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Prediction of Elastic Properties of Micro Particle (B_4C) Reinforced Polymer Composites Using Finite Element Analysis and Analytical Expressions

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Abstract— ***Particle reinforced Composite (PRC) materials are also an important class of polymer composites and these are also used for different engineering applications. Improvements in mechanical properties of this class of materials are under research for diversified applications. The present research work is focused on the evolution of the mechanical properties of the PRC where spherical shaped B_4C particles of diameter in microns are reinforced in a Polymer matrix. The effectiveness of the particle contribution regarding Elastic properties of Particle Reinforced Composite at various particle weight fractions is examined by Finite Element Analysis. The experimental approach is the best way to determine the properties of the composite but it is expensive and time-consuming. Therefore, FEM and analytical methods are the viable methods for the determination of the composite properties. The Finite element results were obtained by adopting Micromechanics approach in association with Finite Element Method. Assuming a uniform distribution of particles and considering one unit-cell of the whole array, the properties of the composite materials are determined. The predicted Elastic properties from FEA is compared with analytical results. Results suggested that B_4C particles are good reinforcement for the enhancement of Elastic properties of Polypropylene.***

Keywords— ***Boron Carbide, Micromechanics, Represent Volume Element, Finite Element Method, Young's Modulus, Polymer Composites.***

I. INTRODUCTION

A composite material consists of two or more constituent materials with significantly different properties combined with a recognizable interface between them, to produce a material with characteristics different from its constituents. Composite materials exhibit high mechanical and thermal properties in comparison with the conventional materials such as polymers, metal alloys etc. Two important phases present in the composite materials are the reinforcement and matrix material. The different phases serve different purposes to achieve the characteristics that are possible to composite materials. The reinforcement is characterized as a high stiff and strong phase which is intended for the load carrying purpose. Matrix phase is uninterrupted bonding among fibers to distribute loads through the reinforcement uniformly and protect it from external situations in the environment such as temperature, moisture, chemical reactions etc. Composites are usually described by the variety of matrices, such as a polymer, metal or ceramic and by the nature of reinforcement, such as fibers, particulate, flake or whiskers. Each of the composites is designed and fabricated as per the requirement for specific applications. Most of the composites are fabricated from the matrix materials like Epoxy, Polyester, Polypropylene etc., and reinforcement material particles like Al_2O_3, SiC, WC and TiO_2.

Polypropylene (PP) is a thermoplastic polymer which is being used in various industries including textile, stationery, automotive, laboratory equipment, plastic parts and reusable containers of various types. The PP is commercially available in the form of granules, sheets etc. Boron carbide (B_4C) is an extremely hard ceramic material used in tank armour, bulletproof vests, and numerous industrial applications. Boron Carbide is superior in the mechanical properties and denser than the other ceramic materials like SiC, WC etc.

Polymer matrix composite materials combining polymers and particles (organic and inorganic components) have attracted research attention from the academic and industrial communities due to their diverse functional applications, good processing and relatively low cost. Particle reinforced composites (PRC) have the same strength in all directions and these have attained research attention due to their diversified applications in different areas. And also Polymer composite materials are being used in a wide range of structural applications in the aerospace, construction and automotive industries due to their light weight and high specific stiffness and strength.

Composite strength strongly affected by particle loading, particle/matrix adhesion, particle size, especially particle/matrix adhesion and different analytical expressions to estimate the E of PRC from review presented by Shao-Yun Fu et al. [1]. Kamalbabu P. et al. [2] presented the effect of particle size on polymer composites and it has been observed that with the decrease in the particle size of the reinforcement the Tensile Strength and Young's Modulus will get improved. The interaction between the filler material and the matrix will be better with smaller size particles [2]. The Modulus increases along with the increase in the reinforcement content by F. Asuke et al. [3]. Finite element analysis of the one-eighth of the unit cell model was done for the prediction of the mechanical properties by Hong Teng [4] and [5]. General literature about composites and analytical expressions for properties were also studied [6-10] and The Finite Element Analysis of Various Composites using ANSYS was studied [11].

II. PROBLEM MODELING

A. Problem Objective

The main objective of the present work is to find the Elastic properties of the particle reinforced composite which is having spherical shape particles of micron diameter as reinforcement in the polypropylene matrix. The overall analysis is taken using the ANSYS Software. For the analysis, Micromechanics in association with the finite element method is adopted. The FE results are compared with the Analytical results.

B. Materials and Properties

The materials for the analysis of the particle reinforced composite are polypropylene is shown in Figure 1 and Boron Carbide powder of the spherical shape of size 150 mesh (~100µm) which is shown in Figure 2.

Fig. 1. Polypropylene (granules)

Fig. 2. Boron Caribe Powder (150 mesh)

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The Materials that were taken for the analysis were isotropic in nature. The properties of the materials are listed in Table I.

TABLE I
CONSTITUENTS PROPERTIES

Material	Young's Modulus (GPa)	Poisson's Ratio	Density (Kg/m^3)
Polypropylene	1.1-1.3	0.42	910-940
Boron Carbide#	450-470	0.21	2520

Boron Carbide material properties are taken from article 75 [12]

C. Numerical Homogenization for Particle Reinforced Composite

The main constituents of the Particle Reinforced Composite are Boron Carbide and Polypropylene. The particle distribution in the matrix material is usually non-uniform. But for the analysis of the PRC, periodic distribution of Boron carbide particles in the matrix phase is assumed. The finite element software ANSYS is a very appropriate tool to solve the problem. Uniform distribution of particles in the resin is shown in Figure 3.

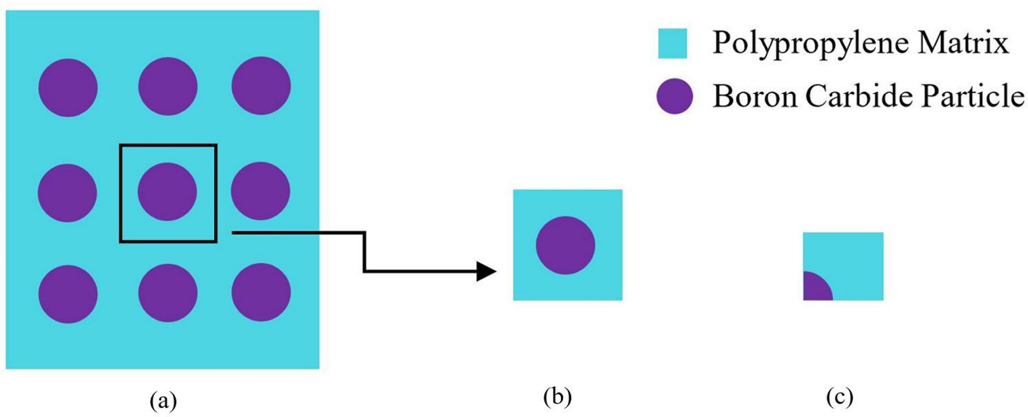

Fig. 3. (a) Uniform distribution of spherical particles in matrix, (b) Isolated Unit cell and (c) One-eighth Model

1) Element Type: For the prediction of the Young's Modulus of the composite accurately, we have to use a suitable element which can calculate the large deflection in all directions. The element used for the present analysis is SOLID186 of ANSYS, which is a higher-order 3-D 20-node solid element that exhibits the quadratic displacement behavior. The element is defined by 20 nodes having three degrees of freedom at each node translation in the nodal x, y, and z directions. The element supports plasticity, hyperelasticity, creep, stress stiffening, large deflection, and large strain capabilities [13].

2) Material Properties: The material properties that were used for the calculation of the mechanical properties of the PP/B_4C Composite are listed in Table II. The properties of PP are taken from the commercially available granules grade of materials.

TABLE II
MATERIAL PROPERTIES OF CONSTITUENTS TAKEN FOR FEA

Material	Young's Modulus (GPa)	Poisson's Ratio	Density (Kg/m^3)
Polypropylene	1.161	0.42	920
Boron Carbide	470	0.21	2520

D. Geometry and Finite Element Modeling

The shape of RVE (representative volume element) taken for the analysis of PRC is a Cube. Due to symmetry regarding geometry, loading, boundary conditions only a one-eighth portion of the RVE is modeled and analyzed. As a one-eighth portion of the unit cell is taken for Finite Element Modeling, the FE model consists of a cube of side 100 units with an embedded one-eighth portion of Boron Carbide Spherical particle of radius 'r_p' at one of the corners of the cube which is also the center of the particle.

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The radius of the boron carbide particle is calculated at different weight fractions of B_4C using the Equation (1). The weight percentages of the B_4C which are taken for the analysis are 5, 10, 15 and 20. The weight percentages are converted into volume fractions. The radius of the particle is calculated by using an equation.

$$r_p = \sqrt[3]{\frac{V_p * 6 * 100^3}{\pi}} \tag{1}$$

Where V_p = Volume fraction of particle
r_p = Radius of the spherical particle

The Finite Element Models were prepared for different volume fractions of the Boron Carbide and Mechanical properties were calculated. Finite Element Model of 20 wt. % of B_4C reinforced polypropylene composite is shown in Figure 4. Converged mesh model of Boron Carbide particles reinforced polymer composite is shown in Figure 5.

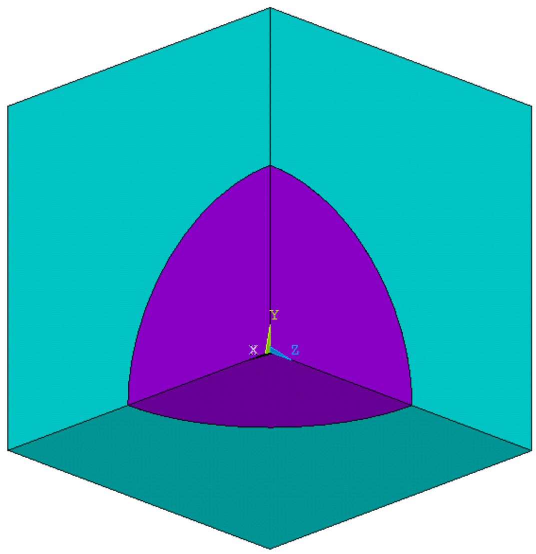

Fig. 4. FE Model of PRC at 20 wt. % of B_4C

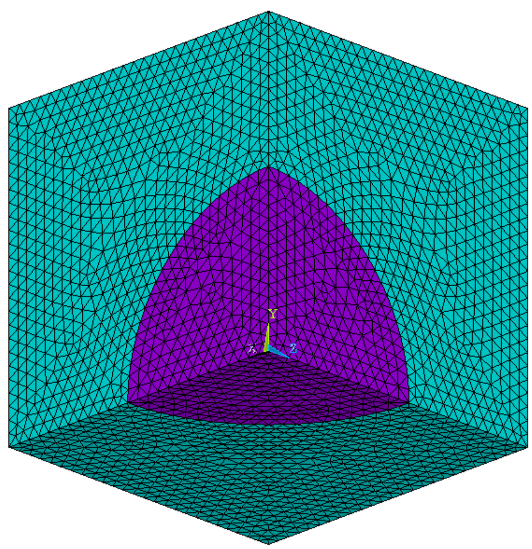

Fig. 5. Converged Mesh Model of PRC at 20 wt. % B_4C

E. Loading and Boundary Conditions

Due to the symmetry of the problem, the following symmetric boundary conditions are used.

At x = 0, $U_x = 0$;
At y = 0, $U_y = 0$;
At z = 0, $U_z = 0$.

In addition, the following multi-point constraints are used.

U_x of all the nodes on the line at x = 100 is same
U_y of all the nodes on the line at y = 100 is same.
U_z of all the nodes on the line at z = 100 is same.

Boundary conditions are imposed on the finite element model in such a way that the model should act as a part of the whole array of composite materials. Due to the symmetry in loading, geometry and boundary conditions, one-eighth of the unit cell is modeled in the analysis and a uniform tensile load of 1 MPa is applied to the Z-face to obtain a Uni-axial state of stress that facilitates the usage of simple hook's law for predicting Young's modulus of resulting composite.
Mesh Convergence is carried out for the FE Model. The converged FE model is used for the prediction of the Elastic properties of the Boron Carbide reinforced polypropylene composite at various weight percentages which are converted to volume fractions. Due to the spherical shape of the particles and symmetrical arrangement of reinforcement, the composite properties are isotropic in nature. The Elastic properties of the PP/B_4C Composite of different weight fractions are calculated.
Because of the isotropic nature and spherical shape of the particle, the following parameters will be equal in magnitude. E_1, E_2 and E_3 are equal. Poisson's Ratio's $\upsilon_{12} = \upsilon_{13} = \upsilon_{21} = \upsilon_{31} = \upsilon_{23} = \upsilon_{32}$. So the Elastic Properties of PRC are taken as E, υ and G.

III. FINITE ELEMENT RESULTS

The Elastic properties of the particle reinforced composites are calculated by using the FE Models prepared for different volume fractions of reinforcement.

A. Young's Modulus of PP/B_4C Composites

Figure 6 shows a variation of Young's Modulus (E) of PP/B_4C composites with respect to wt. % of B_4C. The Young's modulus increases with the increase in the weight percentage of the reinforcement in the matrix material.

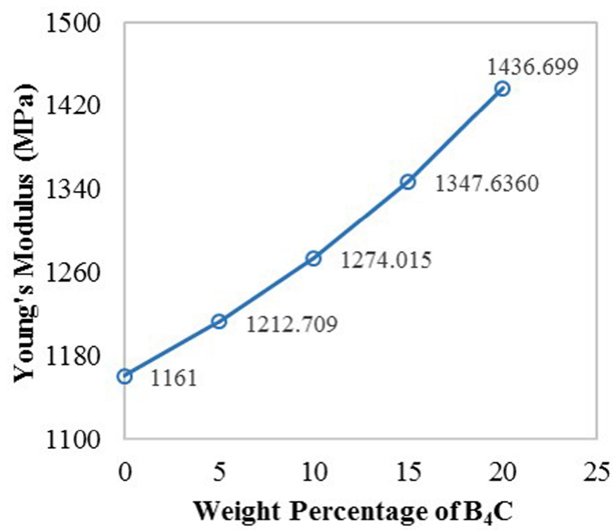

Fig. 6. Young's Modulus (E) with respect to wt. % of B_4C

B. Poisson's Ratio of PP/B_4C Composites

The Finite element procedure is further extended to determine Poisson's ratio of PP/B_4C composite. Figure 7 shows the variation of Poisson's ratio (υ) of PP/B_4C composite. The Poisson's Ratio is decreasing with the increase in the weight percentage of reinforcement.

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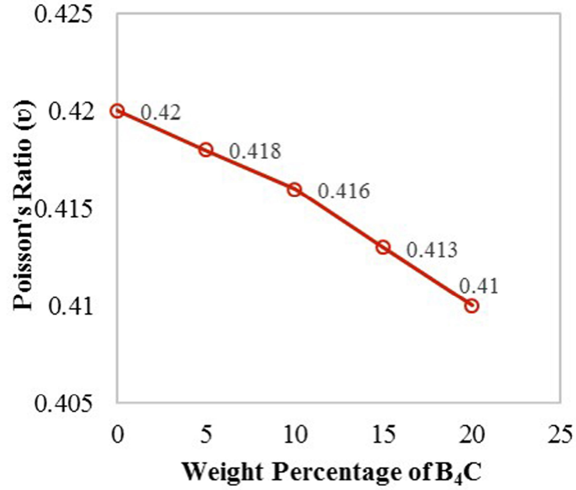

Fig. 7. Poisson's Ratio (υ) with respect to wt. % of B_4C

The Young's Modulus (E) increased with the increase in the weight percentage of reinforcement since modulus of reinforcement is very high, with the inclusion of these particles the modulus of composite increases. The Poisson's Ratio (υ) decreases with the increase in the weight percentage of reinforcement since with the increment of reinforcement (B_4C) concentration the longitudinal strain decreases and there is no considerable change in lateral strain. As a result, the Poisson's ratio is decreasing with respect to B_4C weight fraction.

IV. ANALYTICAL ANALYSIS

The Modulus of the particle reinforced composites can be predicted by using different analytical expressions suggested by various researchers [1]. The analytical expressions are suggested by Einstein, Kerner, Halpin-Tsai and Nielsen are used to estimate E (MPa) of PRC. The FE results are obtained from FE models are compared with the analytical results.

TABLE III
COMPARISON OF YOUNG'S MODULUS OF PRC

Wt. % of B_4C	FEM	Einstein	Kerner	Halpin-Tsai	Nielsen
5	1212.709	1215.857	1212.205	1216.563	1217.329
10	1274.015	1274.198	1268.872	1278.037	1281.541
15	1347.636	1336.601	1332.17	1346.685	1355.809
20	1436.699	1403.649	1403.487	1424.008	1443.014
30	1680.22	1553.708	1576.911	1611.927	1673.074

The expression (2) suggested by Nielsen gives closer agreement between results.

$$\frac{E_c}{E_m} = \frac{1+A_1B_1V_P}{1-\Psi B_1V_p} \tag{2}$$

$$A_1 = K_E - 1 \quad \text{and} \quad \Psi = 1 + [(1 - V_{p\,max})/V^2_{p\,max}]\, V_p$$

$$B_1 = \frac{\frac{E_p}{E_m} - 1}{\frac{E_p}{E_m} + A_1}$$

Where
E_c - Young's Modulus of Composite
E_p - Young's Modulus of Particle
E_m - Young's Modulus of Matrix
V_p - Volume fraction of Particles

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K_E - Einstein's Coefficient
$V_{p\,max}$ - Maximum packaging fraction

The expression can also be used for the calculation of Poisson's Ratio and Shear Modulus of the particle reinforced composite by replacing respective matrix properties.
The Validation FE models were done by comparing the FE results with the analytical results. The following table shows the Comparison between Elastic properties and % of Error between them.

TABLE III
COMPARISON (THEORETICAL VS. FEA) OF ELASTIC PROPERTIES OF PRC

Wt. % of B_4C	E in MPa		% of Error	υ		% of Error
	Analytical	FEA		Analytical	FEA	
5	1217.3292	1212.7091	0.3795	0.4149	0.4183	-0.8067
10	1281.5415	1274.0151	0.5872	0.4095	0.4163	-1.6442
15	1355.8097	1347.6362	0.6028	0.4037	0.4138	-2.5018
20	1443.0148	1436.6990	0.4376	0.3973	0.4108	-3.4077

It was observed that the FE Models of PRC predicts the less value of Moduli than Analytical value and high value of Poisson's Ratio than Analytical value. Almost zero percent error was observed in Moduli and a negligible error was observed in Poisson's Ratio. It was observed that in the case of PRC the FE results are very close with the analytical results at a lower volume fraction of the reinforcement and these results are deviating (high amount) with analytical results at a higher volume fraction of the reinforcement.

The Shear modulus (G) is calculated and Figure 8 shows a variation of Shear Modulus of PP/B_4C composite with respect to wt. % of B_4C. The Shear modulus increases with the increase in the weight percentage of the reinforcement in the matrix material.

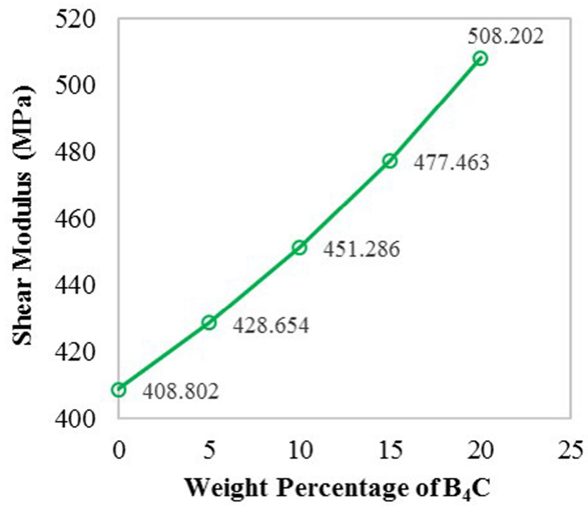

Fig. 8. Shear Modulus (G) with respect to wt. % of B_4C

V. CONCLUSIONS

In the present work, three-dimensional finite element analysis is carried out for finding the elastic properties of PRC at different volume fractions of reinforcement and then results were compared with the theoretical formulations. The influence of volume fraction of reinforcement on Young's Moduli and Poisson's ratios is studied. From the results and discussions, the following conclusions have been made from this present research work.

A. The Elastic properties of PRC are successfully predicted by using RVE and for this analysis Micromechanics in association with Finite Element Method.

B. The Young's Modulus is increasing along with the weight percentage of reinforcement.

C. The Poisson's Ratio is decreasing with the increase in the weight percentage of reinforcement.

D. The Shear modulus is calculated using the analytical expression and it is also increasing along with the reinforcement.

E. The FE models are validated by comparing the elastic properties obtained from the theoretical formulae.

F. A good correlation was observed between Finite Element Results and Analytical results.

G. From the results, it was observed that microparticles will enhance the Elastic Properties of polypropylene highly.

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