Basic and applied

Virtual Modelling and Electromagnetic Absorption Analysis of ZnO/SiO₂-PCL Composites

Daw Mohammad Abdalhadi, Nabeelah Maammar Salih Ahmed²

¹Faculty of Science, Asmarya University, Zliten, Libya ²Faculty of Science, Almergib University, Alkhums, Libya

E-mail:D.sahal@asmarya.edu.ly
*Corresponding author: D.sahal@asmarya.edu.ly

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Abstract: Recent research has focused on developing electromagnetic wave absorbers that exhibit high absorption performance, thin thickness, low density, light weight, low cost, and a broad absorption bandwidth. In this study, a virtual model of a polycaprolactone (PCL)-based composite reinforced with varying proportions of nano zinc oxide (ZnO) and silicon dioxide (SiO₂) was developed using COMSOL Multiphysics. A rectangular waveguide structure was designed to simulate a Network Analyzer (NWA) setup used for wave transmission measurements. The complex permittivity of the composites was calculated for different ZnO and SiO₂ contents. The results revealed that the dielectric constant increased from 2.893 to 3.833, and the dielectric loss factor rose from 0.253 to 0.369 with higher filler loading. Consequently, the reflection loss (RL) decreased to 3.718 dB, while the absorption coefficient increased to 0.110, and the attenuation coefficient reached 3.2393 dB at 10 GHz for an absorber thickness of 0.003 m. These findings demonstrate the potential of PCL/ZnO/SiO₂ composites as lightweight and efficient microwave absorbing materials.

Keywords: Microwave Absorbing, Complex permittivity, Absorption coefficient, Reflection loss.

1- Introduction:

Electromagnetic waves, also known electromagnetic radiation, are produced by the movement of electrically charged particles. These waves can propagate through air, various materials, and a vacuum. Electromagnetic waves with low frequencies are considered electromagnetic fields, whereas those with extremely high frequencies are electromagnetic radiation. Electromagnetic waves contain various frequencies and wavelengths in a wide range of applications. However, they can interfere with one another, potentially harm electronic devices, and may impact human health [1]. Consequently, the demand for preventing electromagnetic interference (EMI) has risen, driven by the growing prevalence and sensitivity of electronic devices, especially radio frequency devices, which are disposed to disrupt digital equipment and electronic instruments related to telecommunications and electric power [2]. The creation of innovative materials to enhance the electromagnetic wave absorption properties of microwave absorbers has attracted global interest due to the increasing demand for these materials. An ideal EM wave absorber should be thin lightweight, exhibit high absorption efficiency, have a wide operational range, allow for tunable absorption frequencies, and possess

capabilities [3]. multifunctional efforts have been dedicated to researching and developing diverse materials in pursuit of these ideal characteristics, and different materials have been used for electromagnetic wave absorption applications. Multilayered carbon nanotubes/silicon dioxide (CNTs/SiO2) fabricated with electromagnetic wave-absorbing ceramic matrix composite material were made by hot-pressed sintering to study the shielding effectiveness (SE) electromagnetic of interference (EMI) and reflecting effectiveness (RE) in the range of frequency 8-12 GHz. The results showed that the gradient multilayered sample had better absorbing effectiveness than the single layered samples, while their SEs were almost the same (Mingxia Chen) et al [4]. There are important requirements to get good absorber material first, the impedance of free space should be the equal intrinsic impedance of the material. Secondly, the incident electromagnetic wave must penetrate the material layer and undergo rapid attenuation [5]. Polymer-based composites have attracted increasing attention for future electromagnetic interference (EMI) applications owing to their unique combination of electrical, mechanical, and optical properties [6]. These materials are promising considered candidates for electromagnetic wave shielding due to their facile processing, structural flexibility, and strong resistance to chemical degradation. In this work, the dielectric response and electromagnetic attenuation characteristics of polycaprolactone (PCL) composites reinforced with zinc oxide nanoparticles (ZnO_{nano}) and silicon dioxide (SiO₂) systematically investigated through numerical simulations in the X-band frequency range (8-12 GHz). When incorporated into a polymeric host such as PCL, these ceramic nanoparticles can induce synergistic effects that enhance impedance matching, interfacial polarization, and multiple attenuation mechanisms, thereby improving microwave absorption performance.

