

Fabrication, Physicochemical Characterization and Antibacterial Evaluation of MgO-Modified PAN/PVP Electrospun Nanofibers

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MgO ile Modifiye Edilmiş PAN/PVP Elektrospun Nanofiberlerin Üretimi, Fizikokimyasal Karakterizasyonu ve Antibakteriyel Değerlendirilmesi

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Abstract

Magnesium oxide (MgO)–reinforced polyacrylonitrile/poly(vinyl pyrrolidone) (PAN/PVP) nanofibers were successfully fabricated via electrospinning, and their structural, thermal, and antibacterial properties were systematically investigated. Owing to its chemical stability and antibacterial properties, MgO was incorporated into the PAN/PVP matrix at loadings of 1, 3, and 5 wt% to enhance multifunctional performance. The effects of MgO content on fiber morphology, structure, wettability, and thermal behavior were evaluated using Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDS), water contact angle measurements (WCA), and thermogravimetric analysis (TGA). The SEM–EDS results supported the incorporation of MgO nanoparticles into the PAN/PVP nanofiber matrix and indicated the presence of Mg- and O-related signals in the MgO-containing samples. Compared to pristine PAN/PVP nanofibers, MgO incorporation resulted in higher residual mass. Uniform, bead-free nanofibers with consistent diameters were obtained from a 15 wt% PAN/PVP solution containing 5 wt% MgO. In in vitro antibacterial tests, samples loaded with 5% weight MgO were found to show measurable inhibition against *Staphylococcus aureus*; the inhibition zone diameters were measured as 17±0 mm and 21±0.5 mm for 10PAN/PVP/5MgO and 15PAN/PVP/5MgO, respectively. Overall, these findings suggest that MgO-reinforced PAN/PVP nanofibers may be promising candidates for antibacterial surface materials, protective coatings, filtration media, and protective textile applications.

Öz

Magnezyum oksit (MgO) ile güçlendirilmiş poliakrilonitril/poli(vinil pirolidon) (PAN/PVP) nanolifler, elektro eğirme yöntemiyle başarıyla üretildi ve yapısal, termal ve antibakteriyel özellikleri sistematik olarak incelendi. Kimyasal kararlılığı ve antibakteriyel özellikleri nedeniyle MgO, çok fonksiyonlu performansı artırmak amacıyla %1, %3 ve %5 ağırlık oranlarında PAN/PVP matrisine dahil edildi. MgO içeriğinin lif morfolojisi, yapısı, ıslatılabilirliği ve termal davranışı üzerindeki etkileri, Fourier dönüşümlü kızılötesi spektroskopisi (FTIR), taramalı elektron mikroskobu-enerji dağılımlı X-ışını spektroskopisi (SEM-EDS), su temas açısı ölçümleri (WCA) ve termogravimetrik analiz (TGA) kullanılarak değerlendirildi. SEM-EDS sonuçları, MgO nanopartiküllerinin PAN/PVP nanofiber matrisine dahil edildiğini destekledi ve MgO içeren numunelerde Mg ve O ile ilgili sinyallerin varlığını gösterdi. Saf PAN/PVP nanofiberlerine kıyasla, MgO ilavesi daha yüksek artık kütleyle sonuçlandı. %15 ağırlık oranında PAN/PVP çözeltisine %5 ağırlık oranında MgO eklenerek, düzgün, boncuksuz ve tutarlı çaplara sahip nanolifler elde edildi. İn vitro antibakteriyel testlerde, %5 ağırlık oranında MgO yüklü numunelerin *Staphylococcus aureus*'a karşı ölçülebilir inhibisyon gösterdiği belirlenmiş; inhibisyon bölgesi çapları 10PAN/PVP/5MgO ve 15PAN/PVP/5MgO için sırasıyla 17±0 mm ve 21±0,5 mm olarak ölçülmüştür. Genel olarak, bu bulgular MgO ile güçlendirilmiş PAN/PVP nanoliflerinin özellikle antibakteriyel yüzey malzemeleri, koruyucu kaplamalar, filtrasyon ortamları ve koruyucu tekstil uygulamaları için umut vadeden adaylar olabileceğini göstermektedir.

Keywords: Antibacterial; Magnesium oxide; Nanofiber; Polyacrylonitrile; Poly(vinyl pyrrolidone).

Anahtar Kelimeler: Antibakteriyel; Magnezyum oksit; Nanofiber; Poliakrilonitril; Poli(vinil pirolidon).

1. Introduction

Magnesium oxide is a widely investigated metal oxide due to its high specific surface area, excellent thermal and dielectric properties, chemical stability, and antimicrobial properties (Farani et al. 2023, Tian et al. 2023, Abinaya et al. 2021, Hornak et al. 2018, Liu et al., 2021). These attributes have driven the incorporation of MgO into

nanofiber systems to improve their functional performance (Hornak 2021, Leonés et al. 2020, Othman et al. 2017). MgO nanoparticles have attracted considerable interest as inorganic antibacterial agents due to their chemical stability, high surface area, and ability to interact with bacterial cell membranes. The antibacterial activity of MgO has been associated with

several possible mechanisms, including reactive oxygen species (ROS) generation, local alkalinity resulting from surface hydration, Mg^{2+} release, and damage to bacterial cell membranes. These effects may induce oxidative stress and membrane disruption, thereby inhibiting bacterial growth. Previous studies have reported that MgO-based materials can be more effective against Gram-positive bacteria such as *Staphylococcus aureus* than against some Gram-negative bacteria, depending on particle size, concentration, surface properties, and bacterial cell wall structure (Sawai et al. 2000; Yamamoto et al. 2002; Tang and Lv, 2014; Coelho et al. 2019; Farani et al. 2023; Liu et al. 2021).

At the nanoscale, MgO exhibits distinct thermodynamic, optical, electronic, and chemical properties, enabling applications in catalysis, water treatment, photocatalysis, and carbon dioxide adsorption (Hashim et al. 2021). Previous studies have demonstrated that MgO nanoparticles can increase the viscosity and electrical conductivity of PAN-based spinning solutions, resulting in the formation of nanofibers with reduced diameters (Dadvar et al. 2014). Furthermore, electrospun MgO-reinforced PVP nanofibers have shown enhanced morphological uniformity and improved antibacterial performance (Liu et al. 2023), while MgO-containing PAN nanofibers have been reported to possess favorable structures for air filtration applications (Dehghan et al. 2016). Despite these advances, the antibacterial behavior of PAN/PVP nanofibers incorporating MgO has not been systematically investigated with respect to MgO loading and polymer concentration. In particular, the concentration-dependent role of MgO in imparting antibacterial functionality while preserving uniform, defect-free fiber morphology remains insufficiently understood. Addressing this gap is essential for the rational design of multifunctional nanofiber systems (Dadvar et al. 2014, Dehghan et al. 2016).

Surface hydrophilicity is an important parameter for nanofiber-based materials because it influences surface interaction with aqueous environments, moisture uptake, and contact-dependent performance (Yuan et al. 2018, Soleimani et al. 2024; Ghanim et al. 2024). Improved wettability may also support the use of nanofiber mats in antibacterial surface-related applications, filtration media, protective coatings, and protective textile systems (Costa et al. 2022, Ferreira et al. 2022; Hawthorne et al. 2022). In MgO-containing nanofibers, changes in surface polarity and hydroxyl group density may contribute to enhanced hydrophilic behavior, as previously reported for MgO-incorporated electrospun membranes showing improved wettability and antibacterial performance

(Peng et al. 2021; Liu et al. 2021; Zhou et al. 2024). In this context, magnesium oxide (MgO) nanoparticles have been shown to significantly improve the wettability of electrospun nanofibers by increasing surface polarity and hydroxyl group density. This enhancement in hydrophilicity may improve water–surface interactions and may contribute to the functional performance of antibacterial and filtration-oriented nanofiber materials. (Niknam et al. 2024; Costa et al. 2022).

Polyacrylonitrile (PAN) is a white, hydrophobic, semi-crystalline synthetic polymer with the formula C_3H_3N . First synthesized in the early 20th century, PAN is characterized by its high thermal stability, with thermal decomposition typically occurring above 300 °C (Hashmi et al. 2019). Due to these properties, PAN has been widely employed in filtration membranes, adsorption materials, and polymer-based composites (Lu et al. 2021, Pourhassan et al. 2022, Huang et al. 2022, Mei et al. 2019). However, strong intermolecular interactions along its polymer chains restrict its solubility, limiting dissolution to highly polar solvents (Pourhassan et al. 2022, Mei et al. 2019). Polyvinylpyrrolidone (PVP) is a hydrophilic, nonionic, linear polymer composed of 1-vinyl-2-pyrrolidone units $(C_6H_9NO)_n$. Its excellent solubility in water and numerous organic solvents, combined with chemical and thermal stability, low toxicity, and strong affinity for both hydrophilic and hydrophobic substances, has led to its widespread use in pharmaceutical, biomedical, and industrial applications (Yanilmaz et al. 2022, Teodorescu et al. 2015). Importantly, PAN and PVP can be co-electrospun to form composite nanofibers, thereby integrating the advantageous properties of both polymers (Mei et al. 2019, Kang et al. 2022, Kim et al. 2020, Zhang et al. 2009). Electrospun PAN/PVP nanofibers have been reported to exhibit high surface area, enhanced porosity, and improved mechanical integrity, making them suitable for multifunctional applications (Kim et al. 2020, Lee et al. 2021).

In this study, PAN/PVP nanofibers with a uniform and smooth morphology containing different concentrations of MgO nanoparticles were successfully produced using the electrospinning technique. The influence of key formulation parameters on fiber morphology and structure was systematically examined. Comprehensive characterization was performed using SEM–EDS, FTIR, and TGA analyses to evaluate morphological features, chemical functionalities, and thermal behavior, while water contact angle measurements were employed to assess surface wettability. The results demonstrated that nanofibers produced from a 15 wt% PAN/PVP solution

containing 5 wt% MgO exhibited the most uniform morphology and favorable physicochemical properties.

Overall, this work provides insight into the structure–property relationships of MgO-reinforced PAN/PVP nanofibers and highlights their potential for antibacterial surface materials, protective coatings, filtration media, and protective textile applications.

2. Materials and Methods

2.1 Chemicals

Magnesium oxide nanopowder/nanoparticles (MgO; purity: 99.95%; average particle size: 45 nm; specific surface area: >45 m²/g, morphology: polyhedral; true density: 3.6 g/cm³; Nanografi, SKU: NG04SO2103) was used as received without further purification. Polyvinylpyrrolidone (PVP; (C₆H₉NO)_n; M_w = 130,000 g/mol) and polyacrylonitrile (PAN; (C₃H₃N)_n; M_w = 150,000 g/mol) were purchased from Sigma-Aldrich. N,N-dimethylformamide (DMF; HCON(CH₃)₂; purity: 99.8%) was purchased from Merck. All chemicals were used as received without further purification.

2.2 Preparation of polyacrylonitrile/polyvinylpyrrolidone (PAN/PVP) solutions

Prior to the electrospinning process, PAN/PVP solutions were prepared at a 1:1 mass ratio with overall polymer concentrations of 10 wt% and 15 wt%. Each mixture was continuously stirred in N,N-dimethylformamide (DMF) using a magnetic stirrer at 40–80 °C for 24 hours to ensure complete dissolution and to obtain a homogeneous, transparent solution (Lee et al. 2021).

2.3 Preparation of PAN/PVP/magnesium oxide (MgO) solutions

For the preparation of MgO-loaded PAN/PVP spinning solutions, 3 g aliquots of the previously prepared 10 wt% and 15 wt% PAN/PVP solutions were transferred into clean glass vessels. Commercial MgO nanopowder/nanoparticles were added to these polymer solutions at 1, 3 and 5 wt% based on the polymer content. The mixtures were magnetically stirred at room temperature for 1 h to obtain initial dispersion of MgO within the polymer solution. Subsequently, the solutions were ultrasonicated for 1 h to improve nanoparticle dispersion and reduce possible agglomeration. Since the MgO nanopowder/nanoparticles were commercially purchased and used as received, no nanoparticle synthesis step was carried out in this study. The prepared solutions were then used directly for electrospinning. The codes assigned to the prepared formulations are summarized in Table 1.

Table 1. Composition and codes of PAN/PVP and PAN/PVP/MgO solutions.

Solution Description	Code
10 wt% PAN/PVP	10PAN/PVP
15 wt% PAN/PVP	15PAN/PVP
10 wt% PAN/PVP/1 wt% MgO	10PAN/PVP/1MgO
10 wt% PAN/PVP/3wt% MgO	10PAN/PVP/3MgO
10 wt% PAN/PVP/5 wt% MgO	10PAN/PVP/5MgO
15 wt% PAN/PVP/1 wt% MgO	15PAN/PVP/1MgO
15 wt% PAN/PVP/3 wt% MgO	15PAN/PVP/3MgO
15 wt% PAN/PVP/5 wt% MgO	15PAN/PVP/5MgO

2.4 Electrospinning of PAN/PVP nanofibers with and without magnesium oxide reinforcement

The electrospinning process was carried out using a 2 mL plastic syringe fitted with a 21-gauge metallic needle, a high-voltage DC power supply (EMCO 4300, 0–30 kV), a syringe pump (New Era Pump Systems Inc., USA), and a grounded flat collector covered with aluminum foil positioned 17 cm from the needle tip. The applied voltage was optimized by testing the range of 10–25 kV, and stable jet formation with continuous fiber production was achieved at 16 kV. The distance between the needle and the collector was varied between 10 and 20 cm, with 17 cm selected as the optimal working distance. PAN/PVP and PAN/PVP/MgO solutions prepared in dimethylformamide at different compositions were electrospun, and the resulting nanofiber morphology was evaluated under these optimized conditions. The electrospun nanofibers were collected on aluminum foil. The electrospinning apparatus used in this study is shown in Figure 1.

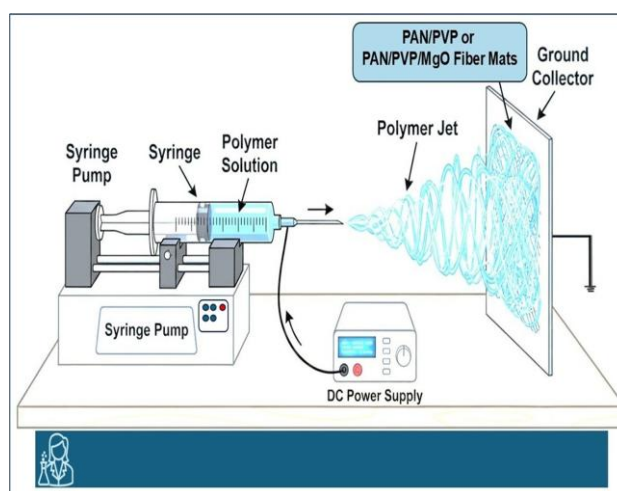


Figure 1. Electrospinning setup.

2.5 Characterization

The structural characterization of the fiber samples was carried out using Fourier Transform Infrared Spectroscopy (JASCO FT/IR 4700) equipped with a diamond ATR accessory. FTIR spectra were recorded in ATR mode over the wavenumber range of 7800–350 cm^{−1}.

with a spectral resolution of 0.4 cm^{-1} , and 32 scans were collected for each sample. The surface morphology of the MgO nanopowder and electrospun nanofiber samples was examined by Scanning Electron Microscopy coupled with Energy-Dispersive X-ray Spectroscopy (SEM-EDS) using an FEI QUANTA FEG 250 instrument. SEM observations were performed under low-vacuum conditions using a secondary electron detector. According to the SEM image metadata, most samples were analyzed at an accelerating voltage of 10 kV with working distances ranging from approximately 12.4 to 14.5 mm, while the 10PAN/PVP fiber sample was examined at an accelerating voltage of 20 kV. The nanofiber samples were mounted on aluminum stubs without any conductive coating prior to SEM observation. Low-vacuum imaging conditions were employed to minimize charging effects during analysis. Fiber diameter measurements were performed from SEM micrographs using image analysis software by measuring randomly selected fibers from different regions of each sample. Elemental composition analyses were conducted using the integrated EDS system. Additionally, thermogravimetric analysis (TGA) was performed using a simultaneous thermal analyzer (HITACHI STA200) to evaluate the thermal stability and degradation behavior of the MgO nanopowder and selected PAN/PVP/MgO nanofiber samples. All measurements were carried out from 25 to 550 °C at a heating rate of 10 °C/min under a nitrogen atmosphere. Nitrogen was used as the purge gas at a flow rate of 200 mL/min, and aluminum pans were used during the measurements. The sample masses ranged from 1.329 to 1.871 mg. Water contact angle (WCA) measurements of the fibers were performed using a Dataphysics OCA 50 Micro contact angle meter. All contact angles were measured immediately after the deposition of 5 μL water droplets to minimize errors caused by evaporation. The measurements were performed in triplicate ($n=3$), and the standard deviation (SD) was reported as the error value.

2.6 Antibacterial activity

The in vitro antibacterial activity of the nanofiber samples was evaluated against Gram-positive (*Staphylococcus aureus*, ATCC 25923) and Gram-negative (*Escherichia coli*, ATCC 25922) pathogens using the disc diffusion method. Bacterial suspensions were adjusted to a concentration of 10^8 CFU/mL , and 100 μL of each suspension was spread onto the surface of Mueller-Hinton Agar (MHA) plates. Subsequently, the nanofiber samples were cut into circular discs (15 mm in diameter), placed on the inoculated agar, and incubated at 37 °C for 24 hours. The diameters of the inhibition zones were measured and

recorded in triplicate. Amikacin 30 μg was used as a positive control.

3. Results and Discussions

3.1 FTIR results

FTIR spectroscopy was employed to assess the potential formation of new chemical bonds or molecular interactions between the PAN/PVP nanofibers and MgO nanoparticles. The FTIR results confirmed the successful incorporation of MgO into the polymeric nanofiber matrix. The spectra of nanofibers formulated with 10PAN/PVP and 15PAN/PVP, as well as their corresponding MgO-loaded counterparts containing 1, 3, and 5 wt% MgO, are presented in Figure 2. The characteristic absorption bands associated with PVP were clearly identified at 1654 cm^{-1} (C=O stretching), 1371 cm^{-1} (CH_2 bending and deformation), and 1283 cm^{-1} (C–N stretching). The PAN component was confirmed by the prominent cyano ($\text{C}\equiv\text{N}$) stretching vibration at 2242 cm^{-1} , along with additional peaks at 1436 cm^{-1} (CH_3) and 1371 cm^{-1} (CH_2), which further validate the presence of PAN-specific functional groups (Aqeel et al. 2015). In the spectra of 10PAN/PVP nanofibers and 10PAN/PVP nanofibers containing MgO (1, 3, and 5 wt%), typical absorption bands of polymer-nanoparticle composites were observed at 1436 cm^{-1} (CH_3), 2242 cm^{-1} ($\text{C}\equiv\text{N}$), 1371 cm^{-1} (CH_2), and 3436 cm^{-1} (O–H). As shown in Figure 2, slight spectral shifts were detected upon the incorporation of MgO. The cyano stretching vibration, originally located at 2242 cm^{-1} in the pristine 10PAN/PVP nanofibers, shifted slightly to 2243 cm^{-1} in the MgO-reinforced samples. Similarly, the O–H stretching band exhibited a shift from 3443 cm^{-1} in the MgO-free nanofibers to 3436 cm^{-1} in the MgO-containing formulations. These subtle shifts are indicative of intermolecular interactions between the polymer chains and MgO nanoparticles (Aqeel et al. 2015, Liu et al. 2023).

FTIR analysis of the 15PAN/PVP nanocomposites incorporating 1, 3, and 5 wt% MgO revealed distinct vibrational bands associated with the polymer matrix and nanoparticles. Prominent peaks were observed at 3411 cm^{-1} (O–H), 2242 cm^{-1} ($\text{C}\equiv\text{N}$ stretching), 1436 cm^{-1} (CH_3), and 1371 cm^{-1} (CH_2). As illustrated in Figure 2, the O–H stretching band of the 15 wt% PAN/PVP fibers incorporating MgO exhibits a significant shift and a decrease in intensity relative to the corresponding spectra of the 10PAN/PVP nanofiber series (Aqeel et al. 2015). Moreover, an increase in MgO content within the 15PAN/PVP nanofibers results in a noticeable reduction in peak sharpness relative to the MgO-loaded 10PAN/PVP samples. This decrease in peak intensity suggests

enhanced polymer–filler interactions in the 15PAN/PVP nanofibers, indicating a stronger interfacial association between MgO nanoparticles and the polymer matrix.

In the spectra of 10PAN/PVP nanofibers containing 1, 3, and 5 wt% MgO, the absorption bands observed between 652 and 402 cm^{-1} correspond to characteristic MgO vibrational modes. A similar pattern is evident in the 15 PAN/PVP nanofibers—particularly in samples incorporating 3 and 5 wt% MgO—where bands appearing between 652 and 400 cm^{-1} are attributed to MgO vibrations (Ferreira et al. 2022). As the MgO concentration increases, a weak band near 837 cm^{-1} becomes discernible, which is associated with metal–oxygen bonding and further confirms the effective integration of MgO within the PAN/PVP nanofiber matrix. Additionally, the incremental MgO loading induces slight shifts in the infrared peak positions, suggesting strengthened polymer–filler interactions while not markedly altering the fundamental chemical structure of the composite (Liu et al. 2023).

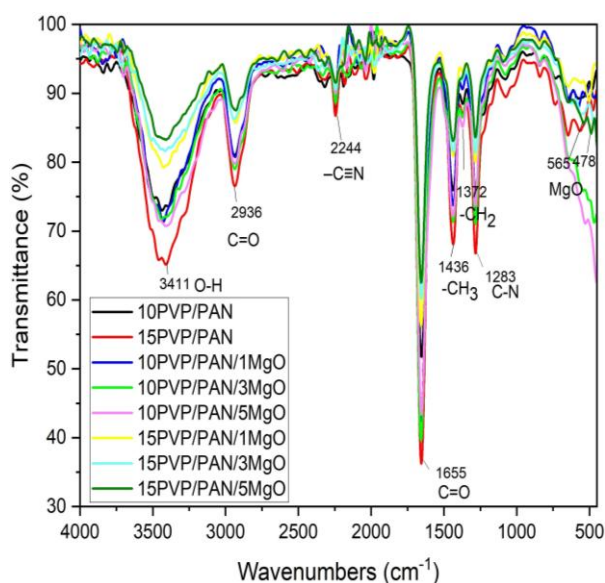


Figure 2. FTIR spectra of 10 and 15 wt% PAN/PVP nanofibers and their corresponding nanocomposites loaded with 1, 3, and 5 wt% MgO.

3.2 SEM results

It is well known that the composition of the polymer solution, its rheological behavior, and the molecular weight of the polymer are the fundamental parameters governing fiber formation during the electrospinning process. Sufficient molecular weight is required to achieve adequate chain entanglement, which is essential for maintaining jet continuity and preventing breakup during elongation. Polymer-based MgO-containing nanofibers have therefore emerged as important materials for both fundamental research and industrial applications. In particular, MgO-loaded nanofibers with

diameters below 1 μm exhibit exceptionally high specific surface areas, facilitating the incorporation of functional groups or surface structures that enhance performance in targeted applications (Hashim et al. 2021).

Several studies have systematically investigated polyacrylonitrile (PAN) under different electrospinning conditions to identify optimal processing parameters (Dehghan et al. 2016). These reports demonstrate that PAN is a versatile polymer owing to its favorable mechanical properties, cost-effectiveness, and ease of processing, making it one of the most widely used polymers for electrospun nanofiber production (Hashim et al. 2021). The fiber diameter of composite systems can be increased by substituting PAN with polyvinylpyrrolidone (PVP) or by blending PAN and PVP at various ratios. It is well documented that increasing polymer concentration results in larger average fiber diameters compared to dilute solutions, which is attributed to enhanced polymer chain entanglement and reduced molecular mobility. These effects increase viscoelastic resistance to jet stretching during electrospinning (Hashim et al. 2021, Dehghan et al. 2016). Before evaluating the morphology of nanofibers produced by the electrospinning method, commercially available MgO nanopowder was examined using SEM-EDS. As shown in Figure 3, the MgO nanopowder exhibited a particulate morphology with nanoscale clustered structures, commonly observed in metal oxide nanopowders due to their high surface energies. The corresponding EDS result confirmed the presence of Mg and O elements, supporting the chemical identity of the MgO nanopowder used in the PAN/PVP/MgO formulations. Subsequently, SEM analyses of PAN/PVP and PAN/PVP/MgO nanofiber samples produced by electrospinning were performed to evaluate the fiber morphology, surface properties, and the effect of MgO addition on the nanofiber structure (Figure 3). The average fiber diameter generally increased as the polymer concentration increased from 10 wt% to 15 wt%. The 10PAN/PVP nanofibers showed an average diameter of 129.31 ± 48.0 nm, whereas the 15PAN/PVP nanofibers exhibited a larger average diameter of 270.83 ± 39.6 nm. This increase may be associated with the higher polymer concentration, which can increase solution viscosity and polymer chain entanglement during electrospinning. The incorporation of MgO also influenced the fiber diameter; however, this effect was not strictly linear. Among all samples, 15PAN/PVP/3MgO exhibited the largest average fiber diameter (402.78 ± 17.8 nm), while 15PAN/PVP/5MgO showed a slightly lower average diameter of 391.6 ± 81.41 nm.

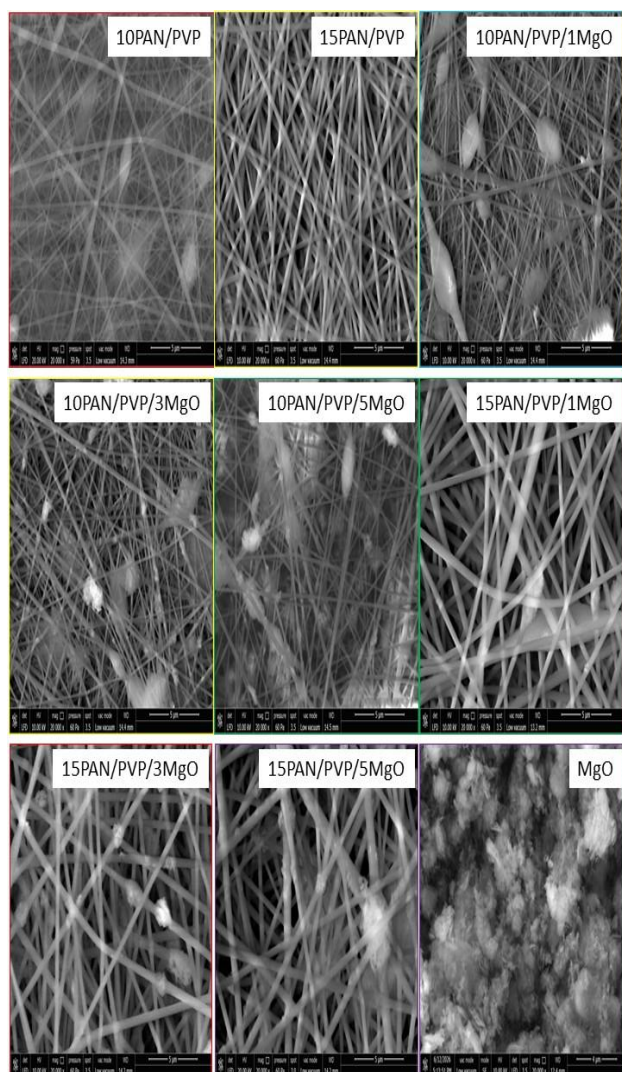


Figure 3. SEM images of 10PAN/PVP and 15PAN/PVP nanofibers and their corresponding nanofibers loaded with 1, 3, and 5 wt% MgO, and SEM image of MgO nanopowder.

This result indicates that fiber diameter is affected by the combined influence of polymer concentration, MgO loading, nanoparticle dispersion, and electrospinning jet stretching. Accordingly, the observed variations in fiber diameter cannot be attributed to a single factor alone. SEM observations showed that the 15 wt% PAN/PVP-based formulations generally produced smoother and more continuous fibers compared with the 10 wt% PAN/PVP-based formulations. In addition, SEM-EDS analysis confirmed the presence of Mg and O signals in MgO-containing nanofiber mats, supporting the incorporation of MgO within the fiber structure. The increase in Mg-related signals with increasing MgO loading was consistent with the initial formulation ratios. Electrospinning performed at an applied voltage of 16 kV, a solution feed rate of 10 $\mu\text{L min}^{-1}$, and a tip-to-collector distance of 17 cm produced a stable electrohydrodynamic jet and continuous, bead-free fibers. In contrast, dilute polymer solutions yielded fibers with smaller diameters but displayed bead-on-string morphologies and localized

jet thinning, indicating insufficient chain entanglement and reduced relaxation time relative to the jet elongation timescale. This observation is consistent with polymer solution theory, which predicts bead formation when the polymer concentration falls below the critical entanglement concentration (C_e) (Hashim et al. 2021, Ewaldz et al. 2022, Barhoum et al. 2019). SEM observations showed that the 15PAN/PVP-based formulations generally produced more continuous and smoother fibers than the 10PAN/PVP-based formulations. This difference may be associated with the higher polymer concentration, which can increase solution viscosity and promote more stable jet formation during electrospinning, as reported in recent electrospinning studies (Islam et al. 2025; Randhawa et al. 2026). Accordingly, SEM observations suggested that both polymer concentration and MgO loading influenced the morphology of the electrospun nanofibers. In general, the 15PAN/PVP-based formulations exhibited smoother, more uniform, and continuous fiber structures with fewer bead-like defects compared with the 10PAN/PVP-based formulations.

The average diameters of the nanofibers varied depending on the polymer concentration and MgO loading. The mean diameter and standard deviation values of the nanofibers are summarized in Table 2.

Table 2. Fiber diameter values of PAN/PVP and PAN/PVP/MgO nanofiber samples.

Sample	Fiber diameter (nm, mean $\pm$ SD)
10PAN/PVP	129.31 $\pm$ 48.0
15PAN/PVP	270.83 $\pm$ 39.6
10PAN/PVP/1MgO	170.22 $\pm$ 81.9
10PAN/PVP/3MgO	147.78 $\pm$ 42.6
10PAN/PVP/5MgO	161.10 $\pm$ 42.2
15PAN/PVP/1MgO	388.4 $\pm$ 37.64
15PAN/PVP/3MgO	402.78 $\pm$ 17.8
15PAN/PVP/5MgO	391.6 $\pm$ 81.41

EDS analysis was performed on 10PAN/PVP and 15PAN/PVP nanofibers containing 1, 3, and 5 wt% MgO to assess the elemental distribution and confirm the compositional characteristics of the nanofibers. EDS analysis confirmed the presence of Mg and O signals in the MgO-containing nanofiber mats, supporting the incorporation of MgO into the PAN/PVP nanofiber structure. The increase in Mg-related EDS signals with increasing MgO loading was generally consistent with the initial formulation ratios (Figure 4). Additionally, EDS analysis was performed to verify the elemental composition of the commercially available MgO nanopowder. The EDS spectrum of the MgO nanopowder showed characteristic Mg and O signals supporting the chemical identity of the nanopowder used in the preparation of PAN/PVP/MgO nanofibers (Figure 4).

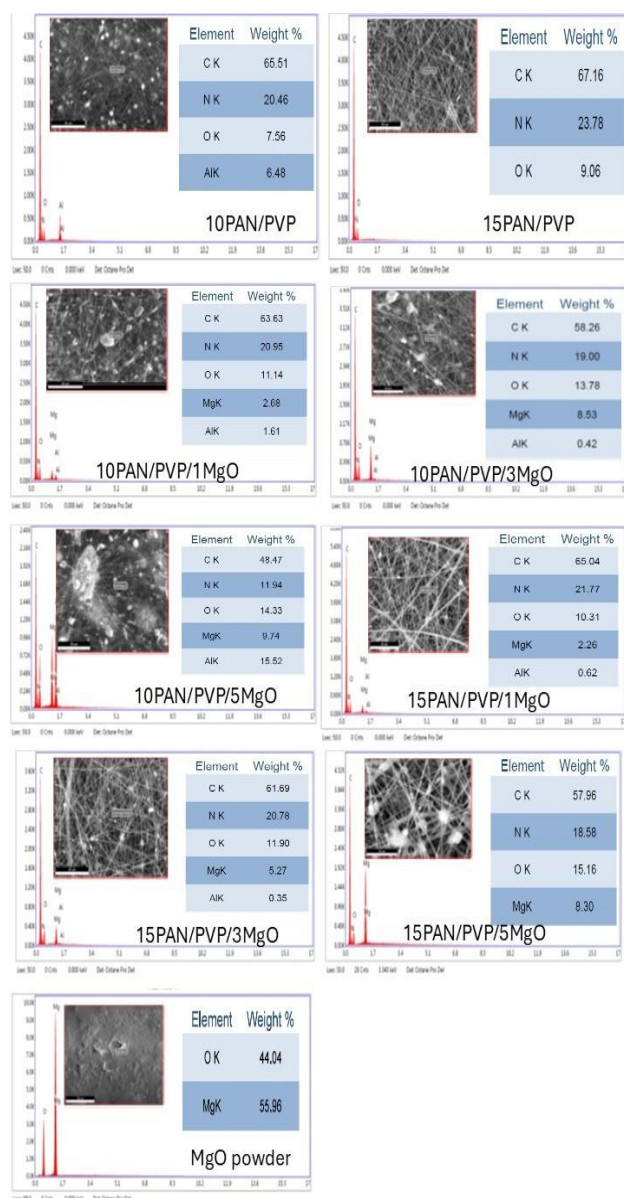


Figure 4. Elemental (wt%) content of nanofiber samples and MgO nanopowder.

Morphological examination by SEM indicated that the 15 wt% PAN/PVP-based formulations generally exhibited smoother and more continuous nanofiber structures compared with the 10 wt% PAN/PVP-based formulations. The presence of Mg and O signals in the EDS spectra of MgO-containing samples supported the successful incorporation of MgO into the nanofiber mats.

3.3 Water contact angle measurements

Water contact angle of the fiber samples was measured and presented in Figure 5. The hydrophilic or hydrophobic nature of polymeric nanofibers plays a pivotal role in determining their suitability for targeted applications (Hashmi et al. 2021). Surface wettability is typically quantified via water contact angle (WCA) measurements. In this study, the surface wettability of PAN/PVP and PAN/PVP/MgO composite nanofiber mats was

investigated by measuring their water contact angles. Polyacrylonitrile (PAN) is known to be inherently hydrophilic, a property attributed to the presence of polar nitrile ($-\text{C}\equiv\text{N}$) groups within its structure. It has been reported that PAN nanofibers produced by the electrospinning method exhibit low water contact angle values ($14\pm 1^\circ$) due to their polar surface groups. This behavior is associated with the strong dipole-dipole interactions between nitrile groups and water (Aflaha et al. 2024a, Aflaha et al. 2024b). Beyond surface chemistry, morphological factors also play a decisive role; decreasing the nanofiber diameter increases surface roughness, which significantly impacts the contact angle (Szewczyk et al. 2019). Nanofiber morphology, along with surface chemistry, can also influence the measured water contact angle. Variations in fiber diameter, mat porosity, and surface roughness can affect water diffusion on electrospun nanofiber surfaces; this has been reported for electrospun fiber materials where both surface chemistry and structural properties contribute to wettability behavior (Bhushan and Jung 2011; Ma et al. 2017). Therefore, the wettability behavior of PAN/PVP/MgO nanofiber mats can be related to the combined effects of PAN/PVP surface chemistry, MgO addition, and nanofiber morphology. The 10PAN/PVP and 15PAN/PVP nanofibers exhibited low contact angles of $29.72\pm 0.66^\circ$ and $22.96\pm 0.52^\circ$, respectively, reflecting the inherent hydrophilicity imparted by the combination of PAN and PVP. The addition of MgO nanoparticles into PAN/PVP nanofibers showed a bidirectional effect in the water contact angle, both increasing and decreasing it. Specifically, a low concentration of MgO (1 wt%) resulted in a slight increase in the contact angle. This observation aligns with literature reports suggesting that metal oxide nanoparticles can modulate the hydrophilic/hydrophobic character of polymer composites (Xia et al. 2018). In contrast, a significant decrease in the contact angle was observed at higher MgO contents (3% and 5%). This behavior demonstrates that the incorporation of MgO nanoparticles into the polymer matrix leads to a decrease in water contact angle, thereby enhancing the hydrophilicity of the nanofibers. This observation aligns with previous studies reporting that MgO improves the surface affinity towards water (Xia et al. 2018, Rinovian et al. 2024, Yu et al. 2024, Xing et al. 2019). This situation can also be explained by the hydrophilic nature of MgO and the increase in $-\text{OH}$ groups on the surface (Xia et al. 2018, Rinovian et al. 2024, Yu et al. 2024).

In the literature, it has been reported that increasing the MgO nanoparticles on polymeric composite surfaces increases hydrophilicity and reduces the contact angle

(Sienkiewicz et al. 2018). The decrease in contact angle at higher MgO loadings may also be partly associated with changes in nanofiber surface morphology. Variations in fiber diameter, porosity, and surface characteristics can influence water spreading behavior on electrospun nanofiber mats (Xue et al. 2017). Therefore, the observed reduction in contact angle is attributed to the combined effects of MgO incorporation, changes in surface chemistry, and possible morphology-related variations. In this context, the contact angle variations observed in PAN/PVP/MgO nanofiber mats can be considered as a result of competitive interactions arising from the polar nitrile groups of PAN, the hydrophilic character of PVP, and the distribution and surface roughness of MgO nanoparticles.

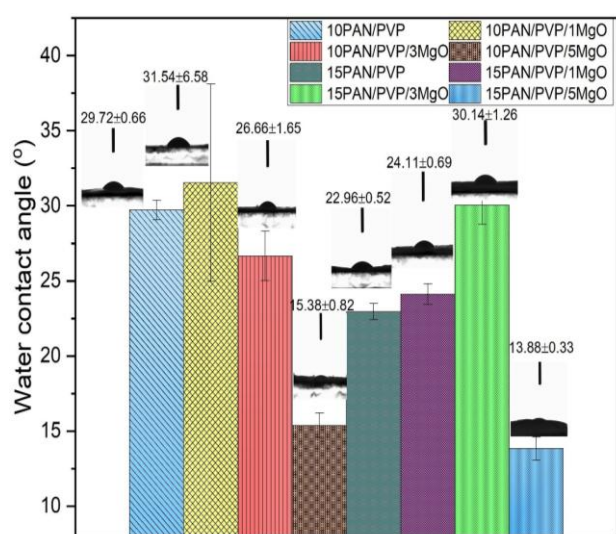


Figure 5. Water contact angle (WCA) analysis nanofibers.

3.4 TGA results

The thermal degradation behavior of the MgO nanopowder and selected 15PAN/PVP/MgO nanofiber samples was evaluated by TGA under a nitrogen atmosphere. As shown in Figure 6, the samples were heated from 25 to 550 °C at a heating rate of 10 °C/min under nitrogen flow. The initial weight loss at lower temperatures can be attributed to the evaporation of physically adsorbed moisture and residual solvent. The main degradation region observed between approximately 250 and 350 °C is associated with the thermal decomposition of the PAN/PVP polymer matrix as commonly reported for polymer-based electrospun nanofiber systems (Hashmi et al. 2019; Liu et al. 2023). The MgO-containing nanofibers exhibited higher residual masses than the neat PAN/PVP nanofibers at 550 °C. However, this increase should be interpreted cautiously, since the higher residue is mainly associated with the inorganic MgO content remaining after polymer decomposition rather than direct evidence of improved

polymer thermal stability alone. Similar interpretations have been reported for inorganic nanoparticle-containing electrospun composite membranes, where increased residual mass is mainly related to the non-degradable inorganic phase (Liu et al. 2021). Therefore, the thermal behavior of the composite nanofibers was evaluated based on the weight-loss profile and residual mass. Among the investigated samples, 15PAN/PVP/5MgO showed the highest residual mass, retaining 46.8% at 550 °C, which is consistent with its higher MgO loading. The weight-loss region above approximately 350–460 °C may be related to further degradation/carbonization of the remaining polymeric residues, while no pronounced additional mass loss was observed above approximately 460 °C (Liu et al. 2023, Xu et al. 2017).

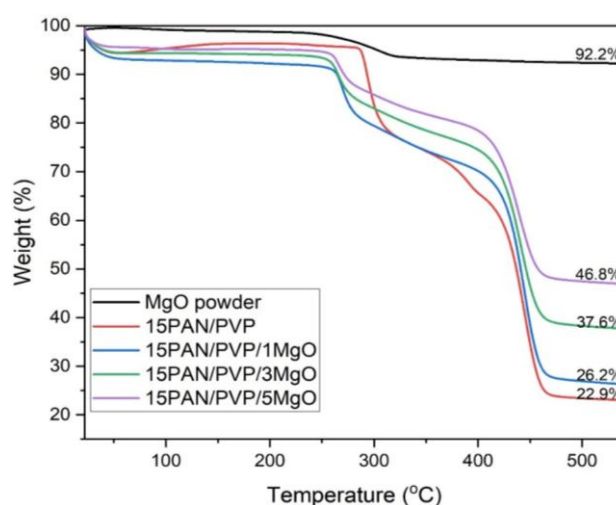


Figure 6. TGA curves of MgO nanopowder and 15PAN/PVP nanofibers containing 1, 3 and 5 wt% MgO.

3.5 In vitro antibacterial activity

The antibacterial activity of the fabricated nanofiber samples was evaluated against Gram-positive *Staphylococcus aureus* and Gram-negative *Escherichia coli* using the disc diffusion method. As shown in Table 3 and Figure 7, the neat PAN/PVP nanofibers and the samples containing 1 and 3 wt% MgO did not produce measurable inhibition zones against either bacterial strain. In contrast, the 5 wt% MgO-loaded samples showed antibacterial activity against *S. aureus*, with inhibition zone diameters of 17±0 mm for 10PAN/PVP/5MgO and 21±0.5 mm for 15PAN/PVP/5MgO. No inhibition zone was observed against *E. coli* under the tested conditions. Although MgO nanoparticles have been reported to exhibit antibacterial activity against both Gram-positive and Gram-negative bacteria, their antibacterial response strongly depends on MgO concentration, particle size, surface properties, agglomeration behavior, test method, bacterial density, and the degree of direct contact between MgO particles

and bacterial cells (Sawai et al. 2000; Nguyen et al. 2018). In the present study, the absence of inhibition against *E. coli* indicates that the prepared PAN/PVP/MgO nanofibers did not show broad-spectrum antibacterial activity under the applied disc diffusion conditions. This result may be associated with limited MgO release/diffusion from the nanofiber matrix and reduced direct interaction with the Gram-negative outer membrane. The outer membrane of Gram-negative bacteria, which contains lipopolysaccharides, can act as an additional permeability barrier and may restrict the interaction of antibacterial agents with the cell wall and cytoplasmic membrane. In contrast, the measurable inhibition zones observed against *S. aureus* suggest that the antibacterial effect of MgO became evident at 5 wt% loading, particularly in the 15PAN/PVP/5MgO sample. The stronger response against *S. aureus* may be related to the absence of an outer membrane in Gram-positive bacteria, which can allow more direct interaction

between MgO-containing fiber surfaces and the bacterial cell wall. In addition, higher MgO loading may increase the availability of active MgO sites at or near the nanofiber surface, thereby enhancing contact-dependent antibacterial effects such as local alkaline stress, reactive oxygen species generation, and membrane/cell wall disruption. This concentration-dependent behavior is consistent with previous MgO-based antibacterial studies reporting stronger antibacterial activity with increasing MgO content and, in some cases, higher susceptibility of *S. aureus* compared with *E. coli* (Yamamoto et al. 2002; Sawai et al. 2000; Coelho et al. 2019; Liu et al. 2021). For example, Coelho et al. (2019) reported complete inhibition of *S. aureus* growth in granules containing 3–4 wt% MgO. Therefore, the antibacterial activity observed in the present study indicates that MgO became effective at 5 wt% loading in the PAN/PVP nanofiber structure, while the prepared samples did not exhibit antibacterial activity against *E. coli* under the tested conditions.

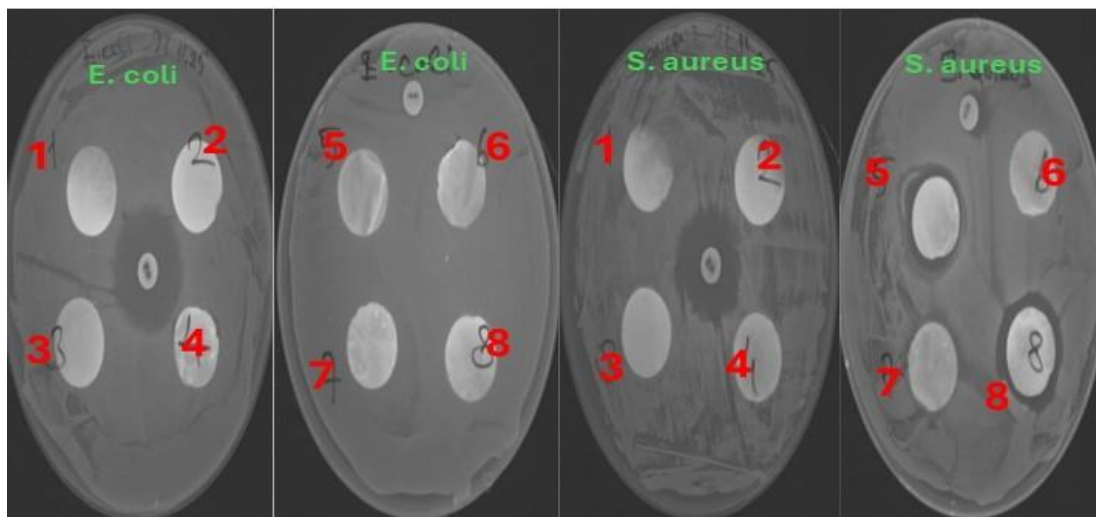


Figure 7. Antibacterial activity of PAN/PVP and PAN/PVP/MgO composite nanofibers evaluated by the disc diffusion method against *S. aureus* and *E. coli*. Sample codes: (1) 10PAN/PVP, (2) 15PAN/PVP, (3) 10PAN/PVP/1MgO, (4) 10PAN/PVP/3MgO, (5) 10PAN/PVP/5MgO, (6) 15PAN/PVP/1MgO, (7) 15PAN/PVP/3MgO, and (8) 15PAN/PVP/5MgO.

Table 3. Inhibition zone diameters of PAN/PVP and PAN/PVP/MgO nanofiber samples against *S. aureus* and *E. coli*.

Sample	Inhibition zone diameter against <i>S. aureus</i> (mm)	Inhibition zone diameter against <i>E. coli</i> (mm)
10PAN/PVP (1)	0	0
15PAN/PVP (2)	0	0
10PAN/PVP/1MgO (3)	0	0
10PAN/PVP/3MgO (4)	0	0
10PAN/PVP/5MgO (5)	17±0	0
15PAN/PVP/1MgO (6)	0	0
15PAN/PVP/3MgO (7)	0	0
15PAN/PVP/5MgO (8)	21±0.5	0
Amikacin 30µg	15±0.5	19±0

4. Conclusions

In this study, PAN/PVP and PAN/PVP/MgO nanocomposite fiber mats were successfully fabricated via the electrospinning technique. Morphological analysis revealed that increasing the polymer concentration to 15% by weight reduced bead formation and resulted in smoother and more even nanofibers. EDS analysis confirmed the effective and homogeneous incorporation of MgO nanoparticles into the fiber structure, with elemental distribution increasing proportionally to the loading content. FTIR spectra corroborated the chemical interactions between the polymer matrix and the nanoparticles, evidenced by significant shifts in the characteristic O–H and C≡N bands. In terms of surface wettability, the addition of MgO enhanced the hydrophilic nature of the nanofibers. This behavior may be attributed to the inherent water affinity of MgO, together with possible contributions from changes in surface morphology and fiber structure. Based on their superior morphological and antibacterial performance, the 15 wt% PAN/PVP nanofiber series was further evaluated via TGA, which demonstrated that the nanocomposites maintained improved thermal behavior. Overall, the developed PAN/PVP/MgO electrospun nanofibers exhibited promising structural, hydrophilic, thermal, and antibacterial properties, indicating their potential as antibacterial surface materials and filtration media; however, cytotoxicity, biocompatibility, and application-specific biological evaluations should be addressed in future studies to further assess their suitability for biomedical-related applications.

Declaration of Ethical Standards

The authors declare that they comply with all ethical standards.

Credit Authorship Contribution Statement

Author-1: Conceptualization, investigation, methodology, software, visualization, validation, formal analysis, writing – review and editing.

Author-2: Investigation, methodology, project administration.

Declaration of Competing Interest

The authors have no conflicts of interest to declare regarding the content of this article.

Data Availability Statement

The authors declare that the main data supporting the findings of this work are available within the article. Datasets are available on request. The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

AI Tool Disclosure

Generative AI tools were used only for English language editing, grammar correction, and improvement of textual clarity.

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