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Modelling and prediction of impact resistance and electromagnetic shielding in graphene-reinforced carbon fiber composites: A critical review

Ajay Kumar Singh, Rajesh Rathore
Department of Engineering, Vikrant University, Gwalior, Madhya Pradesh, India
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Abstract
Graphene-reinforced carbon fibre polymer (G-CFRP) composites have attracted considerable attention for aerospace, automotive, and defence applications due to their high strength-to- weight ratio, enhanced electrical conductivity, and multifunctional performance. The incorporation of graphene nanoplatelets into conventional CFRP systems can significantly improve mechanical properties such as impact resistance while also enabling functional capabilities such as electromagnetic interference (EMI) shielding. However, predicting the behaviour of these hybrid composite systems remains challenging because of the complex interactions between carbon fibres, polymer matrices, and nanoscale graphene reinforcements. This study presents a critical analytical review of predictive modelling approaches used to evaluate the mechanical and electromagnetic performance of graphene- reinforced carbon fibre composites. The review examines key modelling frameworks reported in the literature, including micromechanical models, finite element simulations, multiscale modelling techniques, electromagnetic modelling approaches, and emerging data-driven methods. These modelling strategies are evaluated in terms of predictive capability, computational complexity, and applicability to multifunctional composite design. The analysis highlights the limitations of existing modelling approaches and emphasizes the need for integrated hybrid modelling frameworks that combine physics-based simulations with data-driven techniques to improve predictive accuracy and support the development of advanced multifunctional composite materials.

Keywords: Graphene-reinforced composites, carbon fibre reinforced polymers, impact resistance modelling, electromagnetic interference shielding, multiscale modelling, finite element modelling, machine learning in composites

Introduction

Background

The growing demand for lightweight and high-performance materials in aerospace, automotive, and defence industries has intensified research into advanced composite materials. These sectors require structural materials that deliver high mechanical performance while reducing overall system weight. Lightweight materials improve fuel efficiency, reduce emissions, enhance payload capacity, and increase operational efficiency in modern engineering systems (Baker et al., 2004; Soutis, 2005; Campbell, 2010) [3, 5, 36].

Among advanced materials, fiber-reinforced polymer composites have gained significant attention due to their high strength-to-weight ratio, corrosion resistance, and fatigue durability compared with traditional metallic materials (Chukov *et al*., 2019; Luo, 2023) [7, 21]. Carbon fiber reinforced polymer (CFRP) composites are now widely used in aerospace structures, including aircraft fuselages, wings, and satellite components (Sánchez *et al*., 2022).

Advances in nanotechnology have further enhanced composite materials through the incorporation of nanoscale reinforcements into polymer matrices. Nanomaterials such as graphene, carbon nanotubes, and graphene nanoplatelets can significantly improve mechanical, electrical, and thermal properties of polymer composites (Stankovich *et al*., 2006; Kuilla *et al*., 2010; Kim *et al*., 2010) [16, 18, 37]. Their integration into conventional fiberreinforced systems has enabled the development of multifunctional composites capable of providing structural reinforcement along with electrical conductivity and electromagnetic protection (Gibson, 2010) [12].

Among these nanomaterials, graphene has emerged as a particularly promising reinforcement material. Graphene is a two-dimensional carbon nanostructure consisting of a single layer of carbon atoms arranged in a hexagonal lattice.

Since its discovery, graphene has attracted considerable attention due to its exceptional mechanical strength, electrical conductivity, and thermal transport properties (Novoselov *et al*., 2004; Geim & Novoselov, 2007) [10, 25]. These characteristics make graphene an attractive candidate for improving the performance of advanced composite materials.

Graphene Reinforcement in Carbon Fiber Reinforced Polymer Composites

Graphene-reinforced carbon fiber polymer composites (G-CFRPs) represent a new generation of multifunctional composite materials designed to enhance both structural and functional performance. In conventional CFRP systems, carbon fibers provide high strength and stiffness, while the polymer matrix transfers loads and protects the fibers. The incorporation of graphene nanoplatelets within the polymer matrix or at the fiber–matrix interface can significantly improve the mechanical and multifunctional performance of these composites (Hadden *et al*., 2015) [14].

Graphene reinforcement enhances load transfer efficiency between fibers and the surrounding matrix due to its high surface area and strong interfacial bonding capability. As a result, graphene nanoplatelets can bridge micro-cracks, delay crack propagation and improve fracture toughness in polymer composites (Pontefisso & Mishnaevsky Jr., 2016; Papageorgiou *et al*., 2017) [28, 30]. Multiscale modelling studies further demonstrate that graphenereinforced interphase regions can enhance stress transfer across the fiber-matrix interface, leading to improved mechanical performance of carbon fiber composites (Le *et al*., 2019) [1].

Beyond mechanical improvements, graphene incorporation can enhance electrical conductivity and thermal transport properties of composite materials. These characteristics enable grapheme-enhanced composites to perform additional functions such as electromagnetic interference (EMI) shielding, lightning strike protection, and thermal management in aerospace systems (Chhetri & Kuila, 2024) [6]. Graphene-based nanomaterials have also been investigated for ballistic and impact-resistant applications due to their high strength and energy absorption capacity (Gaur & Singh, 2019) [9].

Consequently, graphenereinforced composites are increasingly considered promising candidates for next-generation multifunctional aerospace materials.

