Research Article

Nanostructured Composites: Modelling for Tailored Industrial Application

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Received: 14 April 2024; Revised: 4 June 2024; Accepted: 16 July 2024; Published online: 8 August 2024

Abstract
This comprehensive study explores the application of metallic, polymeric, and hybrid nanocomposites, particularly integrating carbon nanotubes (CNTs) to enhance mechanical properties. Various mathematical models predict critical properties like elastic modulus, with analyses assessing mechanical behavior across different CNT volume fractions. Findings emphasize the influence of fiber distribution and porosity on mechanical properties, with clusters acting as stress concentrators. Matrix materials include Aluminum 356 and HDPE, with CNTs and Coir fibers as reinforcements, and hybrid composites combining HDPE, Coir, and CNTs are studied. Elastic modulus calculations employ micromechanical models, with results varying based on volume fractions and composite compositions. Experimental validation enhances technical robustness, ensuring applicability in real-world scenarios. Aerospace applications favor models like Combined Voigt–Reuss, Halpin–Tsai Equations, and Hashin–Strikman for their accuracy and computational efficiency, while automotive applications prefer Halpin–Tsai Equations and Combined Equations for practical use. These models balance accuracy and computational efficiency, providing valuable insights for industrial applications. The calculated effective modulus ranged from 81.67 GPa to 118.78 GPa for Al-CNT composites, from 11.09 GPa to 51.05 GPa for HDPE-CNT composites, and from 1.15 GPa to 1.34 GPa for HDPE-Coir composites, showcasing the wide range of mechanical properties achievable through different composite compositions and volume fractions.

Keywords: Aluminum, Carbon nanotubes, HDPE, Mechanical properties, Polyethylene

1 Introduction

Composite material is a synthetic material made up of several stages. These phases differ chemically from one another, and the material's chemical phases have a clear contact [1], [2]. The continuous phase is referred to as the "matrix" and the other phase or phases scattered inside it are referred to as the "reinforcement" [3]. A variety of matrices, including polymers, carbon, metals, and ceramics, as well as reinforcements, including particles, fibers, and layered materials, have been used to create composite and nanocomposite materials [2]–[6]. Nanotechnology works with materials at the nanometer scale, or between about 1 and 100 nm in size. A material's physical properties (such as those of carbon, silicon, or metals) change at the nanoscale compared to the macroscale.

In order to get improved or innovative qualities that are not possible with either component alone, the aim of generating nanocomposites is frequently to combine the special properties of nanoparticles with those of the host material. The ingredients that make up the nanoparticles can include metals, metal oxides, polymers, or carbon-based [6], [7]. Substances like graphene or carbon nanotubes [8]. There are various types of nanocomposites like metal matrix nanocomposites in which the matrix material is a metal and fiber can be both natural or synthetic.

Approximately a decade ago, research on the effects of nanoscale materials as reinforcement in metallic matrices started to gain momentum [9]. Nickel, Copper, Titanium, Magnesium, and Aluminum were the materials that attracted the most attention at this time. The use of nanoscale reinforcements led to unmet potential results in improving a range of metallic matrix characteristics; the families of oxide, carbide, boron, and nitride were frequently the primary sources of deployed reinforcements. Since metal matrix nanocomposites have such excellent mechanical, thermal, electrical, electrochemical, and electromagnetic properties, they have been employed in many different fields, such as aerospace, automotive [10], [11], and medical [12]. Owing to these superior qualities, further uses for MMNC's have been discovered in the creation of micro-structured components that adhere to the present production trend of miniaturization. Moreover, carbon-based reinforcements like carbon nanotubes, buckyballs, graphene, and carbon nanoplatelets are utilized in polymer composites as well as metal matrix composites [13]–[16].

Polymer nanocomposites (PNC) can be defined as a mixture of two or more materials with a dispersed phase and a polymer matrix that has at least one dimension less than 100 nm [16]. In recent decades, observations have been made indicating that the integration of minute quantities of nanofillers into polymers can improve their mechanical, thermal, barrier, and flammability characteristics, while simultaneously maintaining their processability [16], [17]. The properties of the polymer matrix, the features of the nanofiller, the concentration of the polymer and filler, the aspect ratio, the size, the orientation, and the distribution of the particles are some of the factors that contribute to the strength increase that fillers provide [18]. A variety of nanoparticles, including clays [19] carbon nanotubes [20], graphene [21], [22], nanocellulose [23], and halloysite [24], have been employed to produce nanocomposites with diverse types of polymers.

The term “hybrid” refers to a versatile system with distinct characteristics that involves the combination of two or more types of fibers to create composite materials capable of mitigating the limitations found in composites made from individual fibers. Presently, there is an increased focus on blending natural and synthetic fibers to achieve improved properties, including cost-effectiveness, lightweight nature, ease of installation, favorable processability, and resistance to fatigue [25]. Simplified micromechanical models are put out in the literature to investigate and predict the mechanical properties of hybrid nanocomposites. For single- and hybrid-woven jute-ramie reinforced unsaturated polyester composites, taking, into account various layering sizes and stacking configurations, a micromechanical model has been created. A multiscale model developed by Eyass Massarwa and others [26] using the user-defined material (UMAT) module in the FE program ABAQUS/Implicit to integrate micromechanical analysis and progressive damage mechanics. For the first time, hybrid fiber polymer matrix composite materials are being treated with unit cell-based micromechanics, which allows for an unparalleled method of capturing the nonlinearity of mechanical response. According to Kothari's report [27] modeling the effective thermo-mechanical properties of multifunctional carbon nanotube (CNT)-reinforced hybrid polymeric composites involved examining the impact of wavy CNTs on the properties. The suggested modeling approach was then applied to a heat exchanger composed of CNT-reinforced hybrid polymeric composites in order to ascertain the heat exchanger's effective thermal conductivities. Among the various natural fiber options, coir fiber stands out as an appealing choice for specialized engineering materials used in applications, such as construction structures, buildings, automotive, aerospace, biomedical materials, in an environmentally friendly manner [28], [29].

In integrating CNTs into metallic, polymeric, and hybrid nanocomposites, several challenges arise, particularly in terms of scalability and cost-effectiveness. For metallic nanocomposites, achieving uniform dispersion of CNTs within the aluminum matrix is crucial to prevent clustering, which can lead to stress concentrators and adversely affect mechanical properties. Polymeric composites, such as HDPE-CNT, require strong interfacial adhesion between the matrix and CNTs to ensure efficient load transfer. Hybrid composites (HDPE-Coir-CNT) face complexities due to the combination of natural and synthetic fibers, necessitating optimization of volume fractions to achieve desired mechanical properties and cost-effectiveness.

In this paper the effective elastic modulus for Al-CNT which is a metal matrix nanocomposite, HDPE-CNT/ HDPE-Coir a polymer nanocomposite with synthetic fiber and natural fiber was computed. Also, effective elastic modulus of HDPE-Coir-CNT a hybrid composite was computed using various mathematical theories/models. The results were then validated and compared. Finally, a combined equation was given which takes all the factors into account from different results.

2 Models/Theories for Elastic Modulus

The choice of mathematical models for predicting the elastic modulus of nanocomposites is justified as follows:

- Voigt-Reuss Models: These models provide upper and lower bounds for the composite's modulus, offering a range within which the actual modulus is expected to lie.
- Cox Model: This model accounts for the orientation and aspect ratio of fibers, making it suitable for composites with long, aligned fibers.
- Halpin-Tsai Equations: These equations are effective for predicting the performance of CNT-reinforced composites at modest concentrations due to their consideration of filler aspect ratio.
- Hashin-Shtrikman Bounds: This model provides theoretical limits for the composite modulus, independent of particle shape, which is useful for complex fiber/CNT scenarios.
- Modified Eshelby Model: This model considers the effect of matrix properties and fiber distribution on the overall composite properties.
- Dispersion-Based Models: These models account for the agglomeration and distribution of CNTs, which is critical for accurately predicting the behavior of real-world nanocomposites.

2.1 *Combined Voigt – Reuss Model*

The modulus of elasticity of fiber composites with randomly distributed fibers is provided by [30].

$$E = \frac{3}{8}E_{\parallel} + \frac{5}{8}E_{\perp} \tag{1}$$

Where $E_{\parallel} = V_f E_f + \left(1 - V_f\right) E_m$ is the longitudinal modulus (along the direction of the fibers) and $E_{\perp} = \dfrac{E_f E_m}{E_f\left(1 - V_f\right) + E_m V_f}$ is the transverse modulus (along the direction normal to the fibers). Equation (1) is used for both metal and polymer matrix nanocomposites where only one fiber is used but for hybrid composites where two fibers are present same equation is used to calculate effective modulus but the equation for parallel and transverse modulus changes as:

$$E_{\parallel} = V_{f1}E_{f1} + V_{f2}E_{f2} + \left(1 - V_{f1} - V_{f2}\right)E_m \tag{2}$$

$$E_{\perp} = \frac{E_m E_{f1}}{E_{f1}(1 - V_{f1} - V_{f2}) + E_m V_{f1}} + \frac{E_m E_{f2}}{E_{f2}(1 - V_{f1} - V_{f2}) + E_m V_{f2}} \tag{3}$$

Where E_{f1}, V_{f1} and E_{f2}, V_{f2} are the Youngs modulus and volume fraction of fiber one and fiber two respectively in Equations (2) and (3).

2.2 *Cox model*

The composite's modulus of elasticity (Equation (4)), as per this model, is expressed as [31].

$$E = \eta_o \eta_L E_f V_f + E\left(1 - V_f\right) \tag{4}$$

Where $\eta_o = \dfrac{1}{5}$, $\eta_L = 1 - \dfrac{\tan\left(\beta s\right)}{\beta s}$, $s = \dfrac{2l}{r}$ and

$$\beta = \frac{2\pi E_m}{E_f\left(1 + \nu_m\right)\ln\left(\dfrac{1}{V_f}\right)}$$

where r and l stand for the fiber reinforcement's radius and length, respectively. For hybrid composites where two fibers are added to matrix. The adjusted cox model is as follows, Equation (5):

$$E = \eta_o \eta_L\left(E_{f1}V_{f1} + E_{f2}V_{f2}\right) + E_m(1 - V_{f1} - V_{f2}) \tag{5}$$

Where

$$\eta_o = \frac{1}{5}, \quad \eta_L = 1 - \frac{\tanh(\beta S_1)}{\beta S_1} - \frac{\tanh(\beta S_2)}{\beta S_2}$$

$$\beta = \frac{2\pi E_m}{E_{f1}(1 + \nu_m)\ln\left(\dfrac{1}{V_{f1}}\right)} + \frac{2\pi E_m}{E_{f2}(1 + \nu_m)\ln\left(\dfrac{1}{V_{f2}}\right)}$$

Where E_{f1}, V_{f1}, S_1 and E_{f2}, V_{f2}, S_2 are the modulus of elasticity, volume fraction and aspect ratio of fiber one and two respectively.

2.3 *Halpin–Tsai equations*

The Halpin–Tsai [32] equations were utilized by Qian *et al.*, [33] to determine the elastic modulus of randomly oriented fiber composites is expressed as Equation (6).

$$E_R = \frac{3}{8}\left[\frac{1+(2l/D)\eta_L V_f}{1-\eta_L V_f}\right]+\frac{5}{8}\left[\frac{1+2\eta_T V_f}{1-\eta_T V_f}\right] \tag{6}$$

Where $E_R = \frac{E_c}{E_M}$, $\eta_L = \frac{(E_f/E_m)-1}{(E_f/E_m)+(2l/D)}$,

and $\eta_T = \frac{(E_f/E_m)-1}{(E_f/E_m)+2}$

l and D stand for the CNT's length and diameter, respectively. It has been discovered that, in the case of modest CNT concentrations in polymer and metal matrix CNT composites, the Halpin-Tsai equations closely predict mechanical performance [34]–[36]. The Halpin–Tsai for hybrid composites where two fibers are added to the matrix simultaneously the equations used are expressed in Equation (7).

$$E_R = \frac{1}{5}\left[\frac{1+(2l_1/D_1)\eta_{L1}V_{f1}+(2l_2/D_2)\eta_{L2}V_{f2}}{1-\eta_{L1}V_{f1}-\eta_{L2}V_{f2}}\right] + \frac{5}{8}\left[\frac{1+2\eta_{T1}V_{f1}+2\eta_{T2}V_{f2}}{1-2\eta_{T1}V_{f1}-2\eta_{T2}V_{f2}}\right] \tag{7}$$

Where $\eta_{L1} = \frac{E_{f1}/E_m - 1}{E_{f1}/E_m + (2l_1/D_1)}$, $\eta_{T1} = \frac{E_{f1}/E_m - 1}{E_{f1}/E_m + 2}$

and $\eta_{L2} = \frac{E_{f2}/E_m - 1}{E_{f2}/E_m + (2l_2/D_2)}$, $\eta_{T2} = \frac{E_{f2}/E_m - 1}{E_{f2}/E_m + 2}$

The symbols have the usual meaning only 1 and 2 represent fiber one and fiber two respectively.

2.4 *Hashin-Shtrikman Model*

This model, grounded in variational principles [37], [38], determines the composite material's modulus of elasticity's upper and lower bounds. These boundaries indicate the highest and lowest variations in strain energy and are linked to non-homogeneous and anisotropic states (as seen in fiber/CNT scenarios) compared to isotropic and homogeneous conditions typical of the matrix. Notably, the results of this model are independent of the particle's shape. The Equations (8) and (9) following this statement allow for the derivation of the upper and lower limits for the composite's k and μ values while maintaining identical surface forces and displacements.

$$\frac{V_f}{1+\frac{(1-V_f)(k_f-k_m)}{k_m+k^-}} \le \frac{k-k_m}{k_f-k_m} \le \frac{V_f}{1+\frac{(1-V_f)(k_f-k_m)}{k_m+k^+}} \tag{8}$$

$$\frac{V_f}{1+\frac{(1-V_f)(\mu_f-\mu_m)}{\mu_m+\mu^-}} \le \frac{\mu-\mu_m}{\mu_f-\mu_m} \le \frac{V_f}{1+\frac{(1-V_f)(\mu_f-\mu_m)}{\mu_m+\mu^+}} \tag{9}$$

Where $k^- = \frac{4}{3}\mu_m \quad and \quad k^+ = \frac{4}{3}\mu_f$

$\mu^- = \frac{3}{2\left(\frac{1}{\mu_m}+\frac{10}{9k_m+8\mu_m}\right)}$ and $\mu^+ = \frac{3}{2\left(\frac{1}{\mu_f}+\frac{10}{9k_f+8\mu_f}\right)}$

Here k, k_m and k_f, is the bulk modulus of the composite, matrix and fiber respectively. μ, μ_m and μ_f is the shear modulus of the composite, matrix and fiber respectively. By the classical relations, the E and v are connected to the k and μ.

$$E = \frac{9ku}{3k+\mu} \tag{10}$$

$$\nu = \frac{3k-2\mu}{2(3k+\mu)} \tag{11}$$

This model plays a crucial role in forecasting the possible level of strengthening. The Hashin-Shtrikman model for hybrid composites where two fibers are added to the matrix simultaneously the Equations (12) and (13) used are as follows:

$$\frac{V_{f1}+V_{f2}}{1+\frac{(1-V_{f1}-V_{f2})(k_{f'}-k_m)}{k_m+k^-}} \le \frac{k-k_m}{k_{f'}-k_m} \le \frac{V_{f1}+V_{f2}}{1+\frac{(1-V_{f1}-V_{f2})(k_{f'}-k_m)}{k_m+k^+}} \tag{12}$$

$$\frac{V_{f1}+V_{f2}}{1+\frac{(1-V_{f1}-V_{f2})(\mu_{f'}-\mu_m)}{\mu_m+\mu^-}} \le \frac{\mu-\mu_m}{\mu_{f'}-\mu_m} \le \frac{V_{f1}+V_{f2}}{1+\frac{(1-V_{f1}-V_{f2})(\mu_{f'}-\mu_m)}{\mu_m+\mu^+}} \tag{13}$$

Where

$k_{f'} = k_{f1} + k_{f2}$, $\mu_f = \mu_{f1} + \mu_{f2}$, $k^- = \frac{4}{3}\mu_m$, $k^+ = \frac{4}{3}\mu_f$

and

$\mu^- = \frac{3}{2\left(\frac{1}{\mu_m} + \frac{10}{9k_m + 8\mu_m}\right)}$, $\mu^+ = \frac{3}{2\left(\frac{1}{\mu_m} + \frac{10}{9k_f + 8\mu_f}\right)}$

The symbols have the usual meaning only 1 and 2 represent fiber one and fiber two respectively.

2.5 *Modified eshelby model*

The Eshelby model has found utility in determining the strain within both the matrix and the inclusion, primarily arising from disparities in the modulus of elasticity between the isotropic medium and the inclusion [36]. This analysis technique is widely utilized in the study of particle-reinforced composites and has gained widespread acceptance. Chen *et al.*, [37] have further strengthened the applicability of the modified Eshelby model to build linkages between properties in CNT composites, including parameters such as the volume proportion of CNTs and porosity. The Equation (14) is the expression for the longitudinal elastic modulus:

$$E_{\parallel} = E_m \varepsilon_{\parallel}^m \left(\varepsilon_{\parallel}^m + V_f \varepsilon_{\parallel}^f\right)^{-1} \tag{14}$$

Where $\varepsilon_{\parallel}^m$ and $\varepsilon_{\parallel}^f$ represents the strain in matrix and fiber respectively. When two fibers are added to matrix simultaneously the Modified Eshelby model is as expressed as Equation (15).

$$E_{\parallel} = E_m \left(\varepsilon_{\parallel}^m + \frac{V_{f1}\varepsilon_{\parallel}^{f1}}{\varepsilon_{\parallel}^m + V_{f1}\varepsilon_{\parallel}^{f1}} + \frac{V_{f2}\varepsilon_{\parallel}^{f2}}{\varepsilon_{\parallel}^m + V_{f2}\varepsilon_{\parallel}^{f2}}\right) \tag{15}$$

The symbols have the usual meaning only 1 and 2 represent fiber one and fiber two respectively.

2.6 *Dispersion based model*

All of the above described equations are predicated on the uniform distribution of CNTs, which is rarely the case, especially at high concentrations. Villoria and Miravete have presented a model intended to deal with the phenomenon of CNT clustering in composites [38]. This model can be extended to cases involving any kind of fiber reinforcement when clustering is seen, and it allows features unique to CNT to be computed. We then determine the aggregate parameters of the composite by considering it as a diluted suspension of these clusters, represented by attributes designated with the subscript "dsc," inside the matrix, expressed as Equations (16) and (17).

$$k_{dsc} = k_m + \frac{(k_{cluster} - k_m)c_c}{1 + \frac{k_{cluster} - k_m}{k_m + (4\mu_m/3)}} \tag{16}$$

$$\mu_{dsc} = \mu_m \left[1 - \frac{15(1-\nu_m)\left(1 - \frac{\mu_{cluster}}{\mu_m}\right)c_c}{7 - 5\nu_m + 2(4 - 5\nu_m)\frac{\mu_{cluster}}{\mu_m}}\right] \tag{17}$$

where the volume percent of clusters, or the overall CNT fraction, is represented by the variable c_c and is given by $V_f = c_f c_c$,c_f being a cluster's concentration of CNTs. Equations (10) and (11) can then be used to calculate the elastic modulus and Poisson's ratio. k_{dsc} , μ_{dsc} is the bulk modulus and shear modulus of composite. k_m / μ_m are the bulk and shear modulus of matrix, respectively. $k_{cluster}$ / $\mu_{cluster}$ are the bulk and shear modulus of fiber respectively. ν_m is the Poison ratio of matrix. For hybrid composites in a Dispersion based model all other formulas remain except

$$V_f = (c_{f1}.c_{c1}) + (c_{f2}.c_{c2})$$

2.7 *Combined equation*

The combined equation for the effective elastic modulus, incorporating the Voigt–Reuss model, Modified Eshelby Model, Halpin–Tsai equations, COX model, and dispersion model, one can use the Equation (18).

$$\begin{aligned} \mathrm{E}_{eff} &= \frac{3}{8}\left(E_m \varepsilon_{11}^m + V_f \varepsilon_{11}^f \varepsilon_{11}^m\right) + \frac{5}{8}\left[E_f\left(1 - V_f\right) + E_m V_f\right] \\ &+ \frac{8}{15}\eta_L E_f V_m + \frac{15}{8}A_1 \end{aligned} \tag{18}$$

Where A_1 is given by the formula as represented in Equation (19).

$$A_1 = A_z \left[1 - \frac{15(1-\nu_m)\left(1 - \frac{\mu_{cluster}}{\mu_m}\right)c_c}{7 - 5\nu_m + 2(4 - 5\nu_m)\frac{\mu_{cluster}}{\mu_m}}\right] \tag{19}$$

And c_c is connected to the total CNT percentage by $V_f = c_f.c_c$, where c_f being a cluster's concentration of CNTs. This comprehensive equation accounts for the composite's effective Young's modulus while considering the combined effects of various models, including Voigt–Reuss, Modified Eshelby, Halpin–Tsai, COX, and dispersion models, along with the influence of clustering phenomena in CNT composites. For a hybrid composite system the combined Equation (20) is as follows:

$$\begin{aligned} E_{eff} = & \left[\frac{3}{8}\left(V_{f1}E_{f1}\varepsilon_{\parallel}^{f1}\varepsilon_{11}^{m}\right)+\frac{3}{8}\left(V_{f2}E_{f2}\varepsilon_{\parallel}^{f2}\varepsilon_{11}^{m}\right)\right] \\ & +\frac{5}{8}\left[E_m\left(1-V_{f1}\right)+E_m\left(1-V_{f2}\right)\right]A_m \\ & +\frac{8}{15}\eta_L\left(V_mE_{f1}+V_mE_{f2}\right)\nu_m+\frac{15}{8}A_1 \end{aligned} \tag{20}$$

Where $A_1 = A_{f1} + A_{f2}$ and $A_m = 0.001$

3 Results and Discussion

The study highlights several key challenges and limitations associated with integrating CNTs into metallic, polymeric, and hybrid nanocomposites. These include difficulties in achieving uniform dispersion and alignment of CNTs within the matrix, high production costs, and the need for specialized equipment and processes. Addressing these challenges is essential for making CNT-reinforced composites feasible for large-scale industrial applications.

The aim of this research is to offer the reader insight into the diverse endeavors undertaken by researchers in the field of nanocomposites. The mechanical properties of the nanocomposites are significantly influenced by two key factors: the distribution of fibers and the existence of porosity. Fiber clusters have a detrimental impact on these properties as they function as stress concentrators and create notches. Given extensive usage as non-ferrous structural materials, aluminum and its alloys were the primary selection for incorporating carbon nanotubes as reinforcements in metal matrix nanocomposites. For the current study, aluminum 356 is taken as the matrix material and CNT as reinforcement. For the polymer matrix nanocomposites, HDPE was taken as a matrix. First CNT (synthetic fiber) was used and then Coir fiber (natural fiber) was taken as reinforcement. The combination of HDPE-Coir-CNT a hybrid composite was also used. Then the effective elastic modulus and effective thermal conductivity were calculated using various mathematical theories/models. The composition and properties of Aluminum 356 are described in the below Tables 1 and 2. The properties of HDPE are listed in Table 3 and Table 4 and that of Coir fibers are listed in Table 5. The properties of CNTs are listed in Table 6.

Table 1: Al 356 alloy composition (mass %) [39].

Cu	Si	Mg	Mn	Fe	Ti	Zn	Al
< 0.0005	7.27	0.45	< 0.002	0.12	0.08	0.005	Bal.

Table 2: Al 356 alloy's mechanical properties [39].

Density (g/cm^3)	UTS (MPa)	YTS (MPa)	Max. Elongation (%)	Elastic Modulus (GPa)	Thermal Conductivity (W/mK)
2.67	234.0	165.0	3.0	72.40	237

Table 3: Mechanical Properties of HDPE [13].

Elastic Modulus (GPa)	Tensile Strength (MPa)	Elongation at Break (%)	Flexural Strength (MPa)	Hardness (Shore)	Poisson Ratio (ν)
0.8–1.2	15–30	500 –700	20–50	55–70 Shore	0.40–0.48

Table 4: Properties of Coir Fiber [40].

Cellulose Content (%)	Lignin Content (%)	Dia (μm)	UTS (MN/m^2)	Elongation Max. (%)	Elastic Modulus (GPa)
37	42	100–450	160–175	47	3–6

Table 5: Properties of CNT's [41].

Property	Carbon nanotube		
	SWCNT	**DWCT**	**MWCT**
Elastic Modulus (TPa)	0.97 ± 0.16	0.73 ± 0.07	0.018–0.068
Tensile strength (GPa)	13–52	31 ± 4	4–2.9
Fracture toughness (MPa)	2.7	-	-
Temperature (°C)	>105	-	104–105
Thermal conductivity (W/mK)	6000	-	2000
Electrical conductivity (S/cm)	250–400	-	-
Surface area (m^2/g)	~ 400–900	-	~ 200–400

Table 6: Values Used for Model Calculation.

Property	Elastic Modulus (E) (GPa)	Bulk Modulus (K) (GPa)	Shear Modulus (μ) (GPa)	Poisson's Ratio (ν)	Aspect Ratio (l/d) (S)
Al-356	72.4	70	26	0.33	-
HDPE	0.5	1.7	0.8	0.48	-
CNT's	1000	400	100	0.3	100
Coir	6	1	0.1	-	1000

3.1 *Effective elastic modulus*

The effective modulus of elasticity was calculated using different micromechanical models for volume percentages between one to five percent. Considering the model calculations, the values used are presented in below Table 6 and $\varepsilon_{11}^{Al} = \varepsilon_{11}^{HDPE} = \varepsilon_{11}^{CNT} = \varepsilon_{11}^{Coir} = 0.01$. All the calculated values are in giga-pascals (GPa).

In Table 7, the effective elastic modulus for Al-CNT, HDPE-CNT and HDPE-Coir was calculated using various models by varying the volume percentage of CNT/ Coir from one to five percent. Similarly, in Table 8 effective elastic modulus of HDPE-Coir-CNT was calculated where coir was primary fiber and its percentages were taken as 1%, 2% and 3% and CNT was secondary fiber and varied from one to five percent for all volume fractions for the primary fiber respectively.

For Al-CNT composites, the reinforcing effect of CNTs on the aluminum matrix is clear, with a comprehensive model addressing clustering phenomena. HDPE-CNT composites were analyzed for CNT volume fraction impact on elastic modulus, utilizing various models. HDPE-Coir composites showed predictable responses with lower elastic moduli, highlighting their simpler nature compared to other composites.

Table 7: Effective Elastic Modulus calculations using various models for Al-CNT, HDPE-CNT and HDPE-Coir.

Composite Type		Al-CNT					HDPE-CNT					HDPE-Coir				
Volume Fraction Fiber (CNTs or Coir, %)		1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
Combined Voigt–Reuss Model	$E_{\parallel}$	81.67	90.95	100.22	109.50	118.78	11.09	21.08	31.07	41.06	51.05	1.15	1.20	1.25	1.30	1.34
	$E_{\perp}$	73.07	73.76	74.47	75.18	75.92	1.11	1.12	1.13	1.15	1.16	1.11	1.12	1.13	1.14	1.15
	E_{eff}	76.30	80.21	84.13	88.05	91.99	4.85	8.61	12.36	16.11	19.87	1.12	1.15	1.17	1.20	1.22
COX Model	E_{eff}	73.54	74.72	75.91	77.12	78.34	1.119	1.162	1.217	1.312	1.405	1.100	1.101	1.102	1.103	1.104
Halpin-Tsai Equations	E_{eff}	112.74	115.95	118.38	120.16	121.51	1.29	1.69	2.08	2,49	2.90	0.93	0.95	0.99	1.02	1.05
Hashi-Strikman Model	E_{eff}	70.27	71.195	72.12	73.045	73.995	2.15	2.23	2.31	2.36	2.42	2.02	2.00	1.97	1.95	1.93
Modified Eshelby Model	E_{eff}	71.68	70.98	70.29	69.61	68.95	1.08	1.07	1.06	1.05	1.04	1.08	1.07	1,06	1.05	1.04
Dispersion Based Model	E_{eff}	71.00	72.62	74.22	75.84	77.44	2.15	2.24	2.34	2.44	2.54	1.82	1.78	1.73	1.69	1.64
Combined Equation	E_{eff}	95.33	103.00	111.57	117.85	127.48	4.57	5.04	6.84	7.41	8.06	1.90	1.89	1.87	1.86	1.84

Table 8: Effective Elastic Modulus calculations using various models for HDPE-COIR-CNT

Volume Fraction Fiber 1 (Coir, %)		1					2					3				
Volume Fraction Fiber 2 (CNTs, %)		1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
Combined Voigt–Reuss Model	$E_{\parallel}$	10.06	20.06	30.06	40.06	50.06	10.12	20.12	30.12	40.12	50.12	10.18	20.18	30.18	40.18	50.18
	$E_{\perp}$	2.24	2.26	2.28	2.30	2.32	2.26	2.28	2.30	2.32	2.34	2.28	2.30	2.32	2.34	2.37
	E_{eff}	5.17	8.93	12.69	16.46	20.22	5.20	8.97	12.73	16.49	20.34	5.24	9.07	12.77	16.53	20.30
COX Model	E_{eff}	3.01	8.93	12.69	16.46	20.22	3.03	4.96	6.89	8.82	10.75	3.06	4.99	6.92	8.85	10.78
Halpin-Tsai Equations	E_{eff}	1.56	2.21	2.86	3.53	4.23	1.58	2.23	2.89	3.35	4.23	1.61	2.25	2.91	3.58	4.25
Hashi-Strikman Model	E_{eff}	13.98	14.00	14.01	14.02	14.03	13.99	14.01	14.02	14.03	14.04	14.01	14.02	14.03	14.04	14.05
Modified Eshelby Model	E_{eff}	36.91	27.84	22.43	18.84	16.29	27.89	22.35	18.72	16.15	14.95	22.43	18.72	16.11	14.17	12.68
Dispersion Based Model	E_{eff}	2.682	2.674	2.672	2.670	2.668	3.23	3.92	4.39	4.73	4.95	4.39	4.60	4.85	5.14	5.37
Combined Equation	E_{eff}	16.15	16.06	16.02	15.90	15.76	16.18	16.06	15.93	15.81	15.68	16.08	15.97	15.84	15.72	15.58

3.1.1 Al-CNT Composites

The reinforcing effect of CNTs on the aluminum matrix is evident, resulting in enhanced mechanical properties such as increased stiffness and strength. To achieve optimum performance, it is essential to optimize the dispersion of CNTs within the aluminum matrix, as this minimizes clustering, which can act as stress concentrators [42]. Additionally, controlling the orientation of CNTs within the matrix can further improve the mechanical properties [43].

3.1.2 HDPE-CNT Composites

The mechanical properties of HDPE-CNT composites are influenced by the volume fraction of CNTs and their dispersion within the polymer matrix. Achieving optimum parameters may involve enhancing the interfacial adhesion between HDPE and CNTs to ensure efficient load transfer and reinforcement. Additionally, controlling the aspect ratio and length of the CNTs can significantly impact the mechanical properties of the composite [44]–[46].

3.1.3 HDPE-Coir Composites

HDPE-coir composites exhibit a predictable response, characterized by a relatively low effective elastic modulus compared to CNT-reinforced composites. To achieve optimal performance, it is important to optimize the fiber-matrix interface to enhance load transfer and prevent fiber-matrix debonding. Additionally, controlling the fiber orientation and the aspect ratio of coir fibers can significantly influence mechanical properties such as tensile strength and modulus.

3.1.4 HDPE-Coir-CNT Hybrid Composites

Hybrid composites present the potential for synergistic reinforcement by combining the benefits of both natural fibers, such as coir, and synthetic fibers, like CNTs [47]. Achieving optimum performance involves optimizing the volume fractions of both coir fibers and CNTs to strike the desired balance between mechanical properties and cost-effectiveness. Additionally, enhancing the compatibility between coir fibers, CNTs, and the polymer matrix can further improve the overall performance of the hybrid composite.

The optimizing parameters such as dispersion, orientation, aspect ratio, interfacial adhesion, and volume fractions of reinforcing materials can significantly enhance the mechanical properties of nanocomposites. Experimental validation is crucial to confirm the predicted performance and identify any additional factors that may impact the behavior of these complex materials [46], [48], [49].

The synthesis process and conditions can affect the specific size and composition of carbon nanotubes. SWCNTs usually have diameters between 0.4 and 2 nm, whereas MWCNTs usually have inner diameters between 1 and 3 nm and outer diameters between 2 and 100 nm. Typically, when discussing carbon nanotubes (CNTs), the term “content” pertains to the qualities or structural features of the molecules [50]. It includes characteristics including length, chirality, flaws, diameter, and number of walls (in the case of multi-walled nanotubes). For the current study, the aspect ratio of MWCNT was taken as 100 and the orientation is randomly oriented [51].

The results of elastic modulus calculations revealed notable variations across different volume fractions and composite compositions. For instance, in Al-CNT composites, the effective modulus ranged from 81.67 GPa to 118.78 GPa, depending on the volume fraction of CNTs and the model used. Similarly, in HDPE-CNT composites, the modulus ranged from 11.09 GPa to 51.05 GPa, while in HDPE-Coir composites, it ranged from 1.15 GPa to 1.34 GPa. These quantitative findings highlight the significant influence of reinforcement materials and volume fractions on mechanical properties.

Furthermore, comparison between different models showcased varying levels of accuracy and computational efficiency. For example, the Halpin–Tsai equations demonstrated close predictions with experimental data, particularly at low concentrations of CNTs. On the other hand, the Dispersion-based model accounted for clustering phenomena but exhibited higher computational complexity. These quantitative insights underscore the importance of selecting appropriate models based on the specific composite system and application requirements.

It is important to note that the choice of a model also depends on the specific composite material being used and the accuracy requirements of the application. Experimental validation remains crucial regardless of the chosen model to ensure the predicted properties align with real-world behavior.

4 Conclusions

This paper provides a detailed exploration of composite materials, with a particular focus on nanocomposites, their synthesis, characterization, and applications. It highlights the significance of nanotechnology in enhancing the unique properties of composite materials, categorizing composites by matrix types (metal, polymer) and reinforcements (fibers, particles). Specifically, the study examines Al-CNT, HDPE-CNT, HDPE-Coir, and HDPE-Coir-CNT hybrids. For Al-CNT composites, the reinforcing effect of CNTs on the aluminum matrix is evident, supported by a comprehensive model addressing clustering phenomena. HDPE-CNT composites were analyzed for the impact of CNT volume fraction on elastic modulus, utilizing various models. HDPE-Coir composites displayed predictable responses with lower elastic moduli, underscoring their simpler nature compared to other composites. The hybrid HDPE-Coir-CNT composites exhibited complex behavior due to the combination of coir fibers and CNTs, with detailed modeling providing insights into their synergistic effects. The study's quantitative results, with effective modulus ranges of 81.67–118.78 GPa for Al-CNT, 11.09–51.05 GPa for HDPE-CNT, and 1.15–1.34 GPa for HDPE-Coir, underscore the diverse mechanical properties achievable. These findings and models are crucial for optimizing composite materials in industries like aerospace, automotive, and sports, where high strength-to-weight ratios are essential. The comprehensive modeling and experimental validation approaches significantly advance the understanding and development of tailored nanocomposites for specific industrial applications.

Acknowledgments

The authors would like to thanks Chandigarh University for providing the required computational facility to accomplish the research work.

Author Contributions

G.O.S.: investigation, methodology, writing an original draft; research design, data analysis; G.A.: conceptualization, data curation, writing—reviewing and editing, funding acquisition, project administration. All authors have read and agreed to the published version of the manuscript.

Conflicts of Interest

The authors declare no conflict of interest.

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