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Molecular Dynamics Simulation of Polymer Nanocomposites: A Review

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ABSTRACT

Polymer nanocomposites have attracted significant attention from researchers and industries in recent years. This interest stems from their unique combination of properties, including high mechanical strength, remarkable thermal stability, and notable electrical characteristics. Among the available computational tools, molecular dynamics simulation has emerged as one of the most accurate and efficient methods, enabling the investigation of material behavior at the molecular scale. This approach allows researchers to predict and analyze the internal structure and properties of materials without the need for costly and time-consuming experiments. This review compiles and presents the most important scientific achievements in the application of molecular dynamics simulations to the study of polymer nanocomposites. In particular, the role of these simulations in elucidating fundamental mechanical parameters such as elastic modulus, shear modulus, Young's modulus, and fracture behavior is examined. The review also highlights their capability to analyze impact resistance, friction coefficient, and wear rate, alongside investigations into thermal conductivity and the effects of defects on overall material performance. Furthermore, insights into stress-strain behavior, vibration characteristics and natural frequency, as well as the analysis of conductivity performance, are presented. Collectively, these simulation-based approaches provide a deeper understanding of interfacial interactions between the polymer and nanoparticles, identify key reinforcement mechanisms, and uncover the intricate structure-property relationships that govern material behavior.

Literature Review

In 2008, Zheng [1] carried out a multi-scale simulation of polymer matrix nanocomposites and found that the addition of fillers can enhance the matrix's mechanical behavior in several ways: (1) fillers themselves improve the toughness and strength of the matrix due to their inherent high mechanical strength, (2) they act as barriers against crack propagation, and (3) they modify the structure of the polymer layer close to the filler, which further strengthens the nanocomposite.

In 2014, Shokrieh [2] investigated the hardness prediction of graphene/epoxy nanoplatelet nanocomposites. By analyzing four models under periodic boundary conditions and constant density, each with one to four graphene layers, it was determined that the mechanical properties remained nearly unchanged across all configurations.

In 2017, Shen [3] investigated the analysis of the diffusion behavior and dispersion mechanism of polymer grafted nanorods, and the results include: Increasing the removed volume of grafted nanorods, improving the reinforcement/matrix interface, and thus improving the diffusion of grafted nanorods are all due to the increase in bond density and the length of the bond chain.

In 2020, Zhang [4] examined surface modification and properties of graphene/polymer nanocomposites. It was found that increasing polymer functional group polarity improves the interaction with graphene oxide. However, too much polarity causes hydrogen bond formation within the polymer, reducing both interfacial hydrogen bond density and interfacial adhesion.

Shen [5] in 2015 performed simulations on the structural, mechanical, and viscoelastic behavior of grafted polymer nanoparticles. Results indicated that in a homopolymer matrix, higher bond density and longer chain lengths enhanced filler–matrix interactions, thereby improving nanoparticle dispersion. The mechanical strengthening effect was also attributed to the increase in surface area resulting from simultaneously increasing bond density and chain length.

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In 2014, Shen [6] analyzed the nonlinear strain behavior of nanoparticles dispersed within a homopolymer matrix. Findings showed that as strain increased, the elastic modulus dropped and eventually leveled off at a minimum value at higher strain levels.

In 2022, Zhang [7] explored the physical origins behind the unique mechanical behavior of carbon nanotube/polyethylene systems. The study revealed that graphene nanosheet reinforcement enhanced mechanical performance, largely due to longer attached polymer chains and stronger interfacial interactions.

Marcadon [8] in 2013, examined how particle size affects the mechanical response of polymer nanocomposites. It was found that, at a fixed volume fraction, increasing particle radius led to a higher elastic modulus.

In 2015, Fu [9] investigated deformation mechanisms in glass/PE nanocomposites. The study showed that higher nanoparticle volume fractions combined with strong nanoparticle–polymer interactions enable nanoparticles to effectively bridge polymer chains, which prevents localized deformation under tensile loading.

In 2020, Shen [10] investigated stress–strain behavior and reinforcement mechanisms in polymer nanocomposites. The results indicated that mechanical improvements can be achieved either by increasing the nanoparticle volume fraction or by reducing nanoparticle size.

In 2018, Molinari [11] examined how polymer nanocomposites are reinforced and found that at low filler loadings the stress–strain response shows a performance drop. As the filler volume fraction rises, the plastic hardening rate progressively declines, and at sufficiently high loading the material response becomes softer.

Liu [12] in 2016 analyzed polystyrene/silica systems and showed that, for a fixed particle geometry, raising nanoparticle mass fraction increases yield strength; equivalently, increasing particle surface area (by changing shape) has a similar effect. A larger interfacial area also leads to a higher elastic modulus.

In 2019, Izadi [13] reported that C60/carbon-onion-reinforced polymer composites exhibit nearly isotropic elastic behavior, and that raising the reinforcement weight fraction increases the elastic modulus.

In 2016, Islam [14] showed that defects in CNTs significantly influence the Young's modulus of CNT/polyethylene nanocomposites.