Importance of Predictive Modelling

Despite the promising performance of graphene-reinforced composites, their design and optimization remain challenging due to complex interactions between fibers, matrix materials, and nanoscale reinforcements.

Experimental characterization alone is often insufficient to fully understand these interactions because comprehensive testing requires significant time, cost, and material resources.

Predictive modelling approaches have therefore become essential tools for analysing the behaviour of graphene-reinforced composites. Various modelling frameworks have been developed to predict mechanical and functional properties, including micromechanical models, finite element simulations, and multiscale modelling approaches (Odegard *et al*., 2005) [26].

Micromechanical models estimate effective nanocomposite properties by analysing interactions between filler particles and polymer matrices (Elmarakbi & Azoti, 2018) [8]. Finite element modelling is widely used to simulate structural behaviour of graphene-reinforced composites under different loading conditions (Georgantzinos *et al*., 2020) [11].

Multiscale modelling frameworks integrate material behaviour across different length scales, linking nanoscale graphene interactions with macroscopic composite performance (Al Mahmud *et al*., 2019; Hadden *et al*., 2015) [1, 14].

Recent studies have further extended these approaches to analyze hybrid carbon fiber–graphene composites with functionalized graphene nanoplatelets (Al Mahmud *et al*., 2021) [2].

In addition to physics-based models, data-driven approaches such as machine learning algorithms are increasingly used in composite material design. These techniques analyze large datasets to identify relationships between material composition and performance characteristics, accelerating the development of advanced multifunctional composites (Guo *et al*., 2025) [13].

Research Gap

Despite substantial progress in graphene-enhanced composites, several challenges remain in understanding and predicting their multifunctional behaviour. Much of the existing literature focuses primarily on experimental investigations of individual properties such as tensile strength, electrical conductivity, or electromagnetic shielding effectiveness rather than providing comprehensive evaluations of predictive modelling frameworks. Previous studies have demonstrated the ability of graphene nanostructures to enhance mechanical reinforcement and multifunctional performance in polymer composites (Stankovich *et al*., 2006; Kuilla *et al*., 2010; Potts *et al*., 2011; Kim *et al*., 2010; Papageorgiou *et al*., 2017) [16, 18, 28, 31, 37]. Similarly, graphene nanoplatelet-reinforced carbon fiber composites have shown improved mechanical strength and electrical conductivity through experimental and multiscale modelling studies (Hadden et al., 2015; Al Mahmud *et al*., 2019) [1, 14].

However, modelling approaches reported in the literature vary widely in methodology, modelling scale, and application focus. Techniques such as micromechanical modelling, finite element simulations, and multiscale frameworks are often applied independently and primarily address specific material properties (Pontefisso & Mishnaevsky Jr., 2016; Georgantzinos *et al*., 2020) [11, 30]. As a result, many studies fail to integrate multiple functional characteristics within a unified predictive framework.

Recent advances in multifunctional composite design emphasize the need for integrated modelling strategies capable of linking nanoscale material behaviour with macroscopic structural performance (Gibson, 2010; Mirabedini *et al*., 2020; Suresh Babu & Mourad, 2021) [12, 22, 38]. Although emerging techniques such as machine learning-assisted material discovery are accelerating composite development (Guo *et al*., 2025) [13], systematic critical reviews comparing predictive modelling frameworks for both mechanical performance and electromagnetic shielding in graphene-reinforced CFRP systems remain limited.

Therefore, a comprehensive analytical review is needed to evaluate existing predictive modelling approaches and assess their effectiveness in predicting multifunctional performance relevant to aerospace, automotive, and defence applications.

Aim of the Study

The primary aim of this study is to critically analyze and synthesize modelling frameworks used to evaluate the mechanical and electromagnetic performance of graphene-reinforced carbon fibre polymer composites. In particular, the study focuses on predictive approaches for impact resistance, electromagnetic interference shielding effectiveness, and multifunctional behaviour of graphene-enhanced composite materials.

This review systematically examines modelling methodologies reported in the literature, including micromechanical models, finite element simulations, multiscale computational frameworks, and emerging data-driven techniques. By comparing these approaches, the study evaluates their strengths, limitations, and applicability in designing advanced multifunctional composite materials.

Furthermore, the study identifies research gaps and methodological limitations in existing modelling frameworks, particularly regarding the integration of mechanical performance prediction with electromagnetic shielding capabilities. Through this analysis, the review aims to support the development of improved predictive modelling strategies for grapheneenhanced carbon fibre composites used in aerospace, automotive, and defence applications.

Methodological Approach for the Critical Analytical Review

1. Review Design and Analytical Perspective

This study adopts a critical analytical review methodology to examine and synthesize modelling approaches used to predict the mechanical and electromagnetic performance of graphene-reinforced carbon fibre composites. Unlike traditional systematic reviews that mainly summarize experimental findings, this study focuses on analysing modelling frameworks, theoretical approaches, and computational strategies reported in the literature.

The review emphasizes predictive modelling methodologies used to simulate composite behaviour, particularly models addressing impact resistance, mechanical performance, and electromagnetic interference (EMI) shielding in graphene-enhanced carbon fibre polymer composites. Priority is therefore given to studies that present modelling frameworks capable of linking nanoscale material interactions with macroscopic composite behaviour.

This analytical approach enables identification of conceptual similarities, modelling limitations, and methodological gaps across predictive frameworks. By synthesizing these modelling approaches, the study aims to clarify how current models represent the multifunctional behaviour of graphene-reinforced composite systems.

2. Analytical Scope of the Review

The analytical scope of this review focuses on predictive modelling approaches developed for graphene-reinforced carbon fibre polymer composites. Although extensive research exists on the experimental synthesis and characterization of graphene-based composites, the present review concentrates specifically on studies employing computational, analytical, or theoretical modelling frameworks to evaluate composite performance.

Within this scope, modelling approaches addressing key performance domains are considered, including mechanical behaviour, impact resistance, electrical conductivity, and electromagnetic interference shielding effectiveness. These properties are particularly relevant for multifunctional composite materials used in aerospace, automotive, and defence applications.

The review therefore includes studies applying modelling techniques such as micromechanical modelling, finite element simulations, multiscale modelling frameworks, and data-driven predictive approaches. These strategies provide insight into composite behaviour across multiple length scales, from nanoscale reinforcement mechanisms to macroscopic structural performance. Studies focused solely on experimental characterization without modelling components fall outside the primary scope of this review.

3. Literature Identification Strategy

Relevant literature was identified through structured searches of major scientific databases containing peer-reviewed research in materials science, nanotechnology, and composite engineering. The primary databases used included Scopus, Web of Science, ScienceDirect, IEEE Xplore, and SpringerLink.

To ensure comprehensive coverage, the search employed combinations of keywords related to graphene composites and predictive modelling. Key terms included graphene-reinforced carbon fibre composites, graphene nanoplatelet polymer composites modelling, multiscale modelling of graphene composites, finite element modelling of graphene nanocomposites, and electromagnetic interference shielding modelling. These keywords were applied individually and in combination across the selected databases.

The search primarily targeted publications from the past decade to capture recent developments in graphene-based composites and modelling techniques. The resulting studies were screened to identify publications specifically addressing predictive modelling or computational analysis of graphene-reinforced composite systems. Relevant studies were then selected for detailed examination in the analytical sections of this review.

4. Model Classification Framework

To enable systematic analysis, modelling approaches identified in the reviewed studies were organized into a conceptual classification framework based on modelling scale and analytical methodology. This framework allows different modelling strategies to be evaluated according to their theoretical foundations and predictive capabilities.

The primary modelling categories considered in this review include:

a. Micromechanical models, which analyze interactions between reinforcement particles, polymer matrices, and fibre structures to estimate effective composite properties.
b. Finite element models (FEM), which simulate structural behaviour under mechanical loading conditions such as stress distribution, deformation, and impact response.
c. Multiscale modelling frameworks, which integrate simulations across multiple length scales to link nanoscale graphene behaviour with macroscopic composite performance.
d. Electromagnetic modelling approaches, which predict electrical conductivity networks and electromagnetic shielding behaviour in conductive composites.
e. Data-driven and machine learning models, which use large datasets of material parameters to predict multifunctional composite properties.

This classification framework provides a structured basis for comparing modelling approaches reported in different studies.

5. Model Evaluation Criteria

To evaluate the predictive modelling approaches identified in the literature, a set of analytical evaluation criteria was established. These criteria allow different modelling frameworks to be compared in terms of their ability to represent the complex behaviour of graphene-reinforced composite materials.

The main evaluation criteria include:

a. Predictive capability, referring to the ability of a model to accurately predict mechanical or electromagnetic performance.
b. Scale of modelling, indicating whether the model operates at nanoscale, microscale, or macroscale levels.
c. Multiphysics integration, referring to the ability to incorporate multiple physical phenomena such as mechanical behaviour, electrical conductivity, and electromagnetic attenuation.
d. Computational complexity, reflecting the computational resources required to implement the modelling approach.

e. Applicability to multifunctional composites, indicating the extent to which the model can simultaneously address structural and electromagnetic performance.

These criteria provide a consistent analytical basis for comparing modelling frameworks across different studies.

6. Analytical Synthesis Process

Following literature identification and model classification, the selected studies were analyzed through a structured synthesis process designed to identify methodological trends and relationships across the literature.

The synthesis involved three main stages. First, model characterization examined each study to identify the modelling methodology, scale of analysis, and composite properties predicted. Second, comparative model evaluation compared modelling frameworks across studies to identify similarities and differences in modelling assumptions and predictive capabilities. Finally, identification of research trends and gaps highlighted emerging directions and limitations in current predictive modelling approaches.

This structured synthesis enables a comprehensive understanding of the modelling landscape for graphene-reinforced composite materials.

7. Limitations of the Review

Although this review provides a structured analysis of predictive modelling approaches for graphene-reinforced composites, several limitations should be noted.

First, the analysis relies on published academic literature and may not capture modelling developments reported in industrial or proprietary engineering studies. Second, variations in modelling assumptions, material systems, and simulation conditions across studies may introduce variability when comparing modelling frameworks. Finally, the rapidly evolving nature of graphene-based composite research means that new modelling techniques may emerge beyond the scope of the literature reviewed.

Despite these limitations, this study provides a comprehensive analytical overview of existing modelling frameworks and highlights important directions for future research in predictive modelling of multifunctional composite materials.

