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Exploring the Potential of PA6-ABS Blend with Reinforcement of Graphene, MWCNT, and its Hybrid Nanocomposites through Simulation

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Abstract

This research investigates the prospective of reinforcing Polyamide 6 (PA6) blended with Acrylonitrile Butadiene Styrene (ABS) using graphene, Multi-Walled Carbon Nanotubes (MWCNT), and their hybrid combinations to enhance mechanical properties. Different weight percentages of MWCNT, graphene, and hybrid reinforcements were used to create twelve distinct nanocomposite structures. Material properties like density, Young's modulus, shear modulus, and Poisson's ratio were predicted using Digimat 2017 software, and finite element analysis was made easier on ASTM D638 standard tensile specimens using CATIA V5R19 Educational software to evaluate deflection behaviour and maximum von Mises stress. The study shows how various nanofiller kinds and concentrations affect the PA6-ABS blend's mechanical response. According to the results, hybrid nanocomposites have better mechanical properties than single-filler systems. The potential of PA6-ABS based nanocomposites for high-performance engineering applications is highlighted in this work, which offers insightful information about the nanoscale reinforcing mechanisms. Results indicate a consistent decrease in deflection across all nanocomposite types (Graphene, MWCNT, and hybrids) as filler content increased, signifying enhanced stiffness. Notably, PA-M15 exhibited the lowest deflection, suggesting maximum resistance to deformation. Through simulation-based evaluation, it will help guide future material selection and design optimization.

Major Findings: *Simulation studies show that adding graphene, MWCNT, and their hybrids to PA6-ABS blends significantly enhances mechanical stiffness and reduces deflection. Hybrid and MWCNT-reinforced composites, particularly PA-M15, exhibit superior mechanical properties. These materials are promising candidates for high-performance engineering applications.*

Keywords: *Acrylonitrile Butadiene Styrene (ABS), Finite Element Analysis (FEA), Graphene, Mechanical Properties, Multi-Walled Carbon Nanotubes (MWCNTs), Nanocomposites, Polyamide 6 (PA6)*

1.0 Introduction

Polyamide 6 (PA6) is a popular engineering thermoplastic because of its superior processability, chemical resistance, and mechanical qualities. Further improvement of its mechanical qualities, such stiffness and strength, is necessary in some applications, though. To modify its characteristics, PA6 is frequently blended with other polymers, such as Acrylonitrile Butadiene Styrene (ABS). ABS is renowned for its resilience to impact and durability. Strength and ductility are two qualities that may be balanced by combining PA6 with ABS. The

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growing demand for lightweight, high-strength materials across various industries is driving research into innovative material solutions. Incorporating nanoscale reinforcements into a polymer matrix to produce polymer nanocomposites may lead to considerable enhancements of properties.

One possible method for greatly enhancing the performance of polymer mixtures is nanocomposite technology. The mechanical, electrical, and thermal characteristics of polymer matrices have been shown to significantly improve with the addition of nanoscale reinforcements such graphene and Multi-Walled Carbon Nanotubes (MWCNTs). They are one-dimensional cylindrical structures with high Young's modulus and aspect ratio, while graphene, a 2-Dimensional (2D) sheet of carbon atoms, is very strong and stiff. This study explores the use of MWCNTs and graphene, 2 nanomaterials known for their exceptional mechanical properties, to strengthen PA6 and ABS, a flexible engineering thermoplastic. Graphene and MWCNTs, either separately or in hybrid combinations, have the potential to improve the mechanical characteristics of PA6-ABS composites. Designing materials for particular technical applications requires an understanding of how these nanofillers affect the composite material's overall performance. By employing modelling techniques, we want to understand how these reinforcements impact the mechanical behaviour of PA6-ABS nanocomposites and identify the optimal material configurations for enhanced performance[1-3].

The mechanical, electrical, and thermal characteristics of polymer nanocomposites have been enhanced by nanofillers like graphene and Multi-Walled Carbon Nanotubes (MWCNTs), resulting in significant advancements in this field. Polyamide 6 (PA6) is a well-liked thermoplastic that is ideal for sophisticated composite applications due to its remarkable mechanical properties and simplicity of processing[4,5]. The distinctive properties of graphene, MWCNTs, and PA6 are examined in this literature review along with their use in nanocomposites and recent developments in the area. PA6 is widely renowned for its strength, durability, and chemical resistance. Its semi-crystalline structure is responsible for its moderate impact resistance and high tensile strength[6,7]. Over a broad temperature range, the toughness of PA6/ABS mixes compatible with SMA was evaluated. By changing the viscosity ratio and raising the PA6 phase viscosity, SMA prevented scattered phase coalescence. According to morphological and mechanical characteristics, the results show a positive interaction among PA6 and ABS[8].

The mechanical properties of PA/ABS blends are hampered by their low miscibility, despite their importance in the automotive and electrical sectors. By employing two multi-monomer melt-grafted compatibilizers, this work creates mechanically improved PA6/ABS blends that have a distinctive "soft shell-encapsulating-hard core" structure and a notable reduction in scattered domain size. The resultant combination exhibits a 1300% increase in impact strength and a 36% improvement in tensile strength[9]. SEBS-g-MA was used to compatibilize PA6/ABS blends, and the effects of compatibilizer and ABS concentration were investigated. Young's modulus dropped as the compatibilizer concentration increased, while tensile strength increased[10].

Mixtures of PA6 and ABS-MA were prepared using a co-rotational twin-screw extruder. Analyzing blends revealed that PA6's qualities can be enhanced by ABS-MA at even low quantities. Impact strength and elongation at break were significantly increased in the PA6/ABS-MA mix with 10% ABS-MA, which demonstrated the most significant balance of characteristics[11]. Blends with reactive compatibilization based on PA6 were created using recycled ABS. When 5 phr SAN-g-MA was added, mechanical characteristics were much improved, showing encouraging outcomes for plastic recycling[12].

Studies show that PA6's mechanical properties are significantly enhanced by the addition of graphene and MWCNTs. MWCNTs improve tensile strength, Young's modulus, and impact resistance by efficiently transferring stress between the nanofiller and polymer matrix. Graphene-based nanocomposites exhibit significantly greater mechanical reinforcement because graphene has superior intrinsic properties compared to other materials[13]. MWCNTs and graphene increase the thermal conductivity of PA6 composites, which reduces thermal expansion and improves heat resistance. As a result, they can be utilized in electronics, high-temperature environments, and automotive parts[14,15]. One of the biggest challenges in producing PA6-based nanocomposites is evenly dispersing nanofillers. Inadequate dispersion can lead to aggregation, which reduces the overall effectiveness of reinforcement. Functionalization and surface treatments have been studied to increase

the compatibility of MWCNTs and graphene with PA6[16,17]. Recent studies aim to enhance the dispersion of nanofillers through the improvement of processing techniques such solution mixing, melt blending, and *in-situ* polymerization. Hybrid nanocomposites including graphene and MWCNTs are also being studied in order to benefit from the complementing qualities of both fillers. Future studies aim to increase the scalability of PA6-based nanocomposites for industrial applications[18,19].

Recent research has demonstrated the significance of graphene-reinforced nanocomposites in enhancing the mechanical, electrical, and thermal properties of polymer matrices such as PA6. Graphene Nanoparticles (GRNPs) improve the tensile strength, compressive and wear resistance, and impact energy of aluminum alloy composites, according to studies employing Digimat-FE simulations and experimental methods[20,21]. These results are applicable to systems that use PA6. A homogeneous distribution of nanofillers is necessary to maximize these properties; higher filler concentrations increase mechanical performance but can cause brittleness and porosity. The addition of GRNPs to polymer matrices offers promising new information for the creation of high-performance polymer nanocomposites meant for industrial usage, as shown by metal-based composites[22,23].

1.1 Research Gap and Scope

While research exists on PA6 nanocomposites and PA6-ABS blends, there is a need for more investigation into the combined effect of graphene and MWCNT reinforcement on the mechanical properties of PA6-ABS blends, particularly using simulation techniques. A systematic study is needed to optimize the composition and structure of PA6-ABS nanocomposites reinforced with hybrid grapheme or MWCNT systems. This study aims to address this gap by employing Digimat and CATIA to simulate the mechanical behaviour of these nanocomposites.

2.0 Materials and Methods

2.1 Material Configurations

As shown in Table 1, 12 distinct PA6 (70%) with ABS (30%) nanocomposite configurations were examined. The weight percentages of graphene and MWCNTs in these arrangements range from 0.5%, 1% and 1.5%, and hybrid combinations with varied ratios such as 1:1 and 2:1 are also included. Polypropylene Grafted Maleic Anhydride (PP-g-MA) as compatibilizing agent enhances the interaction between the PA6 and ABS phases by reacting with the amine end groups of PA6 or interacting with the ABS phase, thereby promoting interfacial adhesion and leading to improved mechanical properties in the resulting blends. Table 2 shows the Design of Experiments (DOE) for PA6-ABS Nanocomposites.

Table 1. Polyamide 6 and acrylonitrile butadiene styrene nanocomposites configurations

Expt. No.	Details PA6 (70%)+ABS(30%)	Label Code
1	PA6+ABS with Graphene 0.5%	PA-G05
2	PA6+ABS with Graphene 1%	PA-G1
3	PA6+ABS with Graphene 1.5%	PA-G15
4	PA6+ABS with MWCNT 0.5%	PA-M05
5	PA6+ABS with MWCNT 1%	PA-M1
6	PA6+ABS with MWCNT 1.5%	PA-M15
7	PA6+ABS with Hybrid 1:1 0.5%	PA-H1105
8	PA6+ABS with Hybrid 1:1 1%	PA-H111
9	PA6+ABS with Hybrid 1:1 1.5%	PA-H1115
10	PA6+ABS with Hybrid 2:1 0.5%	PA-H2105
11	PA6+ABS with Hybrid 2:1 1%	PA-H211
12	PA6+ABS with Hybrid 2:1 1.5%	PA-H2115

2.2 Simulation Methodology

The Digimat 2017 was used to forecast the effective material properties of each nanocomposite structure, including density, Poisson's ratio, shear modulus, and Young's modulus. The density, Young's and Shear modulus, and Poisson's ratio of PA6-ABS nanocomposites are displayed in Table 3. These predicted properties were then entered into FEA simulations using the CATIA V5R19 Educational software. Every model was exposed to the identical geometry and loading circumstances in order to guarantee comparability. Deflection and Max Von Mises stress were calculated from the simulation data.

2.2.1 General Steps in the Digimat MF Workflow

1. New material: Open Digimat MF as shown in Figure 1 and create a new material.
2. Matrix definition: Describe the characteristics of the PA6 (Polyamide 6 or Nylon 6) (density of 1150 kg/m^3,

Table 2. Design of experiments for PA6-ABS nanocomposites

Expt. No.	PA6 (gm) 70%	ABS (gm) 30%	PP-g-MA (gm) 3%	MWCNT (gm)	Graphene (gm)	Label Code
1	135.1	57.9	6	0	1	PA-G05
2	134.4	57.6	6	0	2	PA-G1
3	133.7	57.3	6	0	3	PA-G15
4	135.1	57.9	6	1	0	PA-M05
5	134.4	57.6	6	2	0	PA-M1
6	133.7	57.3	6	3	0	PA-M15
7	135.1	57.9	6	0.5	0.5	PA-H1105
8	134.4	57.6	6	1	1	PA-H111
9	133.7	57.3	6	1.5	1.5	PA-H1115
10	135.11	57.90	6	0.66	0.33	PA-H2105
11	134.41	57.60	6	1.33	0.66	PA-H211
12	133.7	57.3	6	2	1	PA-H2115

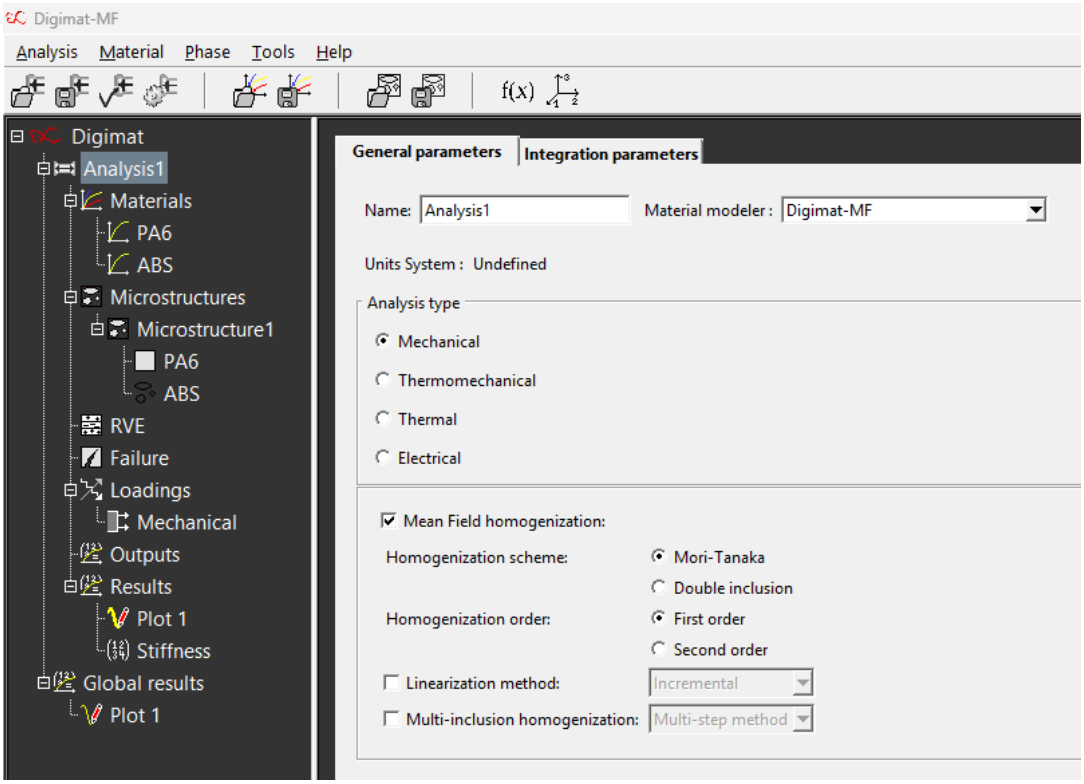


Figure 1. Digimat-MF analysis.

its Young's modulus of 3 GPa, and its Poisson's ratio of 0.375) and ABS (density of 1100 kg/m^3, its Young's modulus of 2.25 GPa, and its Poisson's ratio of 0.35) matrix, as shown in Figure 2A and 2B.

3. Filler definition: Describe the features of MWCNT and graphene, such as aspect ratio and shape descriptors as shown in Figure 3A. (Graphene-X: density 2200 kg/m^3, Young's modulus 1000 GPa, Poisson's ratio 0.16,

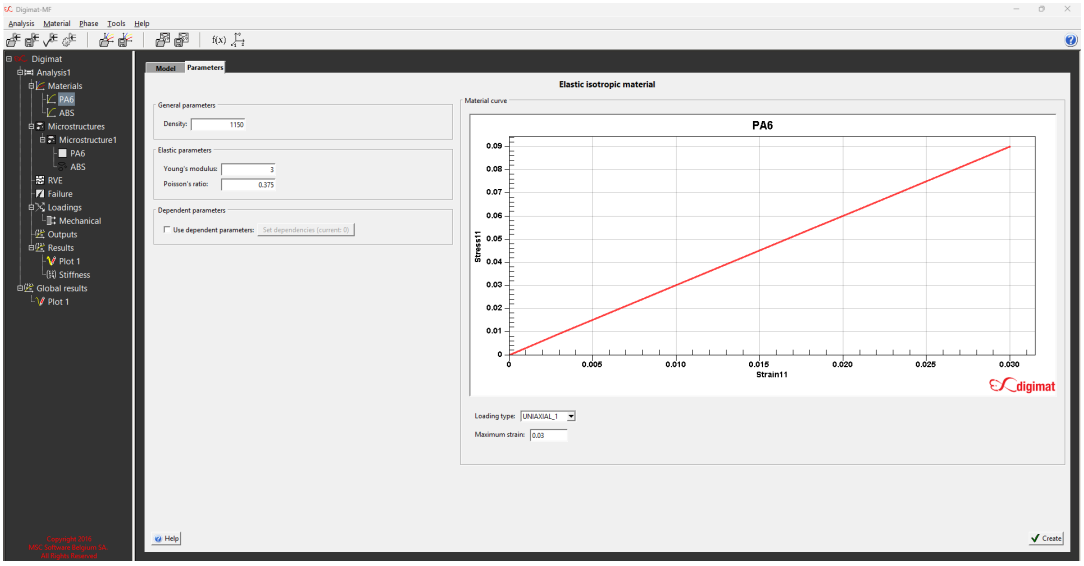


Figure 2 (A). Digimat-MF (PA6 matrix material definition).

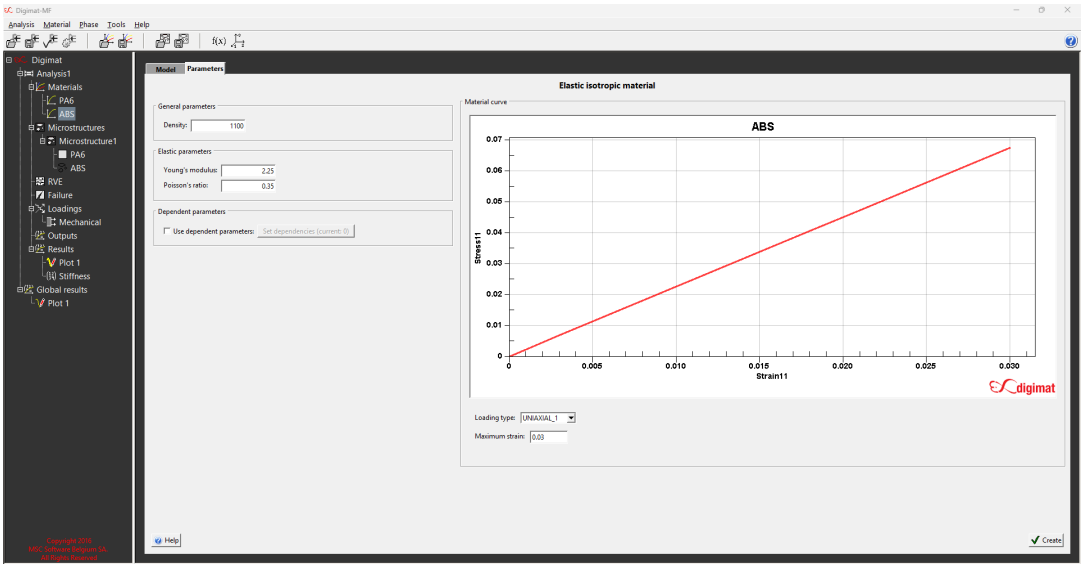


Figure 2 (B). Digimat-MF (ABS matrix material definition).

and MWCNT: density 1875 kg/m³, Young's modulus 1000 GPa, Poisson's ratio 0.225)

4. Micromechanics model: Select the relevant micromechanics model (such as Mori-Tanaka for short fiber reinforced composites).
5. Volume fractions: Enter the MWCNT and graphene volume fractions for every composite formulation as shown in Figure 3B.
6. Interaction: Describe how the matrix and the fillers interact.
7. Homogenisation: Compute the homogenisation. Figure 4 shows the Digimat-MF mechanical loading and Figure 5 shows results of engineering constants.
8. Export: Export the homogenized material properties in a CATIA-compatible format (for example, by creating similar material properties or as a Digimat material file).

2.2.2 ASTM D638: Standard Test Method for Tensile Properties of Plastics

The commonly used standard test technique for figuring out the tensile characteristics of plastics is ASTM D638.

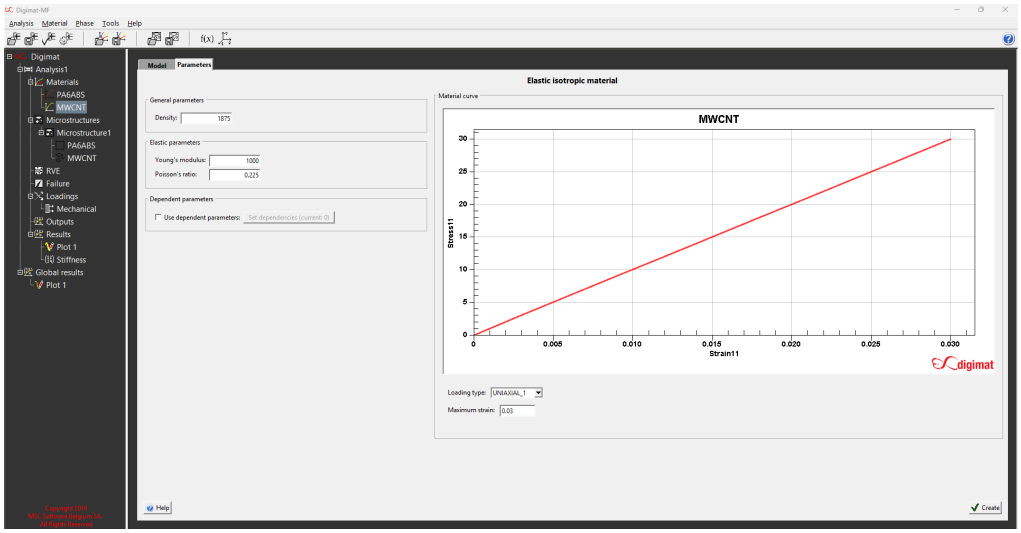


Figure 3 (A). Digimat-MF (MWCNT filler material definition).

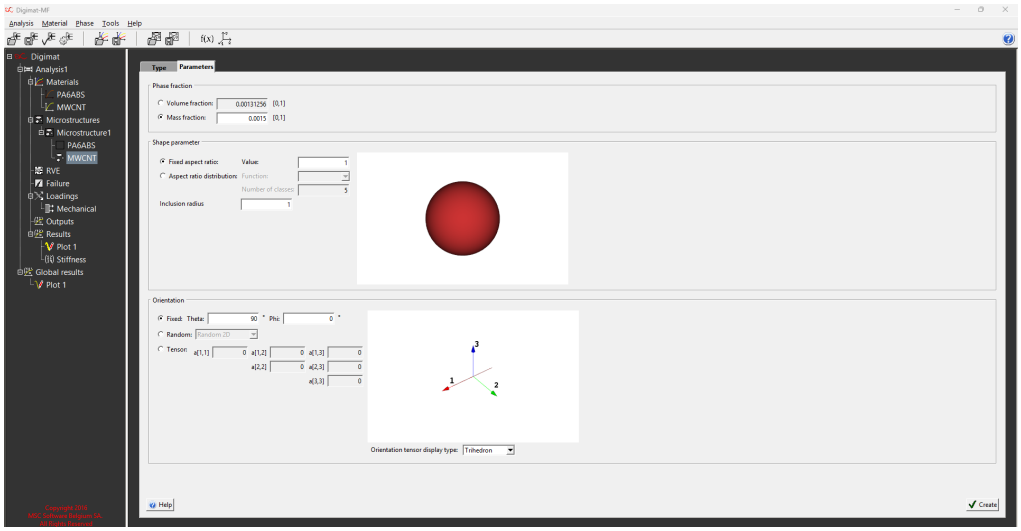


Figure 3 (B). Digimat-MF (MWCNT filler material definition).

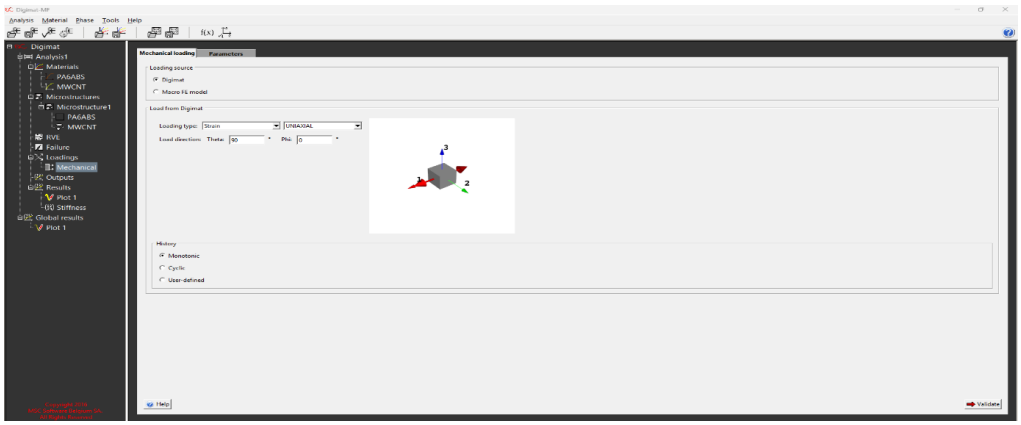


Figure 4. Digimat-MF mechanical loading.

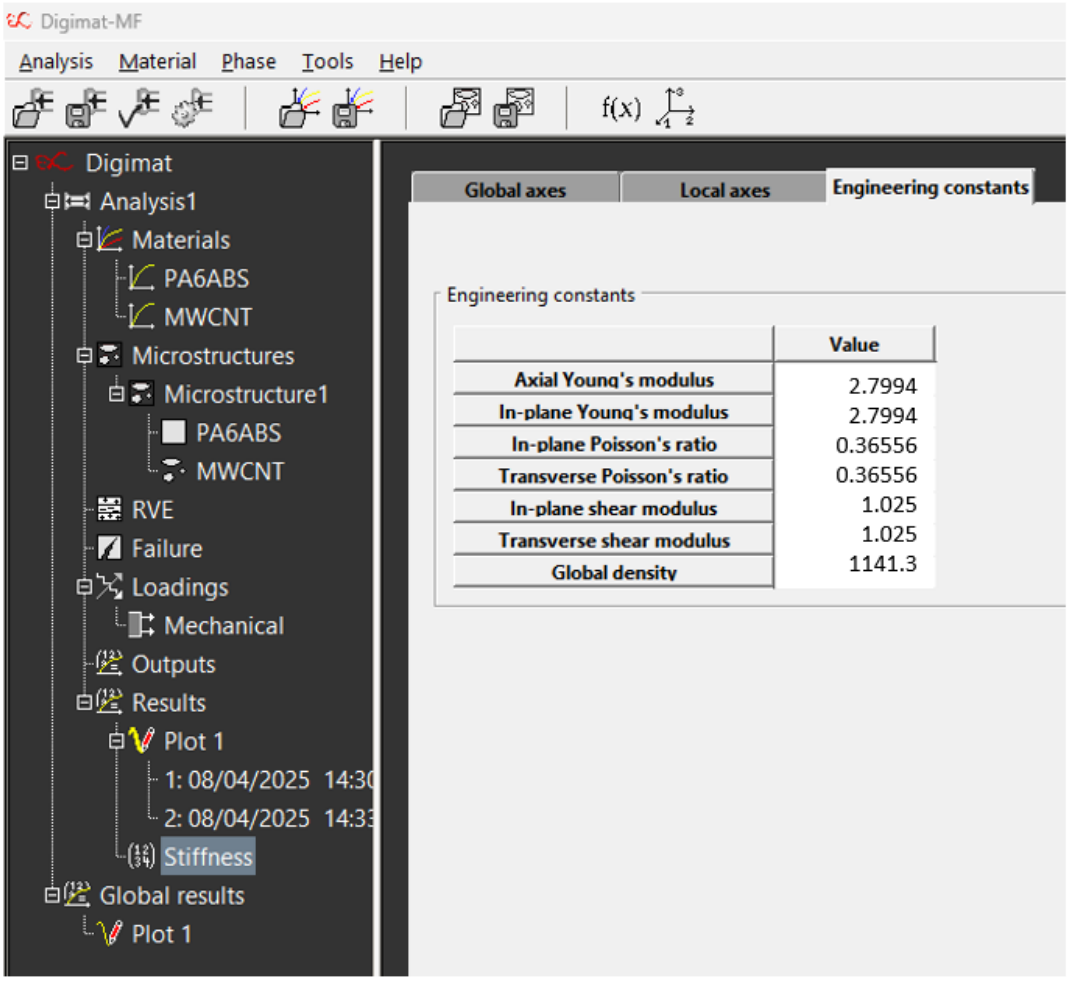


Figure 5. Digimat-MF results of engineering constants.

Table 3. Density, Young's and Shear modulus, Poisson's ratio of PA6-ABS nanocomposites

Expt. No.	Label Code	Density (Kg/m^3)	Young's Modulus GPa	Shear Modulus	Poisson's Ratio
1	PA-G05	1137.3	2.7611	1.0105	0.3662
2	PA-G1	1140	2.7763	1.0162	0.36594
3	PA-G15	1142.8	2.7916	1.022	0.36569
4	PA-M05	1136.7	2.7637	1.0115	0.36616
5	PA-M1	1139	2.7815	1.0182	0.36586
6	PA-M15	1141.3	2.7994	1.025	0.36556
7	PA-H1105	1137	2.7624	1.011	0.36618
8	PA-H111	1139.5	2.7789	1.0172	0.3659
9	PA-H1115	1142	2.7955	1.0235	0.36563
10	PA-H2105	1136.9	2.7628	1.0112	0.36617
11	PA-H211	1139.3	2.7797	1.0175	0.36589
12	PA-H2115	1141.8	2.7968	1.024	0.36561

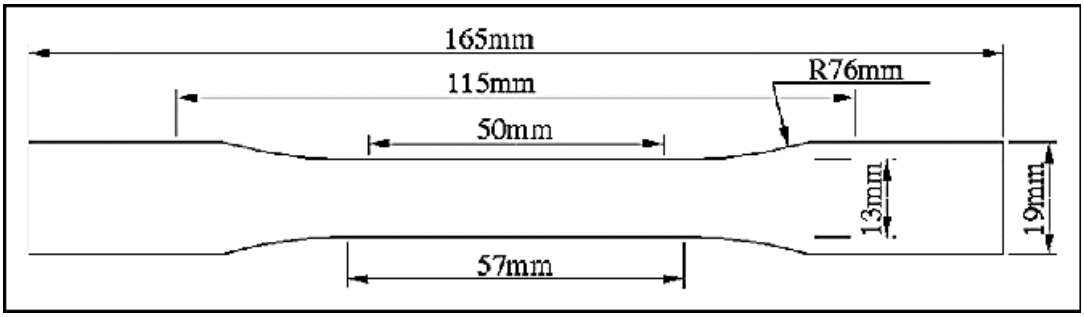


Figure 6. The tensile test specimen (ASTM D638 Type 1, t = 3.36 mm)[1].

The methods for setting up specimens, performing the tensile test, and computing important mechanical attributes are described. 1000N of tensile tension is applied along the Y-axis.

2.2.3 Finite Element Analysis (FEA) in CATIA

1. Model geometry: Using CATIA, create a 3D model of the tensile specimen that has the measurements shown in Figure 6.
2. Material assignment: Assign the relevant CATIA model components to the material attributes produced in Digimat MF.
3. Meshing: Use the model to create a mesh. To make sure that the outcomes are unaffected by the mesh density, do a mesh convergence research. Explain the mesh density and element type that were employed.
4. Boundary conditions and loading: To replicate the tensile test, use the proper loading and boundary conditions, as seen in Figure 7. Indicate the displacement or applied load.
5. Simulation: Use CATIA to run the FEA simulation.
6. Post-processing: Take out the pertinent outcomes of the simulation, namely the deflection and Maximum Von Mises stresses, as seen in Figures 8 and 9.

3.0 Results and Discussions

3.1 Deflection Analysis

A general trend of decreasing deflection with increasing filler content is observed across all filler types (Graphene, MWCNT, H1:1, H2:1). Table 4 shows Deflection (mm) of PA6-ABS Nanocomposites. For example, the graphene-

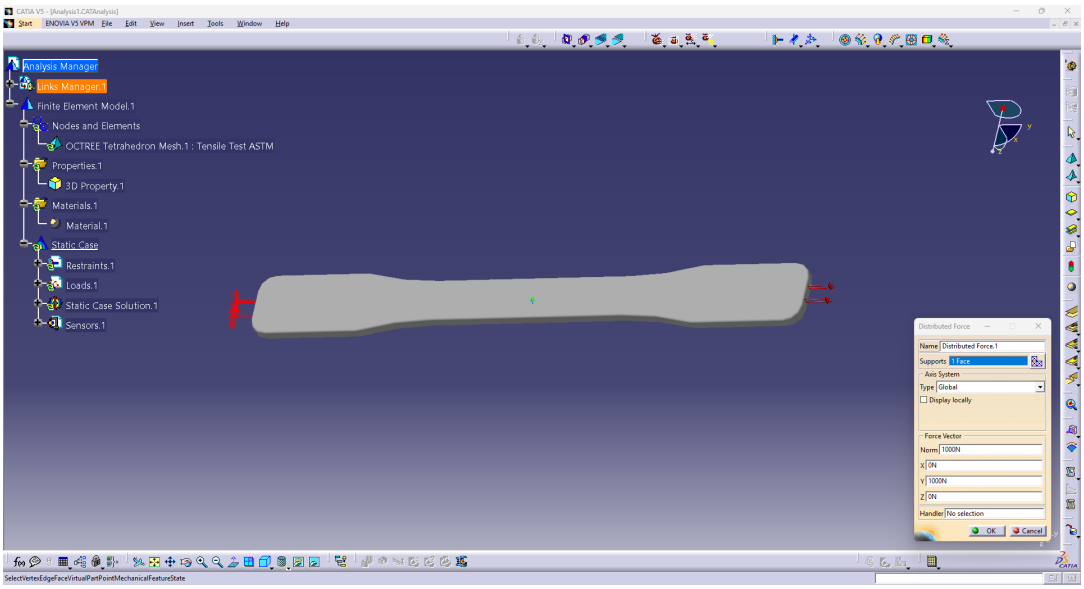


Figure 7. CATIA workbench tensile test specimen under tensile loading condition (1KN).

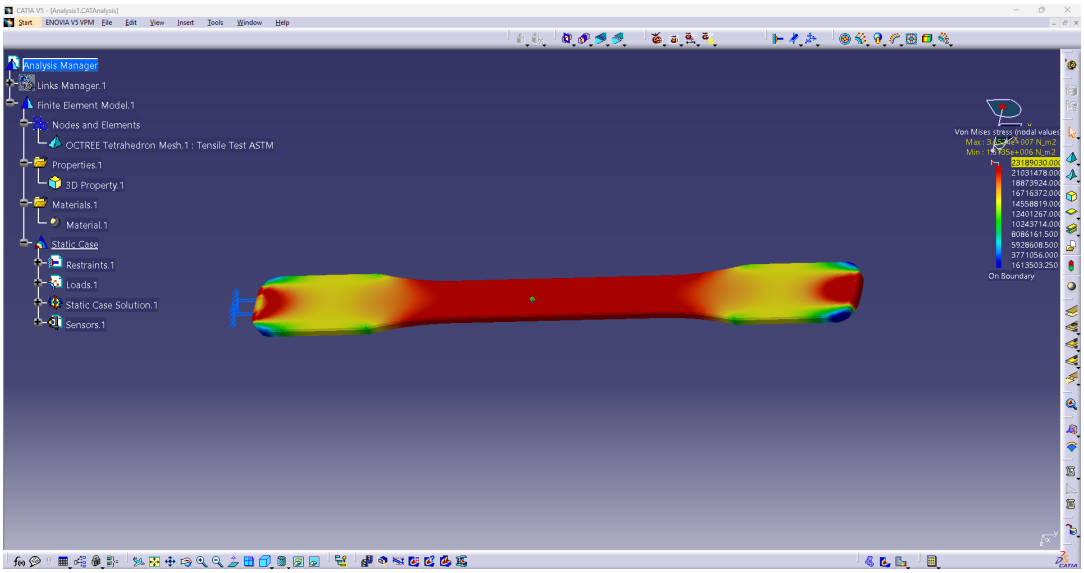


Figure 8. CATIA analysis (maximum Von Mises stresses).

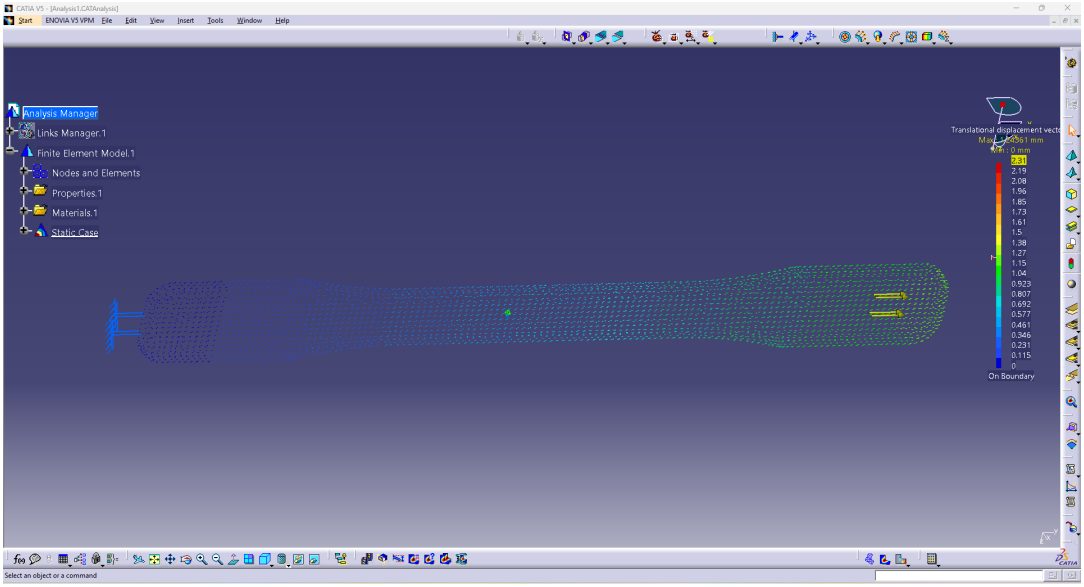


Figure 9. CATIA analysis (deflection).

reinforced samples (PA-G series) show a consistent reduction in deflection from 1.23686 mm (PA-G05) to 1.22336 mm (PA-G15) as filler loading increases. This behaviour is reflected in the MWCNT (PA-M series) and hybrid series (PA-H11 and PA-H21), indicating increased stiffness of the nanocomposite material with higher reinforcement content. Among all specimens, PA-M15 exhibits the lowest deflection (1.21995 mm), suggesting it has the highest stiffness and resistance to deformation under load. This is closely followed by PA-H2115 (1.22109 mm) and PA-H1115 (1.22165 mm).

3.2 Von Mises Stress Analysis

Table 5 shows Max Von Stress (N/m^2) of PA6-ABS Nanocomposites. The maximum von Mises stress values for all configurations lie in a narrow range from approximately 36.5 MPa to 36.6 MPa. Although the changes are subtle, the stress values slightly increase as filler content increases. The highest Von Mises stress was recorded for PA-M15 (36,570,500 N/m^2), indicating that this configuration experienced the highest internal stress concentration under the applied load. This increase

Table 4. Deflection (mm) of PA6-ABS nanocomposites

Expt. No.	Label Code	Deflection (mm)
1	PA-G05	1.23686
2	PA-G1	1.2301
3	PA-G15	1.22336
4	PA-M05	1.2357
5	PA-M1	1.2278
6	PA-M15	1.21995
7	PA-H1105	1.23628
8	PA-H111	1.22895
9	PA-H1115	1.22165
10	PA-H2105	1.2361
11	PA-H211	1.22859
12	PA-H2115	1.22109

Table 5. Max Von Stress (N/m^2) of PA6-ABS nanocomposites

Expt. No.	Label Code	Max Von Stress (N/m^2)
1	PA-G05	36537100
2	PA-G1	36550700
3	PA-G15	36563800
4	PA-M05	36539200
5	PA-M1	36554900
6	PA-M15	36570500
7	PA-H1105	36538100
8	PA-H111	36552800
9	PA-H1115	36566900
10	PA-H2105	36538700
11	PA-H211	36553300
12	PA-H2115	36567900

in stress with increased reinforcement can be attributed to the higher stiffness of the material, which restricts deformation but also leads to greater stress development in localized regions.

Results indicate a consistent decrease in deflection across all nanocomposite types (Graphene, MWCNT, and hybrids) as filler content increased, signifying enhanced stiffness. Notably, PA-M15 exhibited the lowest deflection, suggesting maximum resistance to deformation. Conversely, maximum Von Mises stress showed a marginal increase with higher filler loading, with PA-M15 experiencing the highest stress concentration, likely due

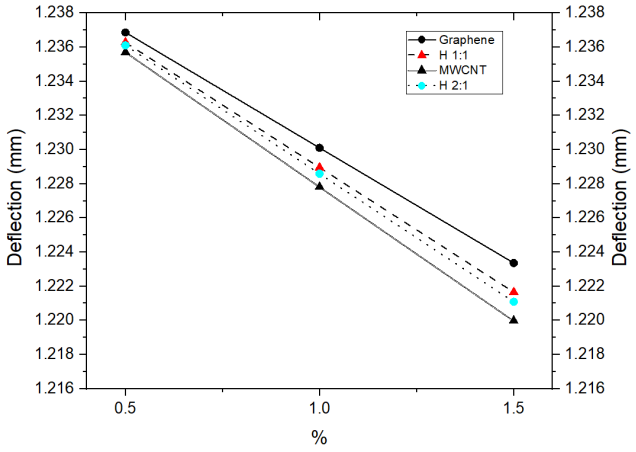


Figure 10. Comparative analysis of deflection in graphene, MWCNT, and Hybrid (H1:1, H2:1) PA6-ABS nanocomposites.

to its increased stiffness restricting deformation and causing localized stress build-up. These findings suggest that while reinforcement enhances stiffness, it can also lead to higher internal stresses under load.

The Figure 10 shows that deflection decreases with increasing filler content for all nanocomposites. MWCNT-reinforced samples show the lowest deflection, indicating the highest stiffness, while graphene-reinforced samples show the highest deflection, indicating the least stiffness. Hybrid fillers (H 1:1 and H 2:1) perform better than graphene alone, with H 2:1 slightly outperforming H 1:1, suggesting improved mechanical performance through hybridization.

The Figure 11 shows that maximum Von Mises stress increases with increasing filler content for all nanocomposites. MWCNT-reinforced composites exhibit the highest stress values, indicating stronger resistance to deformation. Graphene composites show the lowest stress, while hybrid fillers (H 1:1 and H 2:1) fall in between, with H 2:1 performing slightly better. This suggests that MWCNT and hybrid fillers enhance the material's strength more effectively than graphene alone.

Figures 12 to 15 shows, as the filler content increases from 0.5% to 1.5% for all materials (Graphene, MWCNT, H 1:1, H 2:1), deflection decreases, while maximum Von Mises stress, density, Young's modulus, and shear modulus increase, indicating improved mechanical stiffness and strength. Poisson's ratio slightly decreases with filler content, suggesting reduced lateral deformation. Among all, MWCNT and hybrids (especially H 2:1)

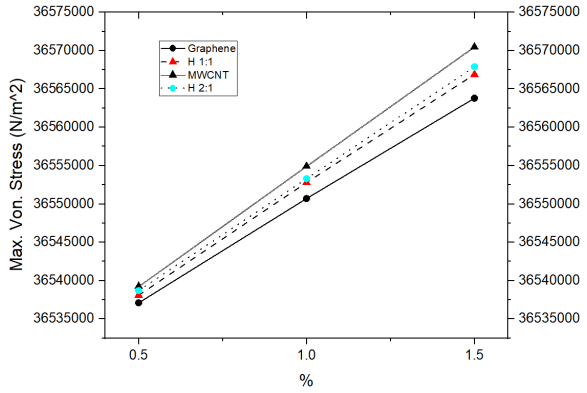


Figure 11. Comparative analysis of maximum von Mises stress in graphene, MWCNT, and Hybrid (H1:1, H2:1) PA6-ABS nanocomposites.

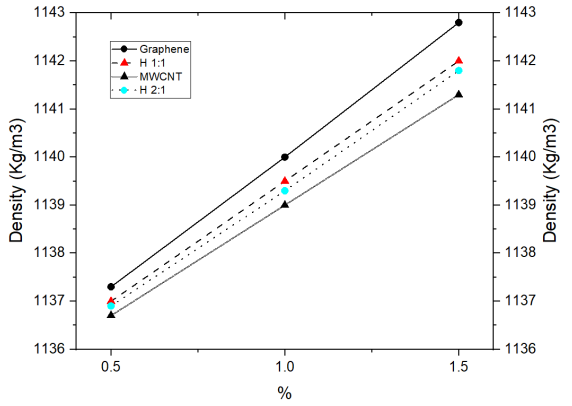


Figure 12. Comparative analysis of density in graphene, MWCNT, and Hybrid (H1:1, H2:1) PA6-ABS nanocomposites.

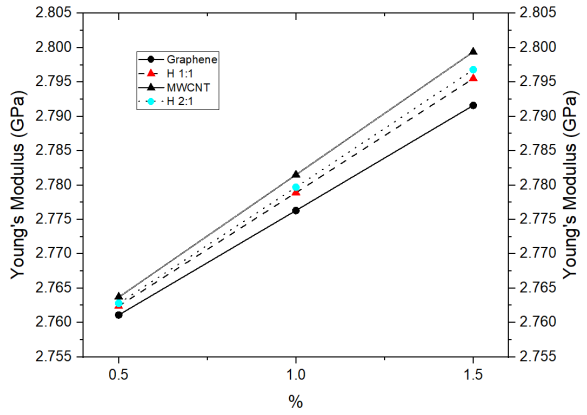


Figure 13. Comparative analysis of Young's modulus in graphene, MWCNT, and Hybrid (H1:1, H2:1) PA6-ABS nanocomposites.

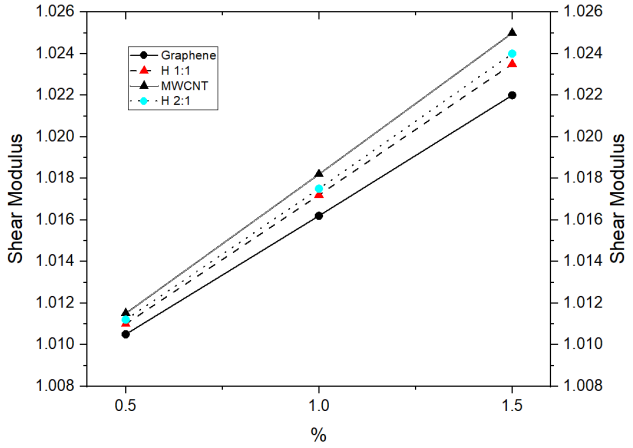


Figure 14. Comparative analysis of Shear modulus in graphene, MWCNT, and Hybrid PA6-ABS nanocomposites.

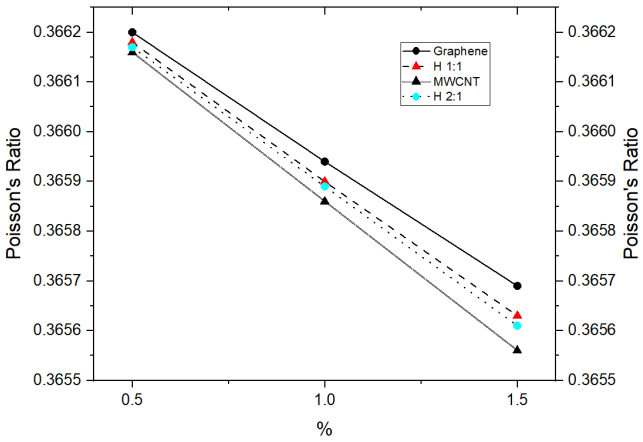


Figure 15. Comparative analysis of Poisson's ratio in graphene, MWCNT, and Hybrid (H1:1, H2:1) PA6-ABS nanocomposites.

show superior improvements in mechanical properties compared to graphene alone. This highlights that hybrid nanofillers provide a balanced enhancement in stiffness, strength, and structural integrity.

4.0 Conclusion

In summary, the addition of nanofillers (Graphene, MWCNT, and their hybrids) to the PA6-ABS matrix successfully decreased deflection, which in turn raised the stiffness of the final nanocomposites. Interestingly, MWCNT reinforcement produced the greatest deflection reduction, suggesting greater stiffness. The highest concentration of stress was found in MWCNT composites; however the maximum Von Mises stress

increased somewhat with filler content, indicating improved resistance to deformation. PA-M15 consistently outperformed other specimens in terms of minimizing deflection while slightly increasing stress. This makes it the most mechanically efficient configuration for applications requiring rigidity. The hybrid materials (PA-H1 and PA-H2 series) also demonstrate promising performance, especially at the 1.5 wt. % reinforcement level, combining low deflection with moderately high stress tolerance. All things considered, these results show that nanofiller reinforcement, especially with MWCNT and hybrid combinations, increases PA6-ABS's mechanical stiffness and strength. However, the enhanced stiffness may also result in higher localized stress under load.

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6.0 Authors Contribution

Both authors equally contributed the work.

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