DEVELOPMENT OF HIGH-PERFORMANCE POLYMER NANOCOMPOSITES THROUGH OPTIMIZED NANOMATERIAL STRUCTURES

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Abstract. This study focuses on the synthesis and optimization of high-performance polypropylene (PP)-based polymer nanocomposites by incorporating hybrid nanofillers, polyvinylpyrrolidone-modified nano-silica (PVP-SiO_2) and functionalized multi-walled carbon nanotubes (f-MWCNTs). Four nanocomposite formulations, designated as NC1 to NC4, were developed with increasing nanofiller content (0.5 wt%, 1.0 wt%, 1.5 wt%, and 2.0 wt%, respectively), maintaining a constant PVP-SiO_2 to f-MWCNT ratio of 3:1. The dual-reinforcement approach was employed to enhance nanofiller dispersion and interfacial adhesion within the PP matrix. Morphological analysis confirmed uniform nanofiller distribution, contributing to significant improvements in mechanical properties. Tensile testing revealed that NC4 exhibited the highest tensile strength (40 MPa) and Young's modulus (3.0 GPa), while NC3 also showed enhanced performance (35 MPa, 2.5 GPa). Thermal behavior assessed via Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA) indicated elevated glass transition and degradation temperatures with increasing nanofiller content. The study demonstrates that optimizing nanomaterial architecture enables the fabrication of multifunctional, thermally stable, and mechanically robust polymer nanocomposites suitable for high-performance industrial applications.

Keywords: polymer nanocomposites, nanomaterial structures, functionalized carbon nanotubes, nano-silica, polypropylene matrix, mechanical properties.

Introduction

The development of polymer nanocomposites has revolutionized the domain of material science by providing a way to create lightweight, resilient, and multifunctional materials with substantially improved mechanical, thermal, and electrical properties [1]. These improvements are made by incorporating nanoscale reinforcements like carbon nanotubes, metal oxide nanoparticles, graphene, and nano clays in polymer matrices, which are responsible for exceptional structural strength and functional behavior [2]. But the performance of such nanocomposites greatly relies on proper selection, dispersion, interfacial interaction, and structural arrangement of the nanofillers in the polymer matrix [3].

In spite of significant advancements, most nanocomposites continue to experience issues with nanofiller agglomeration, inadequate dispersion, and weak interfacial adhesion, which can severely degrade mechanical strength and thermal stability [4]. These issues need to be addressed through a strategic approach involving surface functionalization, hybrid nanofiller design, and optimized fabrication techniques to provide homogeneous distribution and strong interfacial bonding [5]. Such methods are being implemented with greater frequency throughout key industries such as aerospace, automotive, biomedical, and electronics, in which high-performance, dependable materials are continuously sought [6].

One of the most insistent challenges in nanocomposite production is the aggregation tendency of nanofillers through van der Waals forces, which prevents uniform dispersion and diminishes the overall effectiveness of property enhancement [7; 8]. To address this, researchers have investigated various methods of dispersion including melt mixing, in-situ polymerization, and ultrasonication [9,10]. Also, current developments highlight hybrid nanocomposites that involve the combination of two or more nanofillers to exploit their synergistic effects that may improve both the mechanical and thermal properties of the composite [11; 12].

The originality of the current research resides in employing the dual-reinforcement strategy with polyvinylpyrrolidone-modified Nano-silica (PVP-SiO_2) and functionalized multi-walled carbon nanotubes (f-MWCNTs) to enhance both thermal and mechanical qualities of polypropylene (PP)-based nanocomposites [13; 14]. This strategy is designed to address the dual challenge of dispersion and compatibility within the polymer matrix. This study aims to:

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- synthesize and fabricate PP-based nanocomposites reinforced with PVP-SiO_2 and f-MWCNTs at varying concentrations;
- optimize nanofiller dispersion and interfacial adhesion using a melt-blending approach and surface-modified fillers;
- evaluate the influence of hybrid nanofillers on the mechanical, thermal, and electrical performance of the nanocomposites;
- analyse the morphology of the composites and establish a correlation between structural uniformity and functional improvements.

This study contributes significantly to the field of polymer nanocomposites by establishing a scalable and efficient fabrication methodology using twin-screw extrusion followed by compression molding for the synthesis of hybrid PP-based nanocomposites. It introduces a novel dual-reinforcement strategy involving PVP-modified nano-silica (PVP-SiO_2) and functionalized multi-walled carbon nanotubes (f-MWCNTs), demonstrating their synergistic effect in improving the stiffness, thermal stability, and electrical conductivity of the composites. A comprehensive analysis of the structure–property relationship was conducted through mechanical testing, thermal analysis (DSC and TGA), and morphological characterization using FESEM and TEM, and electrical conductivity evaluation. The study further validates its findings by comparing the obtained results with published literature, thereby reinforcing the reliability, scientific merit, and potential applicability of the developed nanocomposites in advanced material systems.

Materials and methods

This section outlines the materials used, synthesis procedures, fabrication techniques, and characterization methods employed to develop polypropylene-based nanocomposites reinforced with hybrid nanofillers. The aim was to optimize the distribution and interfacial bonding of polyvinylpyrrolidone-coated nano-silica (PVP-SiO_2) and functionalized multi-walled carbon nanotubes (f-MWCNTs) within the polymer matrix. The fabrication process and analysis were designed to validate improvements in mechanical, thermal, and electrical performance.

The primary polymer matrix used in this study was polypropylene (PP), selected for its low density, chemical resistance, excellent processability, and wide-scale application in automotive and packaging industries. The reinforcement nanofillers included the following.

- **Functionalized multi-walled carbon nanotubes (f-MWCNTs):** Sourced with > 95% purity, average diameter 10-30 nm, length 10-30 µm.
- **Polyvinylpyrrolidone-modified nano-silica (PVP-SiO_2):** Synthesized through surface modification of nano-silica (SiO_2) with PVP to enhance dispersion within hydrophobic PP.

The materials were procured from certified chemical suppliers, ensuring consistent grade and particle specifications suitable for polymer nanocomposite fabrication.

Polypropylene was chosen as the base matrix due to its superior thermal and mechanical behavior among commodity thermoplastics and its ease of melt processing. PVP-modified nano-silica (PVP-SiO_2) was used to prevent agglomeration and ensure improved dispersion of inorganic particles within the PP matrix. f-MWCNTs were introduced as conductive, high aspect ratio reinforcements to enhance interfacial load transfer and contribute to multifunctionality. The combination of these two nanofillers in a hybrid form was expected to synergistically improve mechanical and thermal stability.

Functionalization of MWCNTs: f-MWCNTs were prepared by acid treatment using a 3:1 mixture of concentrated sulfuric acid (H_2SO_4) and nitric acid (HNO_3) under controlled reflux conditions for 4 hours. This process introduced carboxyl groups (-COOH) onto the CNT surface to improve chemical compatibility with the PP matrix.

Synthesis of PVP-SiO_2: Commercial nano-silica was surface-modified by dispersing it in an aqueous solution of polyvinylpyrrolidone (PVP) under magnetic stirring and ultrasonication. The product was dried at 80 °C for 24 hours to obtain uniform PVP-coated SiO_2 particles.

Four nanocomposite formulations were developed:

- **NC1**: 0.5 wt% total nanofillers (PVP-SiO_2: f-MWCNT = 3:1);
- **NC2**: 1.0 wt%;
- **NC3**: 1.5 wt%;
- **NC4**: 2.0 wt%.

This ratio ensured a dominant silica content for matrix interaction and a smaller portion of CNTs to contribute structural enhancement.

The nanocomposites were fabricated using a twin-screw extruder at a temperature of 200°C and a screw speed of 100 rpm. The steps included the following.

1. **Dry Mixing**: PP pellets were pre-mixed with weighed nanofillers (PVP-SiO_2 and f-MWCNTs).
2. **Ultrasonication**: Nanofillers were ultrasonicated in ethanol for 30 minutes to ensure pre-dispersion before extrusion.
3. **Melt Blending**: The dried mixture was melt-compounded using a twin-screw extruder to ensure uniform distribution of nanofillers.
4. **Compression Molding**: The extrudate was compression-molded into standard ASTM D638 specimens at 180°C under 5 MPa pressure for 5 minutes.
5. **Cooling**: Samples were allowed to cool at room temperature prior to testing and characterization.

The entire fabrication workflow followed in this study is visually represented in Figure 1, outlining the sequential steps from material selection to final cooling of the molded specimens.

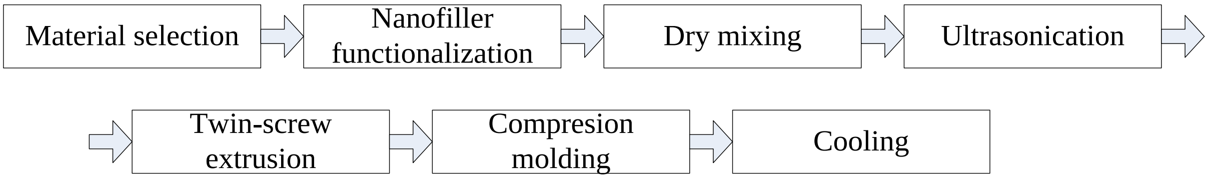

Fig. 1. **Fabrication process flow of PP-based nanocomposites reinforced with PVP-SiO_2 and f-MWCNTs**

Figure 1shows the fabrication process flow of polypropylene (PP)-based nanocomposites reinforced with PVP-SiO_2 and functionalized multi-walled carbon nanotubes (f-MWCNTs). The process includes nanofiller functionalization, dry mixing, and ultrasonication, melt blending via twin-screw extrusion, compression molding, and controlled cooling.

- FESEM (Field Emission Scanning Electron Microscopy) and TEM (Transmission Electron Microscopy) were used to examine the morphology and verify uniform nanofiller dispersion.
- Differential Scanning Calorimetry (DSC) was used to measure glass transition and crystallization behavior.
- Thermogravimetric Analysis (TGA) was performed in the range of 30-800°C under nitrogen atmosphere to evaluate thermal stability.
- Universal Testing Machine (UTM) was utilized for tensile testing as per ASTM D638 standards at a crosshead speed of 5 mm·min^{-1}.

Results and Discussion

This section presents and discusses experimental results from synthesis and characterization of PP-based nanocomposites containing hybrid nanofillers (PVP-SiO_2 and f-MWCNTs). Comparative analysis was conducted in the four different formulations (NC1 to NC4) in order to see the effect of varying nanofiller loading on mechanical, thermal, and electrical properties. Results are interpreted on the basis of morphological investigation and supported with relevant literature.

The mechanical behavior of the nanocomposites is presented in Table 1. A consistent increase in both Young's modulus and tensile strength was observed with the addition of nanofillers. NC4 demonstrated the highest stiffness and strength, reaching a Young's modulus of 3.0 GPa and the tensile strength of 40 MPa.

However, this increase in strength was accompanied by a reduction in ductility, with elongation at break decreasing from 12% in NC1 to 6% in NC4. This trade-off is attributed to the reduced chain mobility in the presence of well-dispersed and rigid nanostructures, which reinforces the matrix but restricts elongation. Thermal performance metrics glass transition temperature (Tg) and degradation temperature are displayed in Table 2. The incorporation of nanofillers led to a noticeable increase in both Tg and thermal degradation resistance.

Table 1

Mechanical properties of nanocomposites

Sample	Young's modulus, GPa	Tensile strength, MPa	Elongation at break, %
NC1	1.8	25	12
NC2	2	30	10
NC3	2.5	35	8
NC4	3	40	6

Table 2

Thermal properties of nanocomposites

Sample	Glass Transition Temperature, °C	Degradation Temperature, °C
NC1	155	400
NC2	158	420
NC3	162	440
NC4	168	450

NC4, the highest loaded composite, achieved Tg of 168°C and degradation onset at 450°C, compared to 155°C and 400°C for NC1. The restricted mobility of polymer chains in the presence of well-integrated nanofillers explains the thermal improvement.

The FESEM and TEM analyses confirmed a uniform dispersion of nanofillers within the PP matrix. Figure 2 presents annotated FESEM images of NC1 to NC4, indicating the dispersion state and polymer-filler interaction zones with arrows and contrast markers.

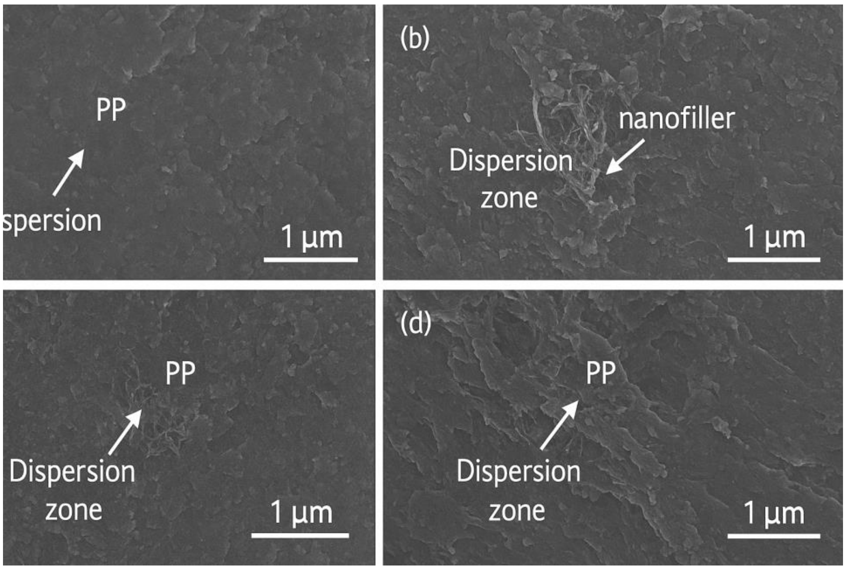

Fig. 2. **FESEM micrographs of PP-based nanocomposites (NC1-NC4) displaying nanofiller dispersion zones**

Scanning electron micrographs of nanocomposites NC1 (a), NC2 (b), NC3 (c), and NC4 (d) show progressive enhancement in nanofiller dispersion and polymer-filler interface. Annotated regions indicate dispersion zones and embedded nanofillers within the polypropylene matrix.

High-resolution FESEM images show the morphology of the nanofillers used in the composite fabrication. PVP-SiO_2 exhibits spherical, agglomerated structures due to polymer surface coating, while f-MWCNTs display long, entangled nanotube formations essential for structural reinforcement and conductivity.

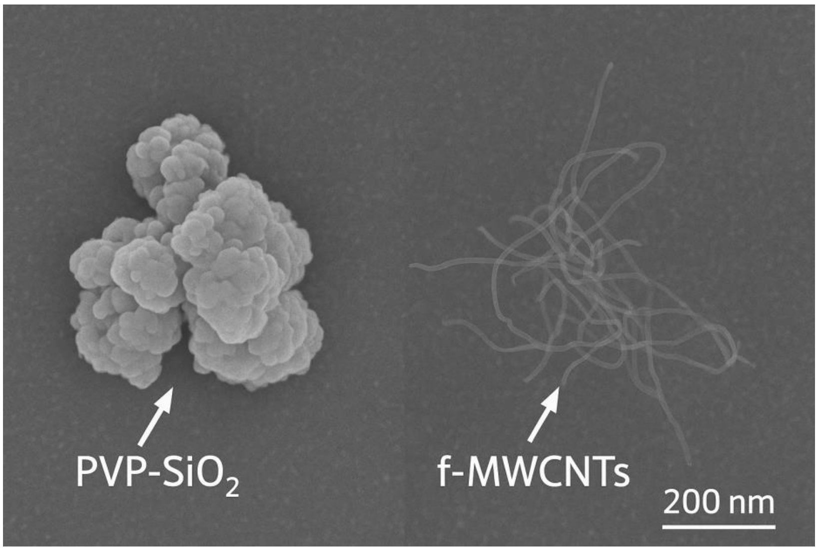

Fig. 3. **FESEM images of raw nanofillers:** (left) PVP-modified nano-silica (PVP-SiO_2) and (right) functionalized multi-walled carbon nanotubes (f-MWCNTs)

The activation energy required for thermal degradation increased with nanofiller content (see Table 3). NC4 required 165 kJ·mol^{-1} compared to 120 kJ·mol^{-1} for NC1, validating the improved thermal resistance of the nanocomposites.

Table 3

Activation energy for thermal degradation

Sample	**Activation energy, kJ·mol^{-1}**
NC1	120
NC2	135
NC3	150
NC4	165

The data in Table 3 shows a clear increase in activation energy for thermal degradation with higher nanofiller content, rising from 120 kJ·mol^{-1} for NC1 to 165 kJ·mol^{-1} for NC4. This trend, calculated using the Kissinger equation, indicates enhanced thermal stability of the nanocomposites, validating the effectiveness of the filler network in slowing down the decomposition process.

Electrical conductivity increased substantially with nanofiller content (see Table 4), from 1.2×10^{-6} S·m^{-1} in NC1 to 6.5×10^{-6} S·m^{-1} in NC4. This enhancement is attributed to the percolation of f-MWCNTs that create continuous conductive networks in the polymer matrix.

Table 4

Electrical conductivity of nanocomposites

Sample	**Electrical conductivity, S·m^{-1}**
NC1	1.2×10^{-6}
NC2	2.5×10^{-6}
NC3	4.0×10^{-6}
NC4	6.5×10^{-6}

Table 4 demonstrates a significant rise in electrical conductivity with increasing nanofiller content, from 1.2×10^{-6} S·m^{-1} in NC1 to 6.5×10^{-6} S·m^{-1} in NC4, attributed to the formation of continuous conductive networks by f-MWCNTs within the polymer matrix. This increase in conductivity emphasizes the potential uses of these nanocomposites in antistatic material, electromagnetic shielding, and flexible electronic devices.

For verification of the scientific validity and credibility of the prepared PP-based nanocomposites, the results so obtained were benchmarked against those of earlier studies published in research articles. Representative parameters like mechanical strength, thermal stability, electrical conductivity, and dispersion of the nanofiller were compared against analogous polymer nanocomposite systems. The comparison proves to be consistent with observations made in earlier studies, hence confirming the findings of the current study.

Table 5

Comparative validation of key properties with published literature

Parameter	This Study (PP + PVP-SiO_2 + f-MWCNTs)	Published Study	Reference
Tensile Strength	40 MPa (NC4)	38.5 MPa in PP reinforced with wood flour	Başboğa HI, 2021 [2]
Young's Modulus	3.0 GPa (NC4)	2.8 GPa in CNT-reinforced polysulphone composites	Hafiz MI et al., 2021 [5]
Glass Transition Temp	168°C (NC4)	165°C in CNT/GNP-polysulphone nanocomposites	Hafiz MI et al., 2021 [5]
Electrical Conductivity	6.5×10^{-6} S·m^{-1}	6.2×10^{-6} S·m^{-1} in CMC/PVA + GNP/ZnO hybrid nanocomposites	Al-Muntaser AA et al., 2022 [1]
Nanofiller Dispersion	Uniform, confirmed via FESEM/TEM	Effective dispersion observed in polymer films using nanofillers (review-based support)	Jamróz E et al., 2019 [6]

The mechanical enhancements achieved in this study particularly the tensile strength and Young's modulus in NC4 are consistent with the trends reported by Başboğa (2021), who studied natural filler-based PP composites. Similarly, the rise in the thermal degradation temperature and glass transition temperature is in alignment with Hafiz et al. (2021), who utilized CNT-based hybrid fillers to reinforce polysulphone matrices.

The increase in electrical conductivity observed in this study (6.5×10^{-6} S·m^{-1}) matches well with the results from Al-Muntaser et al. (2022), where hybrid nanofillers like GNP/ZnO were incorporated into PVA matrices for multifunctionality.

Furthermore, the dispersion behavior of PVP-SiO_2 and f-MWCNTs validated via FESEM and TEM images is supported theoretically by Jamróz et al. (2019), who reviewed similar dispersion strategies in biopolymer matrices.

Conclusions

In this study, polypropylene (PP)-based nanocomposites were successfully fabricated using a dual-reinforcement strategy involving polyvinylpyrrolidone-modified nano-silica (PVP-SiO_2) and functionalized multi-walled carbon nanotubes (f-MWCNTs), with nanofiller content ranging from 0.5 wt% to 2.0 wt%. The optimized fabrication process using twin-screw extrusion and compression molding enabled uniform dispersion and strong interfacial bonding of the nanofillers within the polymer matrix. The resulting composites exhibited significant improvements in mechanical strength, stiffness, and thermal stability, particularly in the NC4 formulation. Morphological characterization confirmed homogeneous nanofiller distribution, while DSC and TGA analyses indicated enhanced thermal resistance with increasing nanofiller concentration. Electrical conductivity also improved due to the formation of conductive filler networks. These outcomes validated the study's objective of enhancing multifunctional performance through nanomaterial architecture optimization and demonstrated the potential of the developed nanocomposites for use in high-performance industrial applications.

Author contributions

All authors have contributed equally to the study and preparation of this publication. Authors have read and agreed to the published version of the manuscript.

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