Results and Discussion

Based on the analytical methodology described in the previous section, this section critically examines the major modelling frameworks used to predict the mechanical and electromagnetic performance of graphene-reinforced carbon fibre polymer (G-CFRP) composites. The discussion focuses on computational strategies for predicting impact resistance, modelling electromagnetic interference (EMI) shielding behaviour, multiphysics simulations, and emerging data-driven approaches. By comparing the capabilities, limitations, and applicability of these modelling techniques, the section provides an analytical overview of current predictive frameworks and their relevance for designing multifunctional composite materials.

1. Modelling Approaches for Predicting Impact Resistance

Predicting the impact resistance of graphene-reinforced carbon fibre polymer (G-CFRP) composites is complex because damage mechanisms occur across multiple length scales. Impact loading can generate matrix cracking, fibre fracture, delamination, and interfacial debonding that evolve simultaneously within composite structures.

Consequently, computational modelling techniques are widely used to analyze the structural behaviour of graphene-enhanced composites under impact conditions (Hadden et al., 2015 [14]; Pontefisso & Mishnaevsky Jr., 2016) [30].

Finite element modelling (FEM) is among the most widely applied approaches for analysing impact behaviour in graphene-reinforced composites. FEM allows detailed simulation of stress distribution, deformation, and damage evolution in multilayer composite laminates. Numerical investigations indicate that incorporating graphene nanoplatelets into polymer matrices improves stiffness, energy absorption capacity, and structural stability of carbon fibre composites. For instance, finite element simulations show that increasing graphene volume fraction enhances natural frequencies and stiffness of composite plates, suggesting improved resistance to deformation under dynamic loading (Georgantzinos *et al*., 2020) [11].

Advanced FEM-based methods have also been applied at smaller structural scales.

Representative volume element (RVE) modelling has demonstrated that graphene monolayers embedded in polymer matrices strengthen the fibre-matrix interphase, thereby improving stiffness and reducing deformation under impact loading (Papa, 2025) [27].

In addition to FEM approaches, multiscale modelling frameworks have been developed to capture reinforcement mechanisms across different length scales. These frameworks integrate molecular-level simulations with micromechanical and continuum models to describe how nanoscale reinforcement influences macroscopic composite behaviour (Odegard *et al*., 2005; Liu & Kumar, 2012) [20, 26].

Hierarchical multiscale modelling combining molecular dynamics and micromechanical analysis has shown that graphene nanoplatelets dispersed in epoxy matrices can enhance transverse mechanical properties of carbon fibre composites (Hadden *et al*., 2015) [14]. Similarly, reactive force-field simulations have been used to analyze interactions between graphene nanoplatelets and polymer matrices in hybrid composite systems (Al Mahmud *et al*., 2019) [1].

Several studies have also investigated the role of graphene-reinforced interphase regions in composite mechanical performance. Multiscale and micromechanical analysis indicate that graphene nanoplatelets embedded within the fibre–matrix interphase improve stress transfer efficiency and increase composite stiffness (Le *et al*., 2019).

Micromechanical modelling further shows that nanoscale morphology and dispersion of graphene fillers strongly influence crack propagation behaviour and damage resistance in polymer nanocomposites (Pontefisso & Mishnaevsky Jr., 2016; Odegard *et al*., 2005) [26, 30].

Despite these advances, challenges remain in accurately predicting impact resistance of graphene-reinforced composites. Many models assume ideal graphene dispersion and homogeneous material behaviour, whereas real composite systems often exhibit filler agglomeration and variability in interfacial bonding. Additionally, multiscale modelling approaches can be computationally demanding, which may limit their application in largescale structural simulations (Suresh Babu & Mourad, 2021) [38].

A summary of the major modelling approaches used for predicting impact resistance in graphene-reinforced CFRP composites is presented in Table 1, highlighting the modelling techniques, key parameters considered, and reported limitations.

Table 1: Summary of Modelling Approaches for Predicting Impact Resistance in Graphene-Reinforced CFRP Composites

Modelling Method	Composite System	Parameters Considered	Major Findings	Limitations	Reference
Multiscale modelling	GNP/CFRP hybrid composites	Interphase, graphene stiffness, load transfer, dispersion	Improved strength, transverse stiffness, and load transfer	High computational cost	Hadden *et al*., 2015 [14]
Reactive force-field multiscale modelling	Graphene-epoxy nanocomposites	Interfacial bonding, nanoscale load transfer, graphene distribution	Enhanced mechanical reinforcement and improved interfacial load transfer	Computationally intensive simulations	Al Mahmud *et al*., 2019 [1]
Finite Element Modelling (FEM)	Graphene-reinforced CFRP laminates	Natural frequency, stiffness, deformation,	Increased stiffness and dynamic stability	Limited nanoscale representation	Georgantzinos *et al*., 2020 [11]
		dynamic stability	with reduced deformation		
Finite Element impact modelling	Graphene nanocomposite plates	Impact load, deformation behaviour	Improved impact resistance and reduced deformation	Simplified microstructural assumptions	Papa, 2025 [27]
Micromechanical modelling	Graphene-polymer nanocomposites	Crack propagation, stress transfer, fracture behaviour	Improved fracture resistance and prediction of structural behaviour	Limited macro-scale structural prediction	Pontefisso & Mishnaevsky Jr., 2016 [30]

While the modelling approaches discussed above primarily focus on predicting the mechanical behaviour of graphene-reinforced composites under impact loading, similar computational strategies have also been developed to analyze their electromagnetic shielding performance.