2- Fundaments of Microwave Absorption

When an electromagnetic wave encounters a material, it experiences three main interactions: absorption, reflection, and transmission. The ability of a material to absorb electromagnetic radiation is determined by its intrinsic loss mechanisms, while reflection primarily arises from an impedance mismatch between the material and the incident medium [7]. These behaviors are generally characterized by three fundamental parameters: complex permittivity (ε), complex permeability (μ) , and attenuation constant illustrated (α) , schematically in Fig. (1)

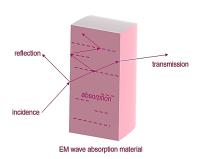


Fig 1. Schematic The general processes of an incident EM wave through an EM absorption

The reflection loss (RL) is a widely used indicator to evaluate the absorption performance of a material

$$R_L = -20log \left| \frac{Z_{in} - 1}{Z_{in} + 1} \right|$$
 (1)

Wherein

$$Z_{in} = \sqrt{\frac{\mu' - j\mu''}{\varepsilon' - j\varepsilon'' - \frac{j\sigma}{\omega\varepsilon_0}}} \cdot tanh\left(jd\frac{\omega\sqrt{(\mu' - j\mu'')(\varepsilon' - j\varepsilon'' - j\sigma/(\omega\varepsilon_0))}}{c_0}\right)$$

And $\omega = 2\pi f$, where Z_{in} is the impedance of incident wave, μ' real part of permeability,

 μ'' Image part of permeability, ε' real part of permittivity, ε'' image part of permittivity, ε_0 permittivity of free space, σ conductivity, ffrequency of EM wave, d thickness of material, and c_0 light speed. When the intrinsic impedance of the absorber matches that of free space, reflection is minimized, and the material achieves optimal absorption efficiency [8]. The complex relative permittivity ε is defined as ε = ϵ' - $i\epsilon''$, where ϵ' represents the dielectric constant (energy storage through polarization) and ε'' is the dielectric loss (energy dissipation due to relaxation). The loss tangent (tan δ = $\varepsilon''/\varepsilon'$) quantifies how efficiently the material converts electromagnetic energy into heat. This behavior is influenced by the relaxation time (τ), which reflects how fast dipoles return to equilibrium under alternating fields [9]. The RL can also be calculated using classical transmission line theory based on the material's electromagnetic parameters.

$$RL = -20log_{10}|S_{11}|$$
 (3)

Additionally, wave attenuation results from a combination of absorption and scattering processes, expressed as the logarithmic ratio between the input and transmitted powers. In this study, the attenuation characteristics of $PCL/ZnO/SiO_2$ composites were obtained using simulated S-parameters (S₁₁ and S₂₁), which provide insight into the energy reflected and transmitted through the composite samples.

$$Attenuation(db) = -20 \log(S_{21})$$
 (4)

3- Electromagnetic wave absorption performance of PCL materials

Microwave absorption performance is closely linked to a material's internal structure, dielectric loss capacity, and synergistic effects between its constituents [10]. Among the various polymer candidates, polycaprolactone (PCL) has attracted attention due to its favorable properties it is biodegradable, nontoxic, semi-crystalline, and electrical insulating [11]. As a type of A-B polymer, polarization in PCL can occur both perpendicular and parallel to its main polymer chains.

PCL possesses a relatively low melting point of approximately 60 °C and a crystallization temperature around −60 °C. It is typically synthesized via ring-opening polymerization of ε-caprolactone using stannous octanoate as a catalyst [12]. The structural formula and synthesis process of PCL are illustrated in Fig.

(2). Depending on its molecular weight, PCL may appear as a waxy solid (for lower molecular weights) or as a hard thermoplastic polymer when the molecular weight exceeds 20,000. The waxy form is often used as an additive, while the solid form is processed into fibers or films at temperatures below 200 °C without thermal degradation [13].

Fig 2. Synthesis and structure of PCL

4- Results and Discussion

Dielectric enhancement of polymeric matrices such as PCL can be achieved through the incorporation of conductive or semi conductive fillers, including carbon-based materials like carbon nanotubes (CNTs) or metallic oxides such as ZnO [14]. One notable study highlighted the effectiveness of ZnO-PCL nanocomposites in microwave attenuation, demonstrating reflection losses up to −18.2 dB. This improvement was attributed to the high specific surface area of the ZnO nano fillers, which facilitates strong interfacial polarization and dielectric loss mechanisms [15]. In the present work, a series of composite samples was prepared by blending polycaprolactone (PCL) with zinc oxide nanoparticles (ZnOnano) and silicon dioxide (SiO₂) at varying ratios. The mixing proportions were as follows:

PCL: 95%, 85%, 75%, 65%, 55% ZnOnano: 3%, 9%, 15%, 21%, 27% SiO₂: 2%, 6%, 10%, 14%, 18%

These composites were studied to assess their electromagnetic wave absorption behavior within the 8-12 GHz frequency range, using a fixed sample thickness of 0.003 m. The investigation relied on virtual modeling and numerical simulation performed using COMSOL Multiphysics software, which emulated measurements obtained from network analyzer (NWA). rectangular waveguide was constructed within simulation environment to model the propagation and interaction of microwaves with the material. The relative permittivity of each composite was calculated using an established mixing rule [16], incorporating experimentally determined complex permittivity values for the pure constituents [17-18]. Based on these formulations, the effective dielectric properties of the composites were estimated and are summarized in Table (1). These values serve as the foundation for analyzing the electromagnetic absorption behavior in the X-band frequency range.

Table 1 Pure values and results of calculating the relative permittivity complex of mixture

the relative permit	tivity complex of mixture
Materials	Relative permittivity
	Complex $\{\varepsilon^* = \varepsilon' - $
	$jarepsilon''$ }
Pure PCL	2.79-0.24J
Pure ZnO _{nano}	6.48-1.41J
PureSiO ₂	3.83-0.0096J
95%PCL	2.893-0.253J
+3%ZnO _{nano}	
+2%SiO ₂	
85%PCL	3.118-0.279J
+9%ZnO _{nano}	
+6%SiO ₂	
75%PCL	3.348-0.308J
+15%ZnO _{nano}	
+10%SiO ₂	
65%PCL	3.587-0.338J
+21%ZnO _{nano}	
+14%SiO ₂	
55%PCL+	3.833-0.369J
27%ZnO _{nano}	
+18%SiO ₂	

The data presented in Table (1) demonstrate that increasing the proportions of ZnOnano and SiO₂ in the composite leads to a noticeable enhancement in both the dielectric constant (ϵ') and the dielectric loss factor (ε''). The dielectric constant reflects the material's ability to store electromagnetic energy through polarization, while the dielectric loss represents the dissipation of this energy as heat due to lagging polarization mechanisms. As the content of ZnOnano and SiO2 increases, both the real and imaginary components of the complex permittivity rise, indicating improved energy storage capacity and stronger attenuation capability [19]. This trend directly enhances the microwave absorption potential of the composite. SiO₂, in particular, contributes significantly to dielectric loss due to interfacial polarization, especially at higher frequencies. Moreover, its inclusion improves impedance matching between the absorber and free space, which is critical for minimizing reflection. In other reported systems, SiO₂ has been employed as an intermediate dielectric layer to optimize impedance matching, as seen in

like CIP-SiO₂-Mn_{0.6}Zn_{0.4}Fe₂O₄, composites absorption performance where improved consistently with increased SiO₂ content [20]. Similarly, studies investigating composites of carbon nanotubes (CNTs) and zinc oxide whiskers (ZnOw) have shown that the complex permittivity increases with higher loading. However, the permittivity tends to slightly decline with increasing frequency due to dispersion effects and reduced interfacial polarization efficiency [21]. The electromagnetic response of the prepared composites was further analyzed through the reflection (S11) and transmission (S21) coefficients, obtained using COMSOL Multiphysics simulations based on the finite element method. These parameters quantify the amount of incident wave energy reflected or transmitted through the material structure.

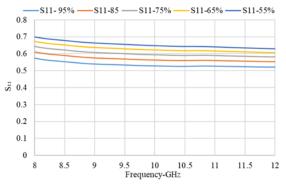


Fig 3. Variation in $|S_{11}|$ for (ZnO+SiO2) content

The reflection coefficient (S11) values increased from 0.548 to 0.651 at a frequency of 10 GHz, correlating with the rising content of ZnOnano and SiO2. As a result, the reflection loss (RL) values also decreased, ranging from 5.519 to 3.718 dB, indicating improved wave absorption. The reflection loss is logarithmically related to S11 and is widely used as a measure of absorber effectiveness in the microwave range. Figure (3) illustrate the observed S₁₁ values decrease with increasing frequency, a typical for dielectric composites due to the diminishing polarization effects at higher frequencies. In contrast, figure (4) shows that the reflection loss RL are increases as the frequency rises. The transmission coefficient (S21) exhibits a consistent upward trend with increasing frequency across all composite samples, as shown in Fig. 5. Notably, S₂₁ values rise from approximately 0.6887 to 0.7852 as the filler concentration decreases from 95% to 55%. This behavior indicates that composites with lower filler loading allow greater electromagnetic transmission due to improved impedance matching between the waveguide and the sample surface. Conversely, higher filler contents lead to stronger impedance mismatch, resulting in increased reflection and reduced transmitted power. This observation is consistent with the energy conservation relationship between the scattering parameters $(|S_{11}|^2 + |S_{21}|^2 \approx 1)$, where an increase in reflection (S11) corresponds to a decrease in transmission (S₂₁). Furthermore, the slight irregularity in the S₂₁ curves suggests non-ideal impedance matching, emphasizing that fine-tuning the ZnO and SiO₂ ratios plays a crucial role in optimizing the electromagnetic absorption capability of the composite system.

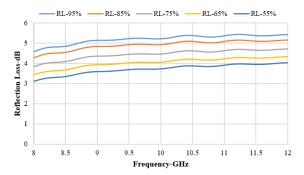


Fig 4. Variation in RL for (ZnO+SiO2) content

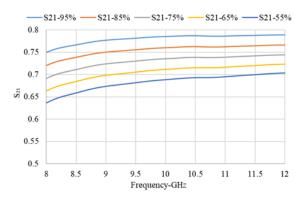


Fig 5. Variation in |S21 | for (ZnO+SiO2) content

The incorporation of SiO₂ significantly contributes to the enhancement of microwave absorption performance. Its role lies primarily in improving impedance matching and promoting dielectric loss, both of which are essential for efficient electromagnetic wave attenuation. Design strategies that employ gradient structures, as demonstrated in CNT-based composites, have proven effective in optimizing both absorption bandwidth and intensity by enabling smoother impedance transitions and multi-scale polarization effects. In addition to dielectric strategies, the

integration of magnetic materials, such as RGO-ZnO-Fe₃O₄, can further enhance absorption by introducing magnetic loss mechanisms and synergistic dielectric-magnetic facilitating interactions [22]. Zinc oxide (ZnO) stands out as an excellent candidate for microwave absorption due to its semiconducting nature, wide bandgap, ease of synthesis, and ability to form welldispersed nanoscale structures. Among various dielectric systems, metal oxide semiconductorbased composites show strong promise owing to their tunable dielectric constants, structural versatility, and balanced dielectric and magnetic loss capabilities. In the present study, as the combined loading of ZnOnano and SiO2 increased, the power loss and absorption coefficient increased with frequency, as illustrated in Fig (6) and Fig (7). This relationship between filler loading and power loss further confirms the effectiveness of the composite in attenuating electromagnetic energy through internal mechanisms, rather than simply reflecting it.

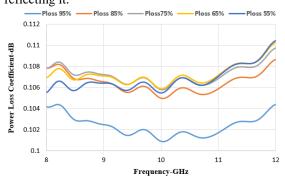


Fig 6. Variation in Power Loss Coefficient Ploss for (ZnO+SiO2) content

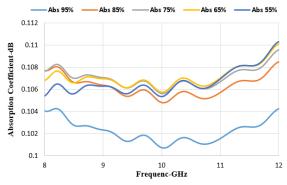


Fig 7. Variation in Absorption Coefficient Abs for (ZnO+SiO₂) content

The electromagnetic attenuation behavior of the composite materials is primarily governed by their dielectric loss characteristics, which arise due to the motion of free and bound charges under alternating electromagnetic fields. In the current study, attenuation values were calculated for the PCL/ZnOnano/SiO₂ composites using equation (4), based on simulated Sparameters across the 8–12 GHz frequency

range. The thickness of the material was maintained at 0.003 m during all simulations. As illustrated in Fig. (10), the attenuation coefficient increased with the rising content of ZnOnano and SiO2, reaching a maximum of 3.281 dB at 10 GHz, while the minimum value observed was 2.1002 dB. These values reflect material's ability dissipate to electromagnetic energy internally rather than allowing wave propagation through the medium. Likewise, Ahmed F. et al. (2016) found attenuation levels of 5.827 dB at 10% NZF filler concentration in a 1 mm thick composite, also within the 8-12 GHz range [23]. Moreover, similar behavior was reported for CNTs/ZnOw composites, where the addition of ZnOw significantly enhanced microwave attenuation [24]. The increased attenuation is attributed to improved interfacial polarization and conductive loss resulting from the effective dispersion of ZnOw nanoparticles within the polymer matrix [25]. Additionally, Figs. (8) and (9) present the trends in dielectric constant and dielectric loss factor versus frequency, confirming that the real and imaginary parts of the permittivity contribute to both storage and dissipation of electromagnetic energy. The combined effect leads to improved shielding effectiveness, which is especially crucial for practical electromagnetic interference mitigation applications.

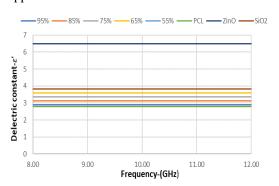


Figure (8) Variation in dielectric constant samples with Frequency

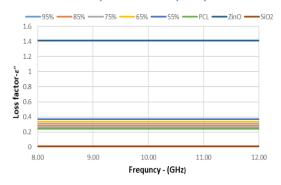


Figure (9) Variation in the loss factor ε'' of samples with Frequency

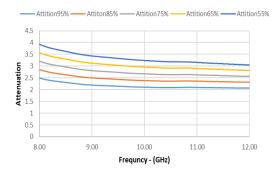


Figure (10) Variation in Attenuation Coefficient for (ZnO+SiO2) content

5- Conclusion

The present study demonstrated that incorporating ZnO nanoparticles (ZnOnano) and SiO₂ into a polycaprolactone (PCL) matrix significantly enhanced the dielectric constant and loss factor of the resulting composites. A higher dielectric constant indicates greater material polarization under an applied field, while the increased loss factor contributes to improved conversion of electromagnetic energy into heat, facilitating efficient attenuation. Moreover, the study showed that increasing the filler content led to improved reflection loss (RL), absorption coefficient, and attenuation coefficient, all of which contribute to stronger electromagnetic absorption. However, an relationship was observed with the transmission coefficient (S₂₁), which decreased with higher filler loading-indicating reduced wave penetration and enhanced shielding behavior. Overall, the simulated results confirm that the PCL/ZnOnano/SiO₂ composites possess favorable characteristics for microwave absorption applications, particularly within the X-band (8-12 GHz). These findings suggest that such composites may offer effective and lightweight solutions for electromagnetic shielding in interference (EMI) advanced electronic and telecommunication systems. Future research may focus on experimental validation, optimization of filler morphology and dispersion, and tailoring sample thickness to further enhance absorption performance and broaden the applicability of these composites.

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النمذجة الافتراضية وتحليل الامتصاص الكهرومغناطيسي لمركبات ZnO/SiO2-PCL

ضو محمد عبد الهادي انبيلة معمر صالح أحمد 2 كلية العلوم، الجامعة الأسمرية، زليتن، ليبيا ا كلية العلوم، جامعة المرقب، الخمس، ليبيا 2

الملخص

ركزت الأبحاث الحديثة على تطوير مواد ماصة للموجات الكهر ومغناطيسية تمتاز بأداء امتصاصي عالى، وسُمكٍ رقيق، وكثافة منخفضة، ووزنٍ خفيف، وتكلفة منخفضة، إضافةً إلى نطاق امتصاص واسع. في هذه الدراسة، تم إنشاء نموذج افتراضي لمركب قائم على بولي كابرولاكتون PCL مدعم بنسب مختلفة من أكسيد الزنك النانوي ZnOولاكتون SiO2. باستخدام برنامج Detwork Analyzer – NWA المستخدم في السالت التقال الموجات، وحُسبت السماحية المركبة للعينة عند تراكيز مختلفة من المضافات النانوية. أظهرت النتائج زيادة في ثابت العزل الكهربائي من 2893 إلى 2893، وارتفاع عامل الفقد العزلي من 2025 إلى 0.369 بزيادة محتوى ZnO و .3032 في المقابل، انخفض فقد الانعكاس PCL/ZnO/SiO2 و 3.2393 لله الزداد معامل الامتصاص إلى 10.110، وبلغ معامل التوهين PCL/ZnO/SiO2 عند تردد وفقالة في امتصاص الموجات الميكروية.