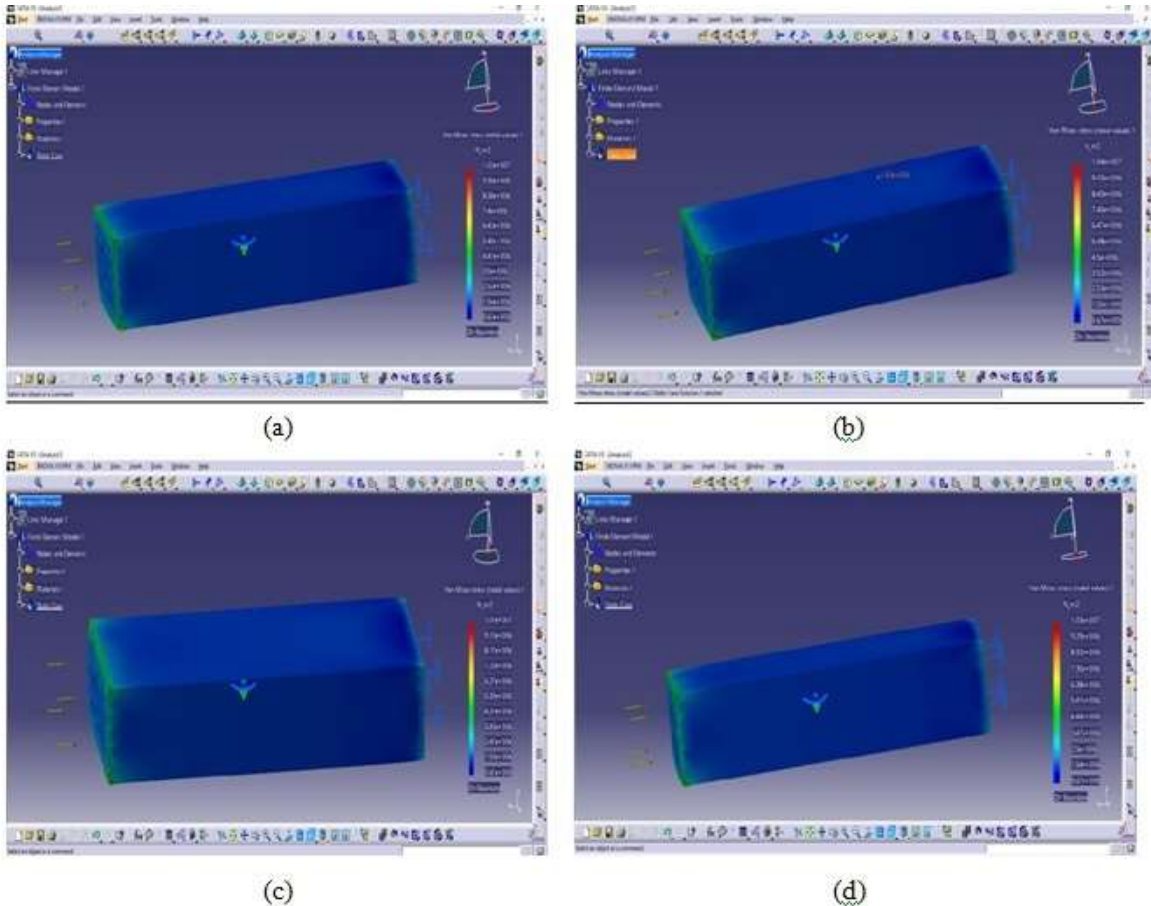


Figure 2: Compressive stress obtained from numerical analysis (a) 10 wt. % filler loading, (b) 20 wt. % filler loading, (c) 30 wt. % filler loading, (d) 40 wt. % filler loading

It can be seen from the table that with increase in hBN content, tensile strength of the composites increases. The measured tensile strength of neat epoxy is 40.5 MPa which increases to 48.8 MPa when 40 wt. % of hBN particles was incorporated in epoxy as shown under measured tensile strength. This increment in tensile strength, as a result of high loading of hBN, may be clarified by the fact that strength of boron nitride particles are more as compared to epoxy matrix.

Similar trend is obtained from numerical analysis which shows that tensile strength of the composite increase with filler content. Though, the rate of increment in the value of tensile strength is more in case of numerical analysis than experimentally obtained values. For 40 wt. % of hBN particles, the value of tensile strength obtained from numerical analysis is 49.5 MPa. Figure 1 shows the trend of tensile stress obtained by numerical analysis when the specific tensile load is applied on it. The difference in value is mainly because of the various defects originated during the actual fabrication of composites which were not taken care-off while doing numerical analysis. This is the reason why the outcome of both the analysis was not perfectly matching with each other.

The dependence of compressive strength of epoxy composites filled with hBN with different filler content is indicated in table 3. For compressive stress, the applied load is kept constant to 2400 N for numerical analysis and the stress under similar condition is taken from experimental analysis. It can be seen from the table that with increase in hBN content, compressive strength of the composites increases. The improvement in compressive strength with filler addition is mainly because of the high compressive strength of filler material.

Also, the increase in compressive strength with increased filler content is due to the favorable deformation processes facilitated by the presence of fillers in the matrix. Under a compressive loading situation, the fillers apparently aid the load bearing capability of a composite, rather than acting as stress raiser as is the case in tensile loading. It can be further observed from the table that values obtained from numerical analysis are in fairly good agreement with the value obtained through experimentation. Figure 2 shows the trend of compressive stress obtained by numerical analysis when the specific compressive load is applied on it. Again, the rate of increment in the value of compressive strength is more in case of numerical analysis than experimentally obtained values which are because of the similar reason as that of difference in value of measured and simulated tensile strength value. The dependence of flexural strength of epoxy composites filled with hBN with different filler content is indicated in table 4. The trend obtained under numerical analysis is shown in figure 3.

Table 4 Flexural stress of epoxy/hBN composites

Set	Measured Compressive Strength (MPa)	Set	Simulated Compressive Strength (MPa)
Set A1	73.5	Set B1	75.2
Set A2	76.8	Set B2	79.6
Set A3	81.2	Set B3	82.5
Set A4	84.5	Set B4	87.3

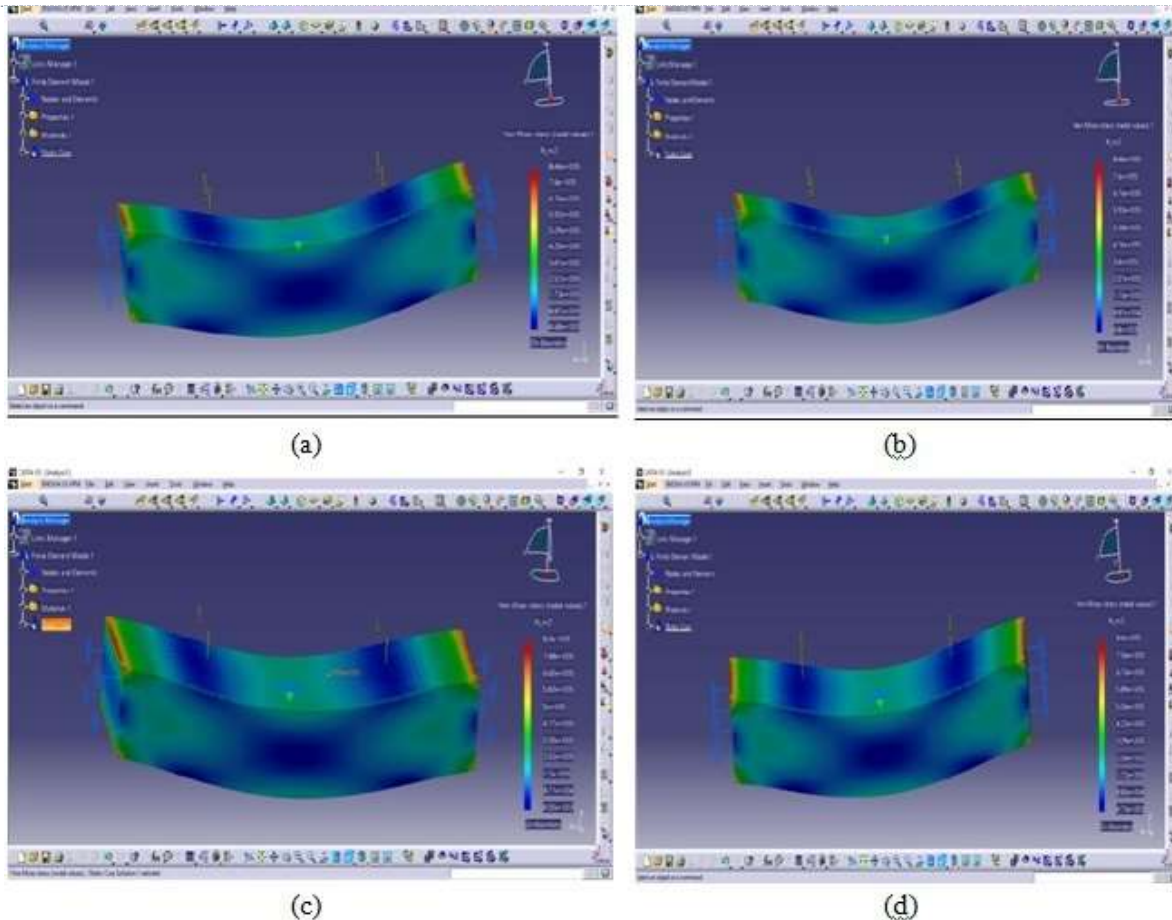


Figure 3: Flexural stress obtained from numerical analysis (a) 10 wt. % filler loading, (b) 20 wt. % filler loading, (c) 30 wt. % filler loading, (d) 40 wt. % filler loading

It can be seen from the table that with increase in hBN content, flexural strength of the composites increases. The load applied for numerical analysis is 500 N the result obtained under numerical and experimental analysis is compared for same condition. From the table it can be seen that both the analysis are providing the similar increasing trend in the value of flexural strength. Again, values obtained under numerical analysis are more compared to obtain from experimental analysis. But the difference is marginal and can be said that the numerical analysis are in fairly good agreement with the value obtained through experimentation.

6. CONCLUSION

This numerical investigation on mechanical properties of epoxy composites filled with micro-sized boron nitride particles has led to the following specific conclusions:

1. Finite element method can be gainfully employed to determine the mechanical properties of epoxy/hBN composite with different amount of filler content. A good agreement of FEM results with those obtained from experimental efforts validates the usefulness of this numerical method.
2. Incorporation of hBN particles results in increase of tensile strength of epoxy and this increment is continue with increase in filler content. For 40 wt. % hBN, maximum value of tensile strength of composite is reported 48.8 MPa for 40 wt. % of hBN.
3. For same content of hBN particle in the composite, the variation in compressive strength provide the gainful results as compressive strength increases with increase in filler content. Experimental values show that compressive strength of composites increases from 85 MPa to 104.4 MPa for 40 wt. % of hBN.

4. For same content of hBN particle in the composite, the variation in flexural strength provide the gainful results as flexural strength increases with increase in filler content. Experimental values show that flexural strength of composites increases from 68 MPa to 84.5 MPa for 40 wt. % of hBN.

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