2. Modelling Approaches for Predicting EMI Shielding

In addition to mechanical reinforcement, graphene-enhanced composite materials have attracted significant attention for electromagnetic interference (EMI) shielding applications. EMI shielding refers to the ability of a material to attenuate electromagnetic radiation and protect electronic components from interference. Graphene nanoplatelets possess high electrical conductivity and large surface area, enabling the formation of conductive networks within polymer matrices that enhance electromagnetic attenuation (Chhetri & Kuila, 2024; Shen *et al*., 2014) [6, 35].

The shielding performance of composite materials is generally governed by three mechanisms: reflection, absorption, and multiple internal scattering of electromagnetic waves. Reflection occurs due to impedance mismatch between the shielding material and incident electromagnetic waves, while absorption results from dielectric and conductive losses within the material. Multiple internal scattering further enhances attenuation

Table 2: Analytical Models Used for Predicting EMI Shielding in Graphene-Based Composites

Model Type	Theoretical Basis	Graphene Composites	Key Parameters Considered	Limitations	Reference
Transmission Line Model (TLM)	Electromagnetic wave propagation through conductive materials	Graphene-based conductive composite materials	Electrical conductivity, conductive thickness, frequency	Simplified assumptions regarding homogeneous material behaviour	Rachidi & Tkachenko, 2008 [33]
Percolation Theory Model	Formation of conductive networks above a critical threshold	Graphene/polymer nanocomposites	Filler volume fraction, filler conductivity, filler dispersion, connectivity	Sensitive to conductive filler dispersion and connectivity	Xu *et al*., 2013
Effective Medium Theory (EMT)	Estimation of effective dielectric and electrical properties	Graphene–polymer composites	Dielectric constant, filler conductivity, filler concentration, matrix properties	Limited accuracy at high filler concentrations	Nayak *et al*., 2023 [24]
Electromagnetic Numerical Simulation Models	Numerical solution of Maxwell's equations	Graphene-based composite structures	Frequency range, dielectric properties, electrical conductivity	Computationally demanding for complex structures	Pittella *et al*., 2022 [29]; Shen *et al*., 2014; Zeng *et al*., 2016 [35, 40]
EMI Shielding Mechanism Models	Theoretical analysis of reflection, absorption, and multiple scattering of electromagnetic waves	Graphene-based EMI shielding composites	Electrical conductivity, shielding thickness, reflection, absorption, scattering	Limited predictive capability without numerical electromagnetic modelling	Kondawar & Modak, 2020; Shen *et al*., 2014; Zeng *et al*., 2016 [17, 35, 40]

Through repeated reflections within the composite structure (Kondawar & Modak, 2020) [17].

Various analytical and computational models have been developed to evaluate EMI shielding behaviour in graphene-based composites (Shen *et al*., 2014; Zeng et al., 2016; Chhetri & Kuila, 2024) [6, 35, 40]. One commonly used approach is transmission line theory, which treats composite materials as electromagnetic transmission media and estimates shielding effectiveness based on wave propagation characteristics (Rachidi & Tkachenko, 2008) [33].

Recent studies combining microwave characterization with electromagnetic simulations have provided further insight into shielding mechanisms in graphene-reinforced composites. For example, modelling investigations have shown that increasing graphene nanoplatelet concentration improves dielectric properties and enhances electromagnetic attenuation in polymer composites (Pittella *et al*., 2022) [29].

Percolation theory is another widely used framework for analysing EMI shielding performance. This theory describes the formation of conductive filler networks within composite matrices, where electrical conductivity increases sharply once the filler concentration exceeds the percolation threshold (Xu *et al*., 2013) [39]. In addition, effective medium theory (EMT) has been applied to estimate the effective dielectric and electrical properties of composites by considering the combined contribution of polymer matrices and conductive graphene fillers (Nayak *et al*., 2023) [24].

Despite these advances, accurately predicting EMI shielding performance remains challenging. Many models assume uniform dispersion of graphene fillers within polymer matrices, whereas real composite systems often exhibit heterogeneous microstructures and agglomeration of conductive fillers. Furthermore, most electromagnetic modelling approaches focus primarily on electrical behaviour and rarely incorporate mechanical effects such as structural deformation or damage, which may influence conductive network formation.

The principal theoretical and computational approaches used for modelling EMI shielding behaviour in graphene-based composites are summarized in **Table 2**.

3. Multiphysics Modelling of Graphene-CFRP Composites

Although mechanical and electromagnetic behaviours are often studied independently, graphene-reinforced composites exhibit strong coupling between structural and electrical properties. This multifunctional behaviour arises from interactions between mechanical reinforcement mechanisms and electrically conductive graphene networks, which has motivated the development of multiphysics modelling approaches.

Coupled mechanical–electrical modelling frameworks have been developed to investigate how mechanical deformation influences electrical conductivity in graphene-reinforced composite materials. Multiscale modelling studies indicate that mechanical loading can modify conductive graphene networks within polymer matrices, thereby affecting electrical conductivity and electromagnetic shielding effectiveness (Al Mahmud *et al*., 2019; Hadden *et al*., 2015) [1, 14]. These findings highlight the strong interdependence between structural and electrical behaviour in graphene-enhanced composites.

Electromagnetic–structural modelling approaches further extend this concept by integrating electromagnetic field analysis with structural mechanics simulations. Finite element modelling techniques have been applied to analyze vibration behaviour and structural response of graphene-reinforced composite laminates under mechanical loading. Numerical studies demonstrate that graphene inclusions enhance both structural stiffness and dynamic response of carbon fibre composite structures, indicating their potential for multifunctional structural applications (Georgantzinos et al., 2020) [11].

Overall, multiphysics modelling frameworks that combine mechanical, electrical, and electromagnetic simulations provide a more comprehensive representation of graphenereinforced composite behaviour. However, these integrated approaches remain computationally demanding and often rely on simplified assumptions regarding graphene dispersion and interfacial bonding. Key multiphysics modelling strategies and their applications in graphene-reinforced composite systems are summarized in Table 3.

Table 3: Multiphysics Modelling Strategies for Graphene-Reinforced Composite Materials

Modelling Scale	Phenomena	Method Used	Key Outcomes	Reference
Multiscale (nano–micro)	Mechanical reinforcement and coupled nanoscale interactions	Molecular dynamics + micromechanics	Enhanced transverse mechanical properties of CFRP composites	Hadden *et al*., 2015 [14]
Multiscale (nano–macro)	Mechanical behaviour and interfacial bonding	Reactive force-field simulations	Improved load transfer between graphene and polymer matrix	Al Mahmud *et al*., 2019 [1]
Macroscale	Structural vibration and mechanical behaviour	Finite Element Modelling (FEM)	Increased stiffness and improved dynamic response of composite laminates	Georgantzinos *et al*., 2020 [11]
Electromagnetic modelling	Electrical conductivity and dielectric behaviour	Microwave characterization and EM simulations	Improved electromagnetic and shielding behaviour in graphene composites	Pittella *et al*., 2022 [29]

4. Emerging Data-Driven Prediction Models

Recent advances in artificial intelligence and data science have created new opportunities for predicting the performance of advanced composite materials. Traditional modelling approaches such as finite element analysis and multiscale simulations often require significant computational resources and detailed material parameters. In contrast, data-driven modelling techniques use statistical learning algorithms to identify relationships between material composition and performance characteristics.

Machine learning algorithms are increasingly applied in materials science to analyze complex composite systems. These approaches can process large datasets of material parameters and identify patterns that influence mechanical, electrical, and thermal properties (Morgan & Jacobs, 2020; Butler *et al*., 2018) [4, 23]. Recent studies demonstrate the potential of machine learning techniques for optimizing multifunctional composite systems. For instance, machine learningassisted modelling frameworks have been used to identify optimal material formulations that balance multiple performance requirements in complex composite materials (Guo *et al*., 2025) [13].

Artificial intelligence-based prediction frameworks can also integrate data from computational simulations and experimental studies, enabling improved prediction of material behaviour. Technology forecasting research suggests that data-driven approaches will play an increasingly important role in the development of next-generation multifunctional composite materials (Huang, 2021) [15]. However, these models have limitations because they require large datasets for training and often provide limited insight into the underlying physical mechanisms governing material behaviour.

The relationships among multiscale modelling, multiphysics simulations, and data-driven prediction approaches are conceptually illustrated in Figure 1, which presents an integrated framework for predicting the multifunctional performance of graphene-reinforced composite systems.

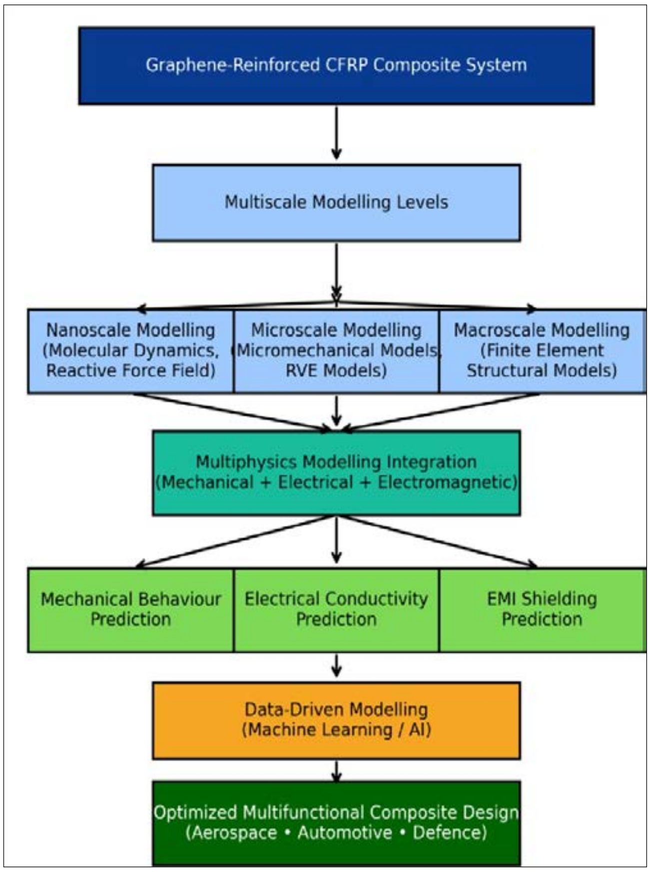

Fig 1: Conceptual framework illustrating predictive modelling approaches for graphenereinforced carbon fibre polymer composites, integrating multiscale modelling, multiphysics simulations, and data-driven prediction methods for multifunctional composite design.

5. Comparative Evaluation of Modelling Frameworks

The modelling approaches discussed in the previous sections demonstrate the wide range of computational strategies used to predict the multifunctional behaviour of graphene- reinforced carbon fibre polymer composites. These frameworks differ in predictive capability, computational requirements, and applicability to industrial composite design.

Finite element modelling (FEM) is one of the most widely used approaches for analysing the structural behaviour of graphene-reinforced composites. FEM enables simulation of stress distribution, deformation behaviour, and vibration characteristics in composite structures. Studies have shown that graphene inclusions within polymer matrices improve stiffness and dynamic response of composite laminates (Georgantzinos *et al*., 2020) [11]. Similarly, FEM simulations of graphene-reinforced nanocomposites indicate improved impact resistance due to enhanced load transfer within the composite structure (Papa, 2025) [27].

Multiscale modelling represents another important framework that links nanoscale reinforcement mechanisms with macroscopic structural performance. These approaches combine molecular dynamics simulations, micromechanical modelling, and continuum analysis. Previous studies have shown that graphene dispersion and interfacial bonding strongly influence the transverse mechanical properties of hybrid composite systems (Hadden *et al*., 2015; Al Mahmud *et al*., 2019) [1, 14]. Micromechanical models also provide insight into effective material properties and crack propagation mechanisms in nanocomposites (Pontefisso & Mishnaevsky Jr., 2016) [30].

For predicting electromagnetic interference shielding behaviour, analytical and computational electromagnetic modelling techniques are commonly applied. Microwave modelling studies demonstrate that graphene nanoplatelet concentration significantly affects dielectric properties and shielding effectiveness of polymer composites (Pittella *et al*., 2022) [29]. In addition, data-driven modelling approaches have emerged as promising tools for predicting material behaviour in complex composite systems by identifying correlations between material composition and performance characteristics (Guo *et al*., 2025; Morgan & Jacobs, 2020) [13, 23].

A comparative summary of the major modelling frameworks, including their predictive capabilities, computational requirements, and industrial applicability, is presented in Table 4.

Table 4: Comparative Evaluation of Modelling Frameworks for Graphene-Reinforced CFRP Composites

Modelling Approach	Scale of Analysis	Predictive Accuracy	Computational Cost	Ability to Analyse EMI Shielding	Industrial Applicability	Reference
Micromechanical models	Microscale	Moderate	Low	Limited	Moderate	Pontefisso & Mishnaevsky Jr., 2016 [30]
Finite Element Modelling (FEM)	Macroscale	High	Medium–High	Limited	High	Georgantzinos *et al*., 2020 [11]; Papa, 2025
Multiscale modelling	Nano–macro scale	Very high	Very high	Moderate	Limited due to modelling complexity	Hadden *et al*., 2015 [14]; Al Mahmud *et al*., 2019
Electromagnetic modelling	Macroscale	High for EMI prediction	Medium	High	Moderate	Pittella *et al*., 2022 [29]
Data-driven / Machine Learning models	Emerging multi-scale	High (data-dependent)	Low–Medium	Potentially high	Potentially high	Guo *et al*., 2025; Morgan & Jacobs, 2020; Butler *et al*., 2018 [4, 13, 23]; Raccuglia et al., 2016

Building on this comparison, a critical assessment highlights clear differences in predictive capability and practical applicability among modelling frameworks. Finite element models provide accurate structural predictions at the macroscale but often depend on experimentally derived parameters and simplified microstructural assumptions.

Multiscale modelling offers deeper insight into graphene–matrix interactions and interfacial mechanics but requires substantial computational resources and complex parameter calibration (Hadden *et al*., 2015; Al Mahmud *et al*., 2019) [1, 14]. In contrast, micromechanical models efficiently estimate effective material properties but are limited in representing complex structural loading conditions.

Electromagnetic modelling techniques, including transmission line and percolation-based models, are effective for predicting EMI shielding behaviour in graphene-based composites. However, these approaches typically treat electrical and mechanical behaviour independently and therefore cannot fully capture the coupled multiphysics response of multifunctional composites (Pittella *et al*., 2022) [29]. More recently, machine learning-based frameworks have shown potential for accelerating composite design by identifying relationships between material parameters and performance outcomes, although their reliability depends strongly on the availability of high-quality datasets (Guo *et al*., 2025; Morgan & Jacobs, 2020) [13, 23].

Overall, no single modelling framework can fully capture the complex multiphysics behaviour of graphene-reinforced composite systems. Hybrid modelling strategies that integrate multiscale simulations, structural modelling, electromagnetic analysis, and data-driven prediction techniques are therefore likely to provide the most effective approach for predicting multifunctional composite performance. This evaluation also highlights the modelling challenges and research opportunities discussed in the following section.

6. Key Modelling Challenges and Research Opportunities

Despite significant advances in predictive modelling of graphene-reinforced composites, several challenges remain in accurately simulating their multifunctional behaviour. A major limitation of current frameworks is the absence of integrated models capable of simultaneously predicting mechanical, electrical, and electromagnetic properties. Most existing approaches address individual performance aspects, such as structural response or electromagnetic shielding, rather than capturing the coupled multiphysics interactions occurring in graphene-reinforced composite systems.

Another key challenge is the limited integration of multiscale modelling techniques within structural simulation frameworks. Previous studies have demonstrated that graphene dispersion and interfacial bonding strongly influence composite mechanical properties (Hadden *et al*., 2015; Al Mahmud *et al*., 2021) [2, 14]. However, translating nanoscale insights into reliable macroscale predictive models suitable for engineering-scale simulations remains difficult.

Bridging this gap between nanoscale material behaviour and macroscopic structural performance therefore represents an important research direction.

A further limitation is the insufficient experimental validation of predictive models. Many computational studies assume ideal graphene dispersion and homogeneous material behaviour, whereas real composite systems often exhibit agglomeration of graphene nanoplatelets and variability in interfacial bonding conditions. These microstructural variations can significantly influence both mechanical performance and electromagnetic shielding effectiveness, emphasizing the need for stronger experimental validation of modelling predictions.

Recent advances in artificial intelligence and data-driven modelling provide promising opportunities to address these challenges. Machine learning algorithms can analyze large datasets and identify complex relationships between material composition, microstructural parameters, and performance characteristics. Such approaches may accelerate the discovery and optimization of multifunctional composite materials by enabling rapid exploration of large design spaces (Guo *et al*., 2025; Raccuglia *et al*., 2016) [13, 32].

Future research is therefore likely to focus on hybrid modelling frameworks that integrate physicsbased simulations with machine learning techniques. These approaches can combine the mechanistic understanding of physics-based models with the predictive efficiency of data-driven algorithms, enabling more accurate prediction of the behaviour of advanced multifunctional composite materials.

Conclusion

1. Summary of Key Findings

This study presented a critical analytical review of predictive modelling frameworks used to evaluate the mechanical and electromagnetic performance of graphene-reinforced carbon fibre polymer (G-CFRP) composites. The review identified several modelling approaches applied across different length scales, including micromechanical models, finite element simulations, multiscale modelling frameworks, electromagnetic modelling techniques, and emerging datadriven prediction methods.

Micromechanical modelling provides insight into interactions between reinforcement phases and polymer matrices and enables estimation of effective material properties in graphene- based nanocomposites (Pontefisso & Mishnaevsky Jr., 2016) [30]. Finite element modelling (FEM) is widely used to simulate structural behaviour of composite materials under mechanical loading conditions such as impact and vibration (Georgantzinos *et al*., 2020; Papa, 2025) [11, 27]. Multiscale modelling frameworks extend these capabilities by linking nanoscale reinforcement mechanisms of graphene nanoplatelets with macroscopic composite behaviour (Hadden *et al*., 2015; Al Mahmud *et al*., 2019) [1, 14].

Electromagnetic modelling approaches are commonly used to predict shielding effectiveness using analytical frameworks such as transmission line theory, percolation theory, and effective medium models (Xu *et al*., 2013; Nayak *et al*., 2023) [24]. In addition, data-driven techniques, including machine learning algorithms, show potential for accelerating the design and optimization of multifunctional composite materials (Guo *et al*., 2025; Morgan & Jacobs, 2020) [13, 23].

Despite these advances, many modelling approaches focus on individual material properties rather than capturing the coupled multiphysics behaviour of multifunctional composites. Furthermore, multiscale models often require significant computational resources, while datadriven models depend on the availability of large datasets. These limitations highlight the need for integrated modelling frameworks capable of simultaneously predicting structural and functional performance in graphene-reinforced composite systems.

2. Implications for Composite Material Design

The findings of this review have important implications for the development of multifunctional composite materials used in aerospace, automotive, and defence applications. In these sectors, structural materials must provide lightweight efficiency, impact resistance, and electromagnetic interference protection simultaneously.

Predictive modelling tools enable engineers to evaluate material configurations and reinforcement strategies before physical manufacturing, thereby reducing development time and experimental cost. Finite element simulations and multiscale modelling techniques can be applied to analyze stress distribution, crack propagation, and energy absorption behaviour in graphene-enhanced composite structures (Hadden *et al*., 2015; Georgantzinos *et al*., 2020) [11, 14]. Similarly, electromagnetic modelling approaches allow prediction of shielding effectiveness and conductive network formation in graphene-based composites (Pittella *et al*., 2022; Chhetri & Kuila, 2024) [6, 29].

Integrating predictive modelling tools into composite design workflows therefore improves the efficiency of developing advanced lightweight structures for high-performance engineering applications.

3. Conceptual Framework for Integrated Composite Performance

Prediction based on the critical evaluation of existing modelling approaches, this study proposes a conceptual framework for predicting multifunctional performance in graphene-reinforced carbon fibre composites. The framework, illustrated in Figure 1, integrates multiple modelling strategies to capture relationships between material parameters, structural behaviour, and electromagnetic performance.

The framework begins with key input parameters defining the composite system, including graphene concentration, fibre orientation, matrix type, and laminate architecture. These parameters influence both mechanical behaviour and electrical conductivity of graphenereinforced composites (Hadden *et al*., 2015; Al Mahmud *et al*., 2019) [1, 14].

Material behaviour is then analyzed using mechanical, electrical, and electromagnetic modelling approaches implemented through computational tools such as finite element structural analysis, electromagnetic simulations, and artificial intelligence-based prediction models. Finite element simulations enable evaluation of structural response under mechanical loading, while electromagnetic simulations provide insight into shielding effectiveness across different frequency ranges (Pittella *et al*., 2022) [29]. Machine learning models further enhance predictive capability by identifying relationships between material parameters and composite performance (Guo *et al*., 2025) [13].

By integrating these modelling approaches, the proposed framework enables prediction of key performance outcomes, including impact resistance, EMI shielding effectiveness, and structural efficiency of graphene-reinforced composite systems.

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