Hou [15] in 2019, found that in grafted-nanoparticle composites, surface hydrogen bonding is strengthened and defective silicate chains are stabilized, which retards crack propagation under load and improves both adhesion and ductility in the C-S-H gel.

Haghighi [16] in 2019, showed that for T6/T14 3D metallic carbon nanostructure reinforcements, increasing the pull-out speed leads to a direct rise in interfacial (surface) work/force.

In 2014, Gao [17] found that upon rupture, stress gradually falls with increasing strain while highly oriented polymer bundles compress. Resistance to failure improves with (1) stronger interfacial interactions, (2) longer nanorods, and (3) a higher density of bulk cross-links.

Gao [18] in 2014, showed that longer, thinner nanorods yield higher mechanical strength under uniaxial loading, with an optimal rod volume fraction for maximizing elastomeric strength. Stronger polymer–nanorod interactions further enhance reinforcement.

In 2021, Zhou [19] investigated SBR/silica interfaces and found the KH550 chemical bond exhibits a surface tensile strength of 760 MPa at 300 K, i.e., over four times that of the unmodified interface.

In 2021, Josep [20] reported that amino-silane outperforms sulfur-silane for strengthening silica/SBR nanocomposites; however, over-adding silane harms interface durability. Increasing nanoparticle count raises tensile strength.

In 2021, Dong [21] explored how glass transition temperature correlates with mechanical behavior in PVA/functionalized graphene oxide composites. Significant gains were reported: with 2.5 wt% tris-graphene oxide, Young's modulus rose by more than 50%, shear modulus by about 46%, and Cauchy stress by 40%. The stronger binding energy between PVA and functionalized graphene oxide, compared to that with pristine graphene oxide, was identified as the reason for the improved mechanical performance.

In 2021, Sliozberg [22] investigated shape memory mechanisms in BP/epoxy nanocomposites at the molecular scale. The study revealed that Young's modulus increased proportionally with CNT content up to a volume fraction of 0.16 (≈40 wt%). Beyond this threshold, a sharp rise in modulus was observed at higher CNT concentrations.

In 2007, Cho [23] examined the elastic response of polymer nanocomposites and found an unexpected effect: smaller nanoparticles led to higher elastic modulus. This was attributed to the dense polymer layer that formed around nanoparticles, acting like a stiff shell that resisted stress, thereby increasing the composite's modulus.

Amraei [24] in 2019 analyzed the role of the interphase region in nanoparticle-reinforced polymer nanocomposites. Results indicated that an interphase model improved elastic properties by over 95% relative to two-phase models with full bonding. The composite's elastic modulus was shown to be highly sensitive to nanoparticle radius and volume fraction.

Ki [25] in 2021 performed an inverse micromechanical analysis of epoxy/POSS nanocomposites. Findings showed that incorporating POSS nanoparticles enhanced Young's modulus and shear modulus to more than three times the values of neat epoxy. Moreover, the thermoelastic behavior improved progressively as the POSS content increased.

In 2007, Adnan [26] investigated how fullerene (buckyball) size influences the elastic response of amorphous PE nanocomposites. Contrary to expectations, smaller buckyballs produced better elastic properties, suggesting size reduction enhanced reinforcement efficiency.

In 2020, Jiang [27] assessed surface characteristics of CNT–polyimide nanocomposites and found that increasing the number of CNT walls was a key factor in enhancing surface stress transfer under tensile loading.

In 2021, Haghigi [28] explored how defects and functional groups impact the mechanics of graphene- and nanotube-based thermosetting nanocomposites. Both features were shown to reduce the elastic modulus of the nanofillers themselves and likewise decreased the modulus of epoxy composites reinforced with continuous nanofillers.

Moeini [29] in 2020 studied temperature and strain rate effects in graphene–epoxy nanocomposites. Higher temperatures reduced composite durability, while the elastic and bending modulus rose significantly with graphene loading up to 0.5 wt%. Beyond this concentration, the modulus increase slowed.

In 2019, Fankhael [30] experimentally investigated interphase elastic properties in nanoparticle/epoxy nanocomposites. Finite element analysis revealed 22–24% increases in elastic behavior for unbonded boehmite/epoxy layers, while bonded layers achieved a larger improvement of 40–42%, confirming the interphase role in strengthening nanocomposites.

In 2019, Hu [31] examined the fracture behavior of polymer nanocomposites containing grafted nanoparticles. Results showed that the fracture properties initially improved but then declined as either the bond density or the bonded chain length increased.

In 2016, Elefthria [32] studied the melt dispersion of graphene/PEG nanocomposites across a broad temperature range. The findings showed only a weak interaction between the polymer and graphene layers, with virtually no polymer bridging the graphene sheets. At the graphene/PEG interface, polymer density increased slightly as temperature decreased, confirming a generally poor material interaction.

Rissanou [33] in 2015 explored the structural behavior of graphene/PEG nanocomposites with 3 wt% graphene. The results indicated that polyethylene chains adjacent to graphene layers were more flexible than bulk chains. Additionally, increasing the graphene sheet size amplified the oscillation range of the chains.

In 2017, Lin [34] investigated the mechanical properties of graphene/PMMA nanocomposites. It was found that elastic and shear modulus improved as the graphene volume fraction increased, but both decreased with rising temperature (300–500 K). The greater the graphene fraction, the more sensitive the nanocomposite was to temperature changes.

In 2020, Farazin [35] analyzed how single-walled CNT dimensions affect CNT/PMMA nanocomposites. Increasing the CNT diameter boosted the longitudinal Young’s modulus by over 3×, the transverse modulus by more than 2×, the shear modulus by ~1.43×, and Poisson’s ratio by ~1.1× compared to smaller diameters.

Locchetta [36] in 2021 examined how particle size and dimensions influence nanocomposite durability. The study concluded that resistance improved as particle size decreased, even when the reinforcement volume fraction remained unchanged. Surface hardness was also confirmed to be size-dependent.

In 2021, Cui [37] evaluated the effects of functional groups on CNT/nitrile rubber composites. Both carboxyl and amide groups improved performance compared to neat nitrile rubber, with amide-functionalized CNTs providing the greatest gains. These enhancements were linked to dipole–dipole interactions and better surface compatibility, which strengthened the mechanical and tribological properties.

In 2021, Wang [38] analyzed the nonlinear vibration behavior of CNT/PMMA plates. Results showed that placing reinforcement near the top and bottom surfaces yielded higher frequencies and greater stiffness compared to reinforcements concentrated in the plate’s mid-layer.

Karatasos [39] in 2019 explored static and dynamic behaviors of graphene/multi-branched polyester (Bolthorne) mixtures. Lowering the temperature gradually stabilized the graphene structure, restricting polymer mobility and causing a significant reduction in molecular motion compared with the molten state.

Holt [40] in 2014 investigated the dynamic and static features of polyvinyl pyridine/silica nanocomposites using dielectric spectroscopy and small-angle X-ray scattering. It was found that the outer polymer layer consistently measured 4–6 nm thick, regardless of nanoparticle density. This contradicted earlier studies, showing that the outer layer was active rather than a so-called “dead layer.”

In 2007, Suchira [41] investigated how reinforcement is achieved in amorphous polymer matrices containing nanoparticles. The findings showed that the key determinant is the particle–polymer interfacial interaction strength, which must be sufficiently high to allow uniform nanoparticle dispersion within the polymer network.

In 2021, Yang [42] examined the role of covalent bonding in nanotube/amorphous PET nanocomposites. Results revealed that covalent functionalization notably enhances surface charge transfer and significantly boosts Young’s modulus under transverse tension and shear. Due to nanotubes’ narrow geometry, the improvement is more pronounced under shear loading. Analysis of internal stress evolution indicated that covalent bonding is a primary contributor to the enhanced charge transfer in these composites.

In 2019, Giannopoulos [43] investigated bone-shaped CNTs as fillers in polyethylene nanocomposites. The study demonstrated that these uniquely structured nanotubes greatly enhance surface strength, which in turn leads to a notable increase in the overall mechanical strength of the composite.

In 2008, Al-Ostaz [44] studied the elastic response of single-walled CNT/polyethylene composites. It was found that SWCNTs display consistent elastic constants across various loads, behaving as linear elastic materials. However, proximity to polymer chains caused the nanotubes to lose circularity, revealing relatively weak transverse mechanical properties.

In 2019, Yang [45] analyzed graphene/PE nanocomposites with oxygen functionalization using both MD and finite element simulations. The oxygen groups were found to disrupt graphene’s structure, reducing both longitudinal Young’s modulus and in-plane shear modulus compared to pristine graphene composites. Both computational approaches confirmed these reductions, attributing them to changes in surface charge transfer capacity.

In 2018, Voljin [46] simulated nanoparticle diffusion in fullerene/thermoplastic polyamide nanocomposites. Results indicated that diffusion dynamics are strongly affected by chemical heterogeneity within polymer chains, especially on length scales comparable to the nanoparticle size. Local chain structure was shown to have a decisive influence on nanoparticle mobility.

In 2013, Rissanou [47] examined graphene nanocomposites with polystyrene, PMMA, and polyethylene. The strength of polymer–graphene interactions followed the order: polystyrene > PMMA > polyethylene. Among the three, polyethylene chains displayed the highest mobility, contrasting with the stronger interactions of the other systems.

In 2018, Skounzos [48] investigated CNT/PMMA nanocomposites, observing that PMMA chains tend to penetrate nanotube interiors, a behavior more pronounced with larger CNT diameters. The composites also exhibited a glass transition temperature about 6 °C higher than that of bulk PMMA, confirming nanotube-induced modifications.

In 2021, Razzaghi [49] evaluated thermal conductivity in graphene/amorphous PE nanocomposites. At a fixed 1% filler fraction, effective conductivity values were ~0.47 W/mK for C2N-PE, ~0.56 W/mK for C3N-PE, and ~0.74 W/mK for graphene-PE. Pure amorphous PE showