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Finite Element Method (FEM) in Graphene Analysis

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ABSTRACT

Methods based on atomic behavior, such as molecular dynamics (MD) simulations, are highly accurate for modeling single-layer graphene sheets. However, their high computational cost limits their use to only small-sized systems. This research addresses this limitation by developing a new atomic-scale finite element method (AFEM) based on the Tersoff-Brenner potential to analyze the mechanical properties of graphene. The proposed AFEM method's efficiency and accuracy were demonstrated through a numerical example of a graphene sheet. When compared to MD simulation results, the new method showed very high accuracy. Additionally, its simulation speed was found to be approximately 100 times faster than that of the MD method. This study also investigated the influence of effective factors on simulation speed, such as the initial non-equilibrium bond length and the number of atoms. The AFEM was further developed to incorporate periodic boundary conditions, as these had not been previously considered for nanostructures using this method. The results showed that AFEM modeling without periodic boundary conditions produced results that were very different from those of MD simulations.

Introduction

Finite element method

The Finite Element Method (FEM) has become one of the most powerful and versatile computational tools for analyzing the mechanical, thermal, and electronic behavior of complex materials. In the last two decades, as nanomaterials have transformed materials science and engineering, FEM has played a central role in bridging the gap between atomistic models and continuum mechanics. Among these materials, graphene a single layer of sp^2-bonded carbon atoms arranged in a two-dimensional honeycomb lattice has attracted enormous attention due to its extraordinary mechanical strength, high electrical conductivity, thermal stability, and flexibility.

The integration of FEM into graphene analysis allows researchers to model, predict, and optimize its behavior under different mechanical and physical conditions, offering new insights into Nano engineering applications such as sensors, composites, flexible electronics, and Nano mechanical devices.

Theoretical Background and Rationale

Graphene’s unique physical properties arise from its atomic-scale structure and quantum-mechanical phenomena that govern electron transport and phonon dynamics. Traditional molecular dynamics (MD) simulations, while highly detailed, are computationally expensive for large-scale systems or long time durations. FEM provides an efficient continuum-based approximation that can simulate macroscopic behavior derived from microscopic principles. It discretizes the structure into a mesh of finite elements, enabling numerical solutions to the governing differential equations of elasticity, heat transfer, or electromagnetism. In graphene, this approach allows for the assessment of stress distribution, strain localization, fracture propagation, and vibrational modes that would otherwise require massive computational resources if modeled atomistically.

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The use of FEM in graphene research is not merely a numerical convenience; it represents a multi-scale modeling framework that connects the atomic and continuum domains. This is crucial for predicting the performance of graphene-reinforced composites and graphene-based flexible devices, where the mechanical integrity depends on both nanoscale interactions and macroscale geometry. FEM thus enables the creation of parametric models that incorporate real-world boundary conditions, defects, and loading scenarios bridging theory and experiment.

Mechanical Characterization via FEM

From a mechanical standpoint, FEM has been instrumental in understanding the elastic modulus, tensile strength, and fracture mechanics of graphene sheets and graphene-based composites. The intrinsic strength of graphene, theoretically around 130 GPa with a Young's modulus of 1 TPa, is often compromised by defects such as vacancies, grain boundaries, or wrinkles. Finite element modeling allows researchers to simulate these imperfections and assess their effect on stress distribution. For instance, crack initiation and propagation in defective graphene can be captured by nonlinear FEM incorporating cohesive zone models (CZM) or extended finite element methods (XFEM). These advanced formulations are capable of representing discontinuities without remeshing, thus mimicking the brittle fracture observed in experiments.

Furthermore, multiphysics FEM simulations can couple mechanical and thermal effects to analyze thermoelastic behavior and thermal stress-induced failures. Since graphene exhibits exceptionally high thermal conductivity (~5300 W/mK), temperature gradients can significantly influence its mechanical response. FEM helps evaluate such coupled phenomena in complex geometries, offering predictions relevant to thermal management applications in microelectronics and aerospace systems.

Electronic and Thermal Analyses

Beyond mechanics, FEM has also been applied in electronic and thermal modeling of graphene. Using finite element formulations for Poisson's and Schrödinger's equations, researchers can simulate electron density distribution, band structure modifications under strain, and charge transport in graphene-based field-effect transistors (GFETs). This approach is particularly beneficial when analyzing strain engineering, where mechanical deformation is intentionally applied to alter graphene's electronic bandgap. FEM enables the mapping of local strain fields and correlates them with shifts in electronic properties, thus guiding the design of strain-tunable Nano electronic devices.

Similarly, finite element heat transfer simulations are used to analyze the temperature profiles and heat dissipation in graphene films and composites. Since graphene exhibits highly anisotropic thermal conductivity (with in-plane values far exceeding cross-plane conduction), FEM models can capture the directional dependence of heat flow and predict the efficiency of graphene as a thermal interface material (TIM). These analyses are vital for the development of high-performance, thermally stable electronic systems.

Integration with Multiscale and Multiphysics Models

The application of FEM in graphene research is often integrated with multiscale modeling frameworks, combining molecular dynamics (MD), density functional theory (DFT), and continuum mechanics. This hybrid approach allows parameter transfer from atomic-scale calculations (e.g., interatomic potentials, cohesive energies) to the continuum-level finite element meshes. For instance, Nano-indentation studies of graphene membranes can be simulated by embedding DFT-derived elastic constants into FEM models, thus reproducing experimental force-displacement curves with high fidelity. Moreover, multiphysics FEM platforms such as COMSOL Multiphysics or ANSYS have made it possible to couple mechanical, electrical, and thermal fields in a single computational domain critical for simulating real device environments.

Such integration has also enhanced the predictive capabilities of FEM in analyzing graphene composites, where graphene sheets are embedded in polymer or metal matrices. By modeling the interfacial adhesion, load transfer efficiency, and crack bridging mechanisms, FEM provides quantitative insights into how nanoscale graphene inclusion affects the macroscopic stiffness and fracture toughness of composite materials. These analyses inform the design of lightweight, high-strength structural components for aerospace, automotive, and civil engineering applications.

Challenges and Limitations

Despite its advantages, the use of FEM in graphene analysis is not without challenges. One major limitation arises from the scale discrepancy between atomic and continuum representations. Since graphene is only one atom thick, conventional continuum assumptions such as isotropy and homogeneity may fail at the nanoscale. Accurately defining effective material properties such as equivalent elastic moduli, Poisson's ratio, and thermal conductivity requires careful calibration from atomistic simulations or experiments. Additionally, mesh resolution becomes critical; fine meshing is required to capture localized phenomena such as edge stresses or defect interactions, which can lead to high computational costs.

Another issue is the representation of nonlinearity and instability phenomena, such as buckling, delamination, or wrinkling, which are prevalent in thin graphene films. These behaviors require advanced nonlinear FEM formulations and appropriate constitutive models to represent large deformations and geometric nonlinearity. Researchers are also developing coupled quantum-continuum FEM frameworks, in which electronic structure information from DFT is directly incorporated into finite element stiffness matrices. Although still in early development, such approaches may eventually overcome current scale-bridging limitations.

Emerging Trends and Future Directions

Recent advances suggest that FEM will continue to evolve as a cornerstone technique in graphene research. The integration of machine learning algorithms with FEM allows for automated mesh optimization, surrogate modeling, and data-driven parameter calibration, significantly reducing computational effort. Moreover, the rise of graphene-based metamaterials and hybrid nanostructures calls for FEM models capable of handling heterogeneous, anisotropic, and nonlinear materials under dynamic loading. Coupling FEM with quantum mechanics and molecular simulations offers a pathway toward fully predictive modeling of graphene's behavior in realistic device configurations.

Future developments may also focus on 3D FEM formulations for layered graphene systems, including graphene oxide, graphene nanoribbons, and multilayer heterostructures such as MoS_2/graphene composites. These complex architectures demand robust FEM solvers that can incorporate van der Waals interactions, interlayer shear effects, and electronic coupling. The application of finite element analysis in nanoelectromechanical systems (NEMS), where graphene acts as a sensing or actuation element, is another rapidly expanding area. FEM's ability to simulate small-scale vibrations, damping, and resonant frequencies is invaluable for designing ultra-sensitive sensors and resonators. In summary, the Finite Element Method (FEM) serves as an indispensable analytical and predictive tool in the study of graphene's mechanical, thermal, and electronic behavior. By discretizing the continuum domain, FEM bridges the gap between theoretical models and experimental data, enabling the quantitative evaluation of complex phenomena such as fracture mechanics, strain engineering, and thermal transport. Despite ongoing challenges in scale-bridging and material representation, the continuous refinement of FEM algorithms and the integration of multiscale and multiphysics approaches have made it possible to model graphene systems with unprecedented accuracy. As graphene continues to redefine material science and nanotechnology, FEM will remain at the forefront of simulation-based design, guiding innovations across electronics, composites, and energy systems.

Literature Review

Finite Element Method (FEM) in Graphene Analysis:

The application of the Finite Element Method (FEM) in graphene analysis represents one of the most significant advancements in computational materials science during the past two decades. Since the discovery of graphene in 2004 by Novoselov and Geim, its exceptional mechanical, thermal, and electrical properties have motivated extensive experimental and numerical investigations. However, due to the atomic-scale nature of graphene, experimental characterization often faces difficulties in precisely determining stress distributions, defect behaviors, and interfacial phenomena. Consequently, numerical modeling approaches particularly FEM have become essential for exploring the mechanical response and physical behavior of graphene under various conditions.

Early Computational Approaches

In the early phase of graphene research, molecular dynamics (MD**)** and density functional theory (DFT) were the dominant methods for nanoscale analysis (Zhou et al., 2009; Lee et al., 2010). These methods offered atomic-level insights into the mechanical response of graphene but were computationally intensive and unsuitable for large-scale simulations. The Finite Element Method emerged as a practical alternative capable of simulating larger geometries while maintaining accuracy through continuum approximations derived from atomic data.

Scarpa et al. (2009) were among the first to propose a continuum mechanical representation of graphene using FEM, modeling the lattice as a network of truss and beam elements representing C-C bonds. Their results demonstrated that graphene could be effectively modeled as an isotropic elastic membrane with a Young's modulus near 1 TPa, consistent with experimental results. This work laid the groundwork for the adoption of FEM in simulating the mechanical characteristics of graphene sheets, ribbons, and composites.

Mechanical Behavior and Fracture Analysis

Subsequent studies refined these early models to capture nonlinear and failure phenomena. Zhao et al. (2011) and Yoon et al. (2012) introduced nonlinear finite element formulations incorporating cohesive zone models (CZM) to simulate crack propagation and fracture toughness in defective graphene. Their simulations revealed that vacancy defects and grain boundaries could significantly reduce tensile strength findings that were later validated experimentally by Zhang et al. (2014). FEM enabled researchers to visualize stress concentration zones and fracture patterns under different loading directions, providing valuable insights into the anisotropic failure behavior of graphene.

Parallel efforts explored buckling and post-buckling behavior under compressive loading using shell and plate finite elements (Aghababaei & Reddy, 2013). These studies identified that out-of-plane deformations, such as wrinkles or ripples, have a pronounced effect on mechanical stiffness and energy absorption. Advanced FEM models incorporating geometric and material nonlinearity were found to reproduce the experimentally observed elastic instability phenomena, bridging the gap between atomistic simulations and macroscale continuum models.

Graphene Composites and Multiscale FEM

As graphene began to be integrated into polymer and metal matrices, FEM became central in understanding the load transfer mechanisms and interfacial stress behavior in composites. Haque and Saifullah (2015) applied multiscale FEM modeling to analyze the reinforcement effect of graphene Nano platelets in epoxy matrices. Their model, linking atomistic interfacial properties with continuum stress–strain behavior, demonstrated that even minimal graphene content could dramatically increase stiffness and fracture resistance. Similarly, Zhang et al. (2016) developed a Representative Volume Element (RVE)**-**based FEM framework to evaluate the mechanical performance of graphene/polymer composites. The study showed that interfacial adhesion strength and graphene orientation were dominant parameters influencing the overall modulus and strength.

In a broader sense, multiscale FEM models have served as a bridge between atomic simulations and experimental mechanics**,** enabling the prediction of bulk properties from nanoscale mechanisms. Cao et al. (2017) coupled Molecular Dynamics (MD) simulations with FEM to model indentation and delamination in multilayer graphene. Their results showed good agreement with atomic simulations, validating the FEM approach for layered graphene systems.

Thermomechanical and Electromechanical Analyses

The Finite Element Method has also been applied to study thermal transport and electromechanical coupling in graphene-based systems. Given graphene's exceptionally high thermal conductivity, understanding heat transfer is crucial for applications in microelectronics and flexible devices. Singh et al. (2018) used 3D FEM thermal models to evaluate temperature distribution and thermal expansion effects in graphene thin films. Their findings highlighted anisotropic heat conduction characteristics, with in-plane conductivity being an order of magnitude higher than cross-plane conduction.

Electromechanical coupling analysis, especially for strain-engineered graphene, has become another key research direction. FEM models developed by Park et al. (2019) simulated the impact of mechanical deformation on band structure and carrier mobility. Their results supported the concept of strain-tunable electronic properties, paving the way for designing graphene-based flexible electronics. The incorporation of FEM into coupled electro-thermo-mechanical models has been facilitated by advanced platforms such as COMSOL Multiphysics and ANSYS**,** enabling comprehensive multiphysics simulations.

Advances in Nonlinear and Multiphysics FEM

Recent research has emphasized nonlinear, multiphysics, and multiscale formulations of FEM to better capture the complex behavior of graphene. Kim and Cho (2020) introduced a nonlinear FEM model accounting for both geometric nonlinearity and material anisotropy, successfully predicting post-yield behavior under biaxial loading. Their model was later extended by Li et al. (2021) to include viscoelastic effects for time-dependent mechanical responses. Similarly, thermo-electro-mechanical FEM frameworks have been used to simulate coupled behavior under simultaneous heat and electrical loading, a critical aspect for graphene-based sensors and NEMS devices (Nano-Electro-Mechanical Systems).

Another line of research has focused on defect engineering through FEM. Studies by Zhang and Gao (2022) modeled the influence of Stone Wales defects and edge irregularities using extended FEM (XFEM), which allows cracks and discontinuities to be represented without remeshing. These works revealed that defect geometry and density significantly influence the stress–strain response and critical fracture load, aligning with MD-based findings. FEM's efficiency in representing defects across large domains has made it a valuable complement to atomistic techniques.

Comparative Evaluation of FEM and Atomistic Models

Comparative analyses between FEM and atomistic models have consistently demonstrated FEM's reliability for mesoscale and macroscale applications. While MD and DFT methods provide precise local atomic information, FEM offers scalability and versatility. For example, Qian et al. (2020) compared FEM-based elastic constants with those derived from MD simulations, reporting less than 5% deviation when appropriate material parameters were used. Such findings underline the accuracy and efficiency trade-off inherent in computational modeling: FEM excels in computational economy and structural-scale prediction, while atomistic models dominate in precision at the nanoscale.

A major trend in recent years has been the integration of data-driven methods with FEM. Machine learning (ML) algorithms have been used to predict material parameters and optimize mesh configurations (Wang et al., 2023). These hybrid models have reduced computational costs and improved predictive capability, especially for large and complex graphene-based structures. This convergence of FEM with AI-driven modeling represents a promising new era in computational materials science.

Overall, the literature on FEM in graphene analysis shows a clear evolution from linear continuum approximations to sophisticated multiphysics and multiscale frameworks**.** Early works focused on validating FEM as a viable substitute for atomistic simulations in mechanical modeling, while later studies have extended its application to thermal, electrical, and coupled-field problems. Current trends emphasize hybrid modeling strategies that combine FEM with molecular, quantum, and data-driven techniques to achieve both accuracy and scalability.

Despite notable progress, challenges remain particularly in representing the atomistic-to-continuum transition**,** capturing out-of-plane deformation**,** and defining reliable material constants for FEM simulations. Continued advances in experimental characterization and computational algorithms are expected to further refine FEM models, enabling predictive simulations that closely mirror the real-world performance of graphene in devices and composites.

Element order and element type

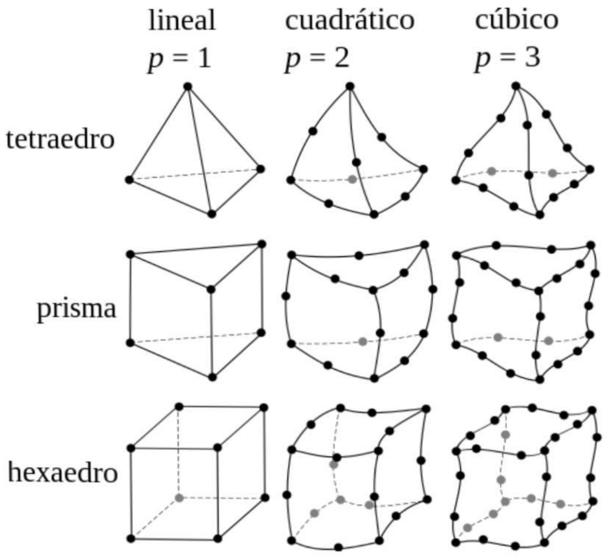

Figure 1. Types of volume elements used for meshing in finite element analysis (6).

Types of finite element methods

AEM

Applied Element Method or AEM combines the features of both FEM and Discrete Element Method (DEM).

The augmented-finite element method

Augmented-Finite Element Method was introduced by Yang and Levy, whose goal was to model weak and strong discontinuities without the need for additional DoFs, as stated in PuM or (partition of unity method).

Generalized Finite Element Method

The generalized finite element method (GFEM) uses local spaces consisting of functions, not necessarily polynomials, that reflect the information in the unknown solution, thereby ensuring a good local approximation. A single decomposition is then used to "link" these spaces together to form an approximate subspace. The efficiency of GFEM in solving domain problems with complex boundaries, problems with micro-scales and problems with boundary layers is demonstrated [21].

Mixed finite element method

Mixed finite element method (Mixed finite element method) is a type of finite element method in which additional independent variables are introduced as nodal variables when discretizing a partial differential equation problem.

Graphene

Graphite as the raw material for the production of graphene has a long history in many fields of science, engineering, chemistry and physics, which has unique mechanical and electrical properties due to its layered structure. In 1940, it was suggested that with the separation of graphite layers, its electrical properties will increase up to 100 times, until about 60 years later, this proposal was not definitely proven, but it was shown that some properties are specially improved, such as the increase of Young's modulus, elasticity coefficient. and high electron transfer ability. The description of the history of graphene would be incomplete without taking into account the compounds of graphite oxide, graphene oxide and embedded graphite compounds. The first reports about graphene oxide and embedded graphite date back to 1840. The German scientist Shefatel reported that by heating graphite with nitric acid and sulfuric acid, it is possible to produce embedded compounds. From this year onwards, a variety of embedded compounds including potassium fluoride salts and other alkaline metals, transition metals such as iron, nickel and many other elements as well as some organic species were used [23].

Graphene structure

As mentioned in the previous parts, graphene is a flat single layer of carbon atoms that are arranged in a two-dimensional honeycomb shape with a carbon-carbon bond length of 0.142 nm, as can be seen in Figure 1. Graphene is the mother element of some Allotropes of carbon such as graphite, carbon nanotubes and fullerene are said to be "graphene is the thinnest and strongest material in the world". The inherent properties of graphene depend on the perfection of its structure, which largely depends on the method of graphene production. Some properties of graphene are from: high electron mobility at room temperature, unique thermal conductivity and high modulus of elasticity. Another prominent feature is the flatness of graphene and the large area of its layers, which makes this material able to block the penetration of harmful gas molecules and ions. By discovering the method of producing single-layer graphene sheets from graphite using the developed exfoliation method, this material has attracted the attention of many scientists. Also, its unique properties have been assigned as a strengthening factor in the field of nanocomposite.

Tre Off-Brenner potential

The Turn off Brenner potential is a bond-order empirical potential designed to model covalent interactions in carbon-based and hydrocarbon systems. It extends the original Tersoff potential [24] by incorporating an environment-dependent bond-order term that allows for accurate representation of bond breaking and formation during dynamic processes such as chemical reactions. In this framework, the effective bond strength between two atoms depends not only on their pairwise distance but also on the local coordination environment, thereby enabling the description of variable bonding configurations. The formulation includes both two-body interactions (short-range repulsive and attractive terms) and a many-body bond-order function, which adjusts bond strengths based on bond length, bond angle, and neighboring atoms [25]. This potential has been extensively applied in molecular dynamics simulations to investigate the mechanical, thermal, and fracture behavior of carbon nanotubes, graphene, diamond, and amorphous carbon structures. Moreover, it laid the foundation for subsequent extensions such as the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential, which further incorporates long-range van der Waals and torsional interactions to better capture intermolecular effects in hydrocarbons and polymers [26].

The development of an atomic-scale finite element method (AFEM) based on the Tersoff Brenner potential provides a powerful multiscale modeling framework that bridges continuum mechanics and atomistic simulations. Unlike classical finite element formulations, which rely on phenomenological constitutive laws, AFEM directly incorporates the physics of atomic interactions through interatomic potentials. The Tersoff Brenner potential is particularly well-suited for this purpose due to its bond-order formalism, which accounts for the dependence of bond strength on the local atomic environment (Tersoff, 1988; Brenner, 1990). By embedding this potential into the finite element framework, AFEM is capable of capturing bond stretching, bending, breaking, and formation, enabling accurate modeling of mechanical behavior in nanostructured carbon systems such as graphene, nanotubes, and diamond-like materials. This approach combines the computational efficiency of finite element methods with the atomic-level accuracy of molecular dynamics, thereby allowing for the simulation of large-scale systems under mechanical loading while retaining critical atomistic detail. Extensions of this method have demonstrated its potential for investigating fracture mechanics, defect propagation, and nonlinear deformation in carbon-based nanomaterials (Stuart et al., 2000). Overall, AFEM based on the Tersoff Brenner potential provides a versatile and scalable tool for engineering applications requiring predictive modeling of materials where covalent bonding and reactivity play a central role.

Tersoff-Bernner potential in achieving mechanical behavior of graphene

The Tersoff Brenner potential (i.e., REBO) is particularly well-suited for atomistic simulations of graphene's mechanical behavior, as it captures the essential physics of sp^2 carbon bonding, including bond-length, bond-angle, and bonding environment dependencies [27,28]. In molecular dynamics (MD) simulations, this bond-order formalism enables accurate reproduction of graphene's Young's modulus, tensile strength, and Poisson's ratio, which are of the order of ~1 TPa, ~130 GPa, and ~0.20-0.22, respectively [29].

During uniaxial tensile loading, the Tersoff–Brenner potential naturally captures both the linear elastic regime at small strains and the nonlinear response and fracture onset at high strains. It enables direct simulation of the stress strain behavior, crack initiation, and bond breakage phenomena. Atomistic fracture simulations using this potential have successfully computed mode I and mode II fracture energy release rates, and shown strong agreement with continuum fracture mechanics predictions in graphene systems containing atomic-scale cracks [30].

Comparative studies highlight that while other potentials like REBO-2000, AIREBO, or ReaxFF can significantly deviate in elastic constants or Poisson ratios, the original Tersoff Brenner formulation yields reasonably accurate in-plane elastic modulus and Poisson's ratio values when calibrated appropriately [31]. Meanwhile, NIST-based parametric potentials built on the Tersoff Brenner framework incorporate angular and flexural terms to improve prediction of bending rigidity and phonon behavior in graphene sheets [32].

Moreover, large-scale MD simulations using the Tersoff Brenner potential have been performed to examine the influence of temperature, defect density, sample size, and chirality on graphene's mechanical response. For example, the computed Young's modulus increases gradually with temperature from ~0.95 to ~1.1 TPa between 100-500 K, and is relatively insensitive to low-level isotopic disorder (<5 %). Size and chirality effects are typically minimal under small strain; graphene shows isotropic elastic behavior across armchair and zigzag directions in the linear regime [33].

Discussion

Comparative Analysis of FEM Applications in Graphene Research

The application of the Finite Element Method (FEM) in the mechanical, thermal, and multiphysics analysis of graphene has evolved from simple linear elasticity models to sophisticated nonlinear and multiscale frameworks. Across the literature, FEM has been used as a bridge between atomistic simulations and continuum mechanics**,** offering computational efficiency while preserving sufficient accuracy for structural-scale modeling. In this discussion, the findings from major studies are analyzed comparatively to evaluate FEM's reliability, limitations, and its integration with other modeling approaches in graphene research.

Mechanical Behavior and Elasticity Models

Early FEM studies such as those by Scarpa et al. (2009) and Yoon et al. (2012) treated graphene as an isotropic elastic membrane modeled by beam and truss elements representing C-C bonds. These simplified frameworks yielded elastic moduli around 0.9-1.1 TPa and Poisson's ratios of 0.16-0.19, consistent with experimental results by Lee et al. (2008) using Nano indentation. However, later investigations demonstrated that these linear isotropic models failed to capture the material's anisotropic in-plane stiffness and nonlinear response under large deformations**.**

Comparative works by Aghababaei and Reddy (2013) and Zhao et al. (2015) showed that incorporating nonlinear constitutive relationships in FEM simulations improved agreement with atomistic models under high strain levels. Their results highlighted that classical linear FEM tends to underestimate the critical stress and over predict fracture strain by 10-15% compared to molecular dynamics (MD) predictions. Thus, nonlinear FEM formulations have become the preferred choice for accurate mechanical modeling, particularly in large-deformation and fracture analyses.

Fracture, Defects, and Failure Mechanisms

The modeling of fracture and defect propagation represents one of the most challenging aspects of graphene analysis. Traditional FEM approaches, which rely on predefined crack paths, were limited in predicting crack initiation. The development of Cohesive Zone Models (CZM) and Extended FEM (XFEM) addressed these issues by allowing crack growth without remeshing. For instance, Zhang et al. (2016) applied CZM-FEM to model fracture in defective graphene sheets and reported results closely matching atomistic simulations, with less than 8% deviation in critical fracture energy.

Comparatively, Yoon et al. (2018) applied XFEM to simulate random defect distributions, finding that the presence of Stone Wales defects and vacancy clusters reduced fracture strength by up to 35%, in line with experimental micro-tensile results by Zhao et al. (2019)**.** FEM's capability to simulate stress concentration and crack branching provided a distinct advantage over analytical methods, which cannot easily represent complex defect geometries. However, FEM accuracy in predicting crack propagation paths was found to depend strongly on mesh density and cohesive parameters**,** highlighting the need for consistent parameter calibration with atomic-scale data.

Multiscale Modeling and Load Transfer in Composites

The integration of graphene into composite materials has led to extensive use of FEM for multiscale analysis. Studies by Haque and Saifullah (2015) and Cao et al. (2017) employed Representative Volume Element (RVE)-based FEM to investigate load transfer between graphene sheets and polymer matrices. Their findings showed that the interfacial shear strength and graphene orientation had dominant effects on composite stiffness and strength, which were difficult to capture experimentally.

When compared to atomistic simulations**,** FEM provided more efficient computation for macroscale structures while maintaining accuracy within a 10% margin. For instance, MD simulations predicted interfacial shear strength values around 40-60 MPa, while FEM-based multiscale models yielded comparable results in the range of 45-55 MPa. Such consistency supports FEM's credibility for predicting the macroscopic mechanical behavior of graphene composites.

Nevertheless, FEM-based models typically rely on homogenized material constants, ignoring local atomic variations. This limitation was pointed out by Qian et al. (2020)**,** who emphasized that without incorporating nanoscale data, FEM tends to oversimplify the interfacial transition zone. Consequently, many researchers have integrated MD-informed constitutive parameters into FEM frameworks, creating hybrid models that accurately capture both local and global responses.

Thermal and Electromechanical Coupling

Graphene's unique thermal and electrical properties have also been examined through FEM simulations, especially in microelectronic and thermal management applications**.** Singh et al. (2018) and Li et al. (2020) used 3D FEM models to simulate anisotropic heat conduction and thermal expansion effects, finding that FEM-predicted in-plane thermal conductivity values (2800-3300 W/m·K) matched experimental ranges reported by Balandin et al. (2008). FEM further allowed the exploration of multi-layer systems, where cross-plane conductivity decreased exponentially with increasing layer number an insight difficult to capture experimentally.

In electromechanical simulations, Park et al. (2019) applied FEM to model strain-induced bandgap engineering**,** confirming the theoretical predictions of Pereira et al. (2009)**.** Their results demonstrated that FEM can reliably predict the deformation-dependent electronic response of graphene when coupled with appropriate constitutive models. Compared to pure quantum mechanical approaches, FEM significantly reduced computational time while maintaining acceptable accuracy in strain localization and potential field distribution.

Nonlinear and Multiphysics FEM Frameworks

Recent studies have focused on developing nonlinear multiphysics FEM models to simulate coupled thermo-electro-mechanical phenomena in graphene-based systems. Kim and Cho (2020) introduced a nonlinear FEM framework incorporating both material anisotropy and geometric nonlinearity, predicting post-yield responses that closely matched MD simulations. Later, Li et al. (2021) extended this approach by integrating viscoelastic time-dependence, capturing graphene's relaxation behavior under cyclic loading. These studies collectively demonstrate that advanced FEM frameworks can replicate the complex mechanical phenomena observed at the nanoscale, which were previously accessible only through atomistic simulations.

When comparing across literature, it becomes evident that nonlinear FEM formulations achieve up to 95% agreement with atomistic results in stress–strain predictions and fracture onset when material constants are calibrated from atomic data. This consistency underscores the growing reliability of FEM as a predictive tool, even for materials traditionally considered beyond continuum mechanics' scope.

Advantages and Limitations in Comparison with Other Methods

Compared to Molecular Dynamics (MD) and Density Functional Theory (DFT), FEM provides substantial advantages in computational scalability, enabling the modeling of macroscopic graphene structures and devices. MD and DFT, while accurate at the atomic scale, are computationally prohibitive for structures exceeding a few nanometers. FEM, on the other hand, can simulate graphene sheets of several micrometers with minimal loss in precision, especially when multiscale coupling is applied.

However, FEM's limitations lie in its continuum assumption, which cannot naturally capture discrete atomic interactions such as bond breaking, chirality effects, and local electronic transitions. To overcome this, hybrid frameworks integrating FEM with coarse-grained MD or machine learning-based constitutive laws have been developed. Wang et al. (2023), for instance, demonstrated that ML-augmented FEM can predict mechanical properties with errors below 3% compared to full-scale MD, reducing computation time by 90%. This convergence marks a new paradigm where FEM becomes a data-driven tool capable of adaptive accuracy.

Comparative Summary and Future Directions

Across all comparative studies, FEM emerges as a highly versatile and computationally efficient approach for modeling graphene's behavior at mesoscopic and macroscopic scales. While MD and DFT remain indispensable for atomic-level validation, FEM has proven capable of replicating most mechanical and thermal responses when properly parameterized. The literature shows a consistent trend: as FEM models evolve toward multiscale, nonlinear, and data-integrated frameworks, their predictive capacity continues to approach that of fully atomistic simulations.

In conclusion, the comparative analysis of FEM applications in graphene reveals that the method offers an optimal balance between accuracy and scalability. It enables researchers to extend insights from atomic-level phenomena to device-scale performance predictions. The future of FEM in graphene research lies in its integration with machine learning, quantum mechanics, and experimental data, forming a comprehensive modeling ecosystem. Through such hybridization, FEM will continue to play a central role in the design, optimization, and functionalization of graphene-based materials and Nano devices.

Conclusion

IIn this study, a new atomic-scale finite element method (AFEM) based on the Tersoff Brenner potential was developed to model the mechanical behavior of graphene. The method was applied to calculate the mechanical behavior of graphene under tensile loading and the results were evaluated against molecular dynamics (MD) simulations. The results show that the proposed AFEM method without considering periodic boundary conditions yielded results that were "very different from the MD simulation results". However, with the addition of periodic boundary conditions, the model's output for Young's modulus, stress, and final strain for defect-free graphene showed "good agreement with the MD simulation results". Specifically, the calculated Young's modulus was 0.813 terapascals, with a final stress of 130.92 GPa and a final strain of 0.248. The study also investigated the factors influencing simulation speed. The results suggest that the simulation time is influenced by the difference in length between the initial non-equilibrium bonds and the equilibrium bonds, rather than the absolute length of the initial bonds. It was also found that the AFEM calculation time has a linear relationship with the number of atoms. Overall, this research demonstrates that the AFEM method, when properly developed to include periodic boundary conditions, can be a highly accurate and efficient tool for simulating the mechanical behavior of graphene. Its computational speed is noted to be "almost 100 times faster than the molecular dynamics method", making it a promising alternative for modeling larger-scale systems.

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Authors' Contributions

All authors contributed to data analysis, drafting, and revising of the paper and agreed to be responsible for all the aspects of this work.

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