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Reviewed Paper

Enhancing the Mechanical Properties of Additively Manufactured Carbon Nanotube Integrated Components: A Simulation-Based Approach

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Abstract

Additive Manufacturing (AM) is becoming an attractive production technology due to its ability to produce complex shapes and reduce raw material usage. However, its strength and durability are not as good as traditional techniques yet. To address this, nanofillers like carbon nanotubes (CNT) are increasingly being introduced in AM processes, especially in Material Extrusion (MEX) processes. CNTs have strong mechanical characteristics that could improve the parts printed of PLA, PETG, or ABS materials. The objective of this study is to explore how the mechanical properties of 3D-printed parts improve by incorporating CNTs. This study explores the influence of CNTs on the mechanical properties of 3D printed parts and demonstrates how simulations replicate real-world processes. Different simulation tools such as Material Designer and Explicit Dynamics within Ansys software were used in the simulation. Material Designer was used to incorporate CNT filler at varying percentages into PLA, ABS, and PETG matrices, and the strength analysis was carried out using Static Structural. Adding 0.5%, 1%, and 2% CNT increases the material strength if we consider the strain relatively close to pure material. Experimental validation will be carried out to substantiate these observations. These findings suggest that polymers reinforced with CNTs show potential for strengthening materials in AM applications thus enabling engineers to develop more effective designs and benefiting the industry.

Introduction

While the popularity of utilization of AM is growing in every aspect of life, its composite printing is also parallelly growing in R&D and Industry [1], [2]. In MEX, fiber-reinforced MEX technologies are pretty common considering their ease of use and low cost [3][4]. There are also several studies with the use of CNT-based nanoscale MEX processes [5] [6] [7]. CNTs are among the most significant nano-allotropes of carbon. They are one-dimensional cylindrical nanocarbons discovered by Iijima in 1991 [8], [9]. Essentially, they are graphene nanosheets rolled into tubes with sp2-bonded carbon atoms. Depending on the number of rolled layers, CNTs are classified as single-walled (SWCNT), double-walled, or multi-walled (MWCNT) (Figure 1). The distinctive C–C bonding and cylindrical form give these nanotubes exceptional strength [10].

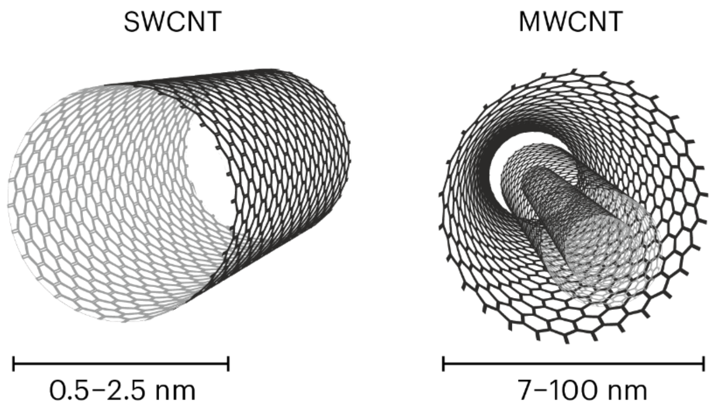


Figure 1. Schematic representation of a SWCNT and a MWCNT [11].

The mechanical properties of CNTs are exceptional, considering their structure based on sp2 hybridization of carbon-carbon bonds. They have Young's modulus of about 1 TPa with tensile strength in the range from 11 to 100 GPa, which makes them very strong, far stronger than steel. Additionally, it is because of delocalized electrons in the z-axis direction that CNTs exhibit very nice electrical and thermal properties such as low thermal expansion coefficient, and high thermal conductivity [12]. These unique properties make CNTs very promising as a reinforcement phase in polymeric composites [13], [14]. Combining polymers with reinforcing fibers or particles enables the customization of mechanical and thermal properties [15].

Nanofillers like CNT are increasingly being introduced in AM processes, especially in the MEX process compared to former studies [16], [17]. The addition of CNTs to a polymer matrix increases its stiffness and strength. In this research, analytical methods and simulations will be used to approximate solutions and visualize results. The Finite Element Method (FEM) will be applied for strength analysis on the specimen, which is modeled according to ASTM International Standards. Several modules and their combinations within ANSYS software will be utilized to conduct the entire simulation.

Material Properties and Homogenization

In the initial phase, engineering data on linear elasticity and plasticity for PLA, ABS, and PETG matrices are accurately sourced from a broad range of references [15], [18], [19], [20], [21], [22], ensuring the selection of the most relevant data for analysis. Within this framework, isotropic elasticity and bilinear isotropic hardening characteristics are defined for the matrices, while the mechanical properties of CNTs are confined to isotropic elasticity. To simulate the composite mixture of the matrices with the nanofiller at varying concentrations, a new Representative Volume Element (RVE) material model (Figure 2) [23] is created using Material Designer. The weight fractions are defined as 0.005, 0.01, and 0.02. Orientation tensors are set to 0.33 in all directions to enable the random generation of nanofillers within the matrices. The CNT diameter is selected to be 50 nm, and the aspect ratio is set at 300 to determine the nanotubes' length.

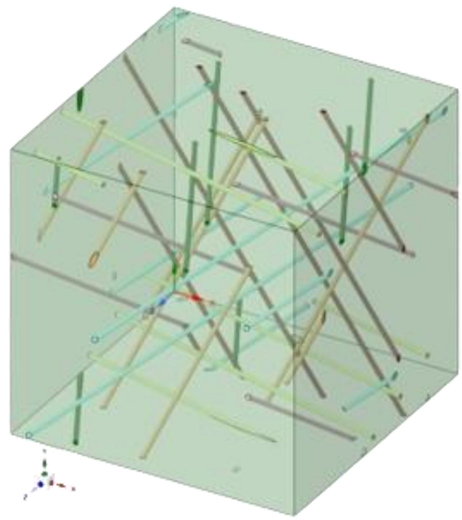


Figure 2. Sample RVE Geometry of Matrices and Nanofiller.

Conformal and periodic (Figure 3) meshing [24] techniques are implemented to ensure uniformity and continuity in the simulation.

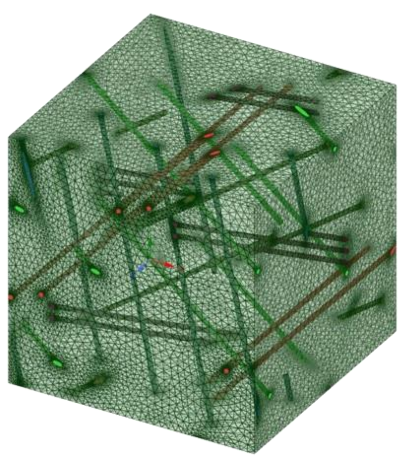


Figure 3. Generated accurate mesh for RVE model for PLA-CNT (1%).

Engineering Constants		
E1	4189.4	MPa
E2	4447.2	MPa
E3	4303.2	MPa
G12	1601.8	MPa
G23	1523.9	MPa
G31	1659.2	MPa
nu12	0.36591	
nu13	0.3949	
nu23	0.35742	

Figure 4. Calculated homogenized properties of PLA-CNT (1%).

After calculating homogenized properties (Figure 4 and 5), they were transferred to engineering data to use in the subsequent analysis. From the results, it can be seen that Young’s Modulus (E), and Shear modulus (G) have been increased. The homogenized material data usually refers to elastic properties. This is because the tool is mainly designed to determine the effective elastic properties of composite materials or heterogeneous structures. It calculates this by subjecting the RVE to various load cases and analyzing its elastic response.

es of Outline Row 6: PLA

A	B	C
Property	Value	Unit
Material Field Variables	Table	
Density	1250	kg m^-3
Isotropic Elasticity		
Derive from	Young's Modulus and Poisson...	
Young's Modulus	3450	MPa
Poisson's Ratio	0.39	
Bulk Modulus	5.2273E+09	Pa
Shear Modulus	1.241E+09	Pa

PLA-CNT (0.5%) C:\Users\mmahmud

ies of Outline Row 3: PLA-CNT (0.5%)

A	B	C
Property	Value	Unit
Density	1.2526E-09	mm^-3 t
Orthotropic Elasticity		
Young's Modulus X direction	3691.7	MPa
Young's Modulus Y direction	3759.5	MPa
Young's Modulus Z direction	3764.3	MPa
Poisson's Ratio XY	0.38525	
Poisson's Ratio YZ	0.37559	
Poisson's Ratio XZ	0.38726	
Shear Modulus XY	1355.7	MPa
Shear Modulus YZ	1336.6	MPa
Shear Modulus XZ	1368.4	MPa

PLA-CNT (1%) C:\Users\mmahmud

es of Outline Row 3: PLA-CNT (1%)

A	B	C
Property	Value	Unit
Density	1.2553E-09	mm^-3 t
Orthotropic Elasticity		
Young's Modulus X direction	4189.4	MPa
Young's Modulus Y direction	4447.2	MPa
Young's Modulus Z direction	4303.2	MPa
Poisson's Ratio XY	0.36591	
Poisson's Ratio YZ	0.35742	
Poisson's Ratio XZ	0.3949	
Shear Modulus XY	1601.8	MPa
Shear Modulus YZ	1523.9	MPa
Shear Modulus XZ	1659.2	MPa

PLA-CNT (2%) C:\Users\mmahmud

es of Outline Row 3: PLA-CNT (2%)

A	B	C
Property	Value	Unit
Density	1.2591E-09	mm^-3 t
Orthotropic Elasticity		
Young's Modulus X direction	5825.5	MPa
Young's Modulus Y direction	4338.5	MPa
Young's Modulus Z direction	3765.6	MPa
Poisson's Ratio XY	0.33424	
Poisson's Ratio YZ	0.52311	
Poisson's Ratio XZ	0.40443	
Shear Modulus XY	1422.1	MPa
Shear Modulus YZ	1630.6	MPa
Shear Modulus XZ	1340.1	MPa

Figure 5. Comparison of engineering data for PLA-CNT (0.5%, 1%, and 2%) and PLA.

From the results in Figure 5, it can be seen that Young's Modulus increased from 3450 MPa to 3691 MPa (X direction), 3759 MPa (Y direction), and 3764 MPa (Z direction) for the 0.5% mixture.

For the 1% mixture, the increment is from 3450 MPa to 4189 MPa (X direction), 4447 MPa (Y direction), and 4303 MPa (Z direction).

However, on the 2% mixture, the values have been increased but in different multitude in different directions. This is because of the greater concentration of CNTs in the X direction.

Analysis information

The engineering data obtained are utilized for the static structural analysis. The process begins with importing the specimen's 3D model, which is subsequently discretized into elements of high quality. For mesh generation, a specific sizing method is implemented, setting the element size at 3mm based on the geometry size and small details, and then the quality of the elements is checked (Figure 6). The mesh quality is considered excellent based on the element metrics, with skewness values ranging between 0 and 0.25 [25].

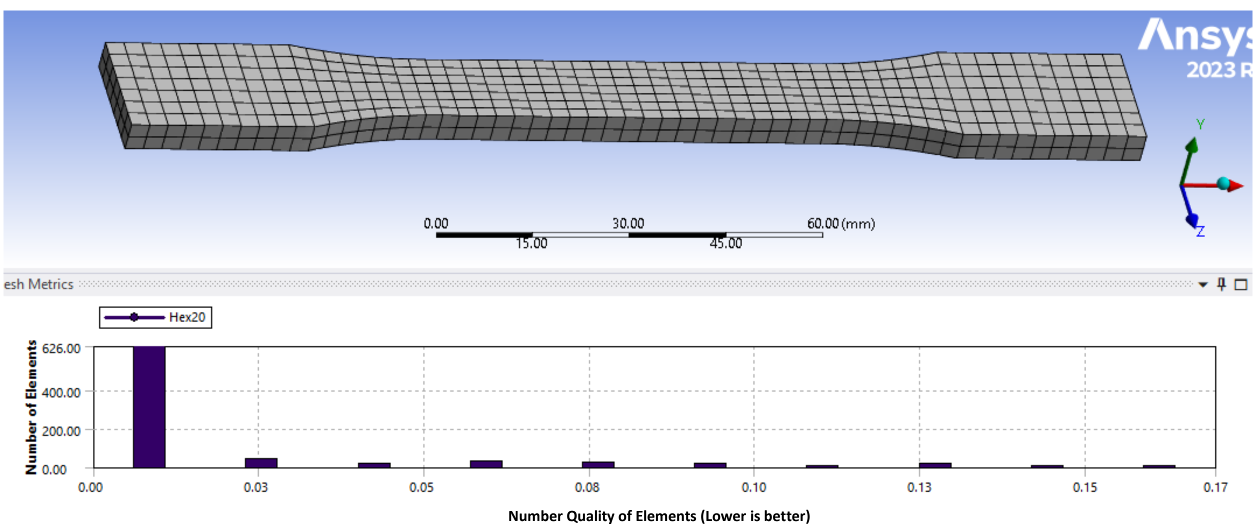


Figure 6. Meshing and Element Metrics.

The analysis requires concentration on a specific node, element, or section of the specimen's extent. Thus, a designated area is selected as the area of interest (Figure 7). Subsequently, the boundary conditions are applied.

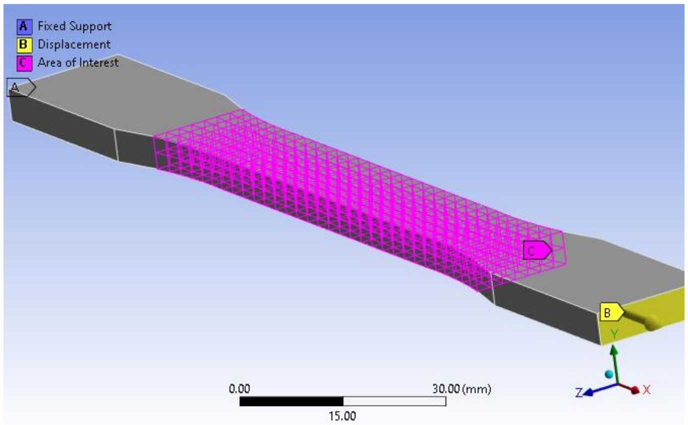


Figure 7. Boundary Conditions and Area of Interest

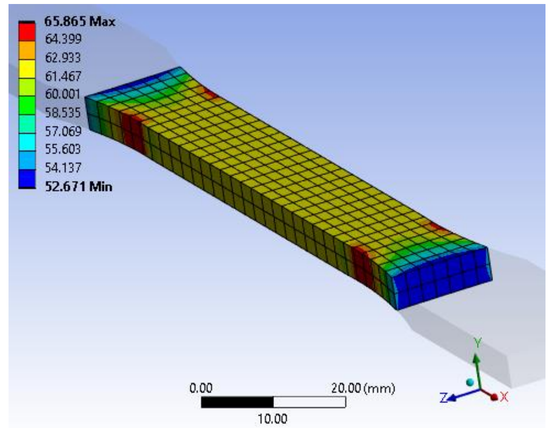
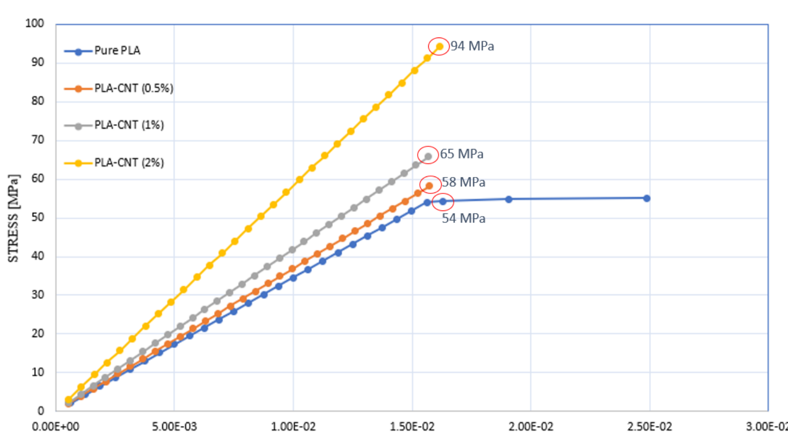


Figure 8. Normal Stress along X

Results and Comparisons

Following 21 simulation runs, the results (Figure 9) necessarily enable the approximation and comparison of the tensile strength of pure PLA, ABS, and PETG materials and their composites mixed with CNTs at concentrations of 0.5%, 1%, and 2%. Due to the homogenized material data and calculated effective elastic properties of composite materials, plastic data are not given in the plot for mixed materials and the analytical analysis assumes that the mechanical bonding between the nanofiller and matrices is maintained. Therefore, the strain value is also maintained at the pure matrices level to estimate relevant stress increment and to demonstrate the extent to which the nanofiller maximizes the strength. A Stress-Strain curve is plotted using the data derived from these calculations. The results demonstrated that the influence of CNT increases the Young's Modulus of the matrices significantly. The increment in tensile strength might also be observed from 54 MPa for pure PLA to 58 MPa, 65 MPa, and 94 MPa respectively for PLA/CNT composites with concentrations of 0.5%, 1%, and 2% (Figure 8). Figure 9 also illustrates the results for ABS and PETG blends.



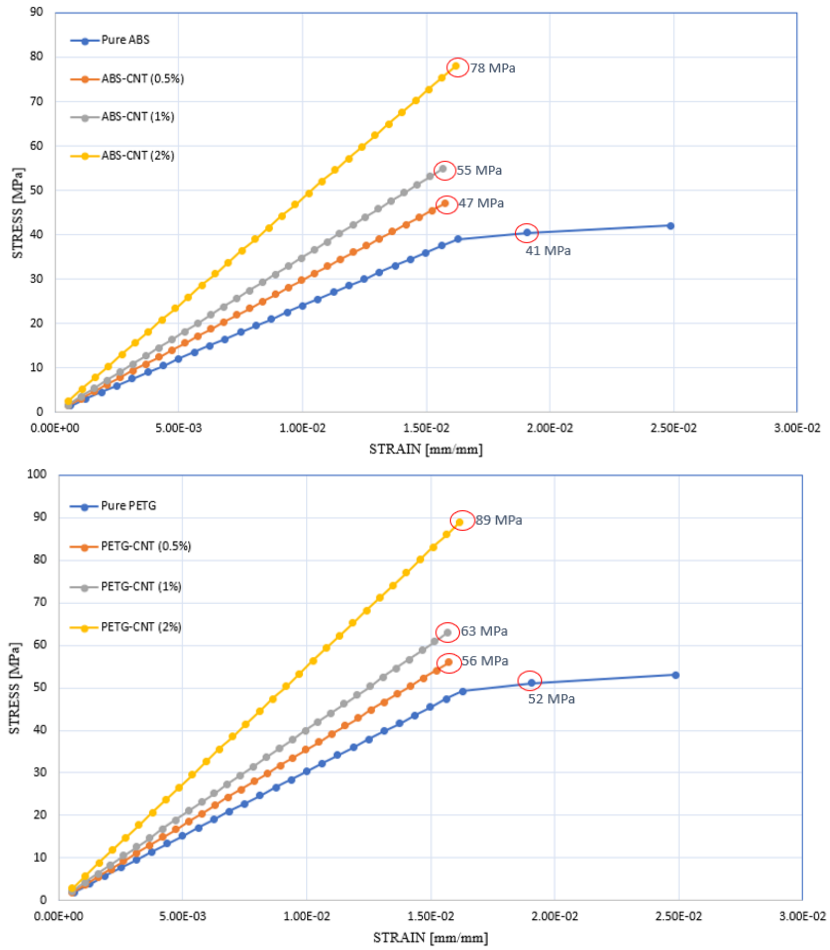


Figure 9. Stress-strain curve (PLA, ABS, and PETG mixtures).

Challenges and Future Research

Despite these promising properties of CNTs, some larger challenges have to be overcome for their general application within polymer composites. Among them, the uniform dispersion of CNTs within the polymer matrix is one of the biggest challenges due to the high agglomeration tendency of CNTs due to strong van der Waals forces. Moreover, the interfacial bonding between the CNTs and the polymer matrix should also be optimum for the realization of better mechanical performance [13].

When the CNT content was increased to 1.5 wt.%, the tensile strength decreased because higher filler content led to agglomeration. The study revealed that increased MWCNT content resulted in poor interfacial adhesion between the polymer matrix and the MWCNTs, leading to aggregation and clumping of the nanofillers [26], [27].

Besides dispersion and agglomeration challenges, the aspect ratio of CNTs significantly impacts the longitudinal elastic modulus. CNTs generally have a high aspect ratio, but their performance in polymer composites depends heavily on the type of polymer matrix used.

According to Arash et al. [28], who studied the effect of CNT aspect ratio on Young's modulus and yield strength in CNT/polymethyl methacrylate (PMMA) composites, increasing the CNT aspect ratio resulted in enhanced Young's modulus of PMMA and increased strength.

Conclusion

In the conclusive view of these exceptional strengths, stiffness, electrical, and thermal properties of CNTs, they have huge potential to enhance mechanical performance in the polymer composite. This is evidenced through versatility and application in many diversified industries. This research study presented that adding CNTs to a polymer matrix has shown increased values in Young's and Shear Modulus. While AM is known as low in mechanical properties, these kinds of analytical studies show its potential to increase the strength of polymers by adding nanofillers like CNTs. While this study was conducted, it was seen that some dispersive and interfacial bonding-related issues have to be addressed to exploit the great potential of polymer composites reinforced with CNTs in future applications. Comprehensive analytical and real-world experiments are necessary to substantiate this research and identify methods to consistently enhance polymer properties under specific conditions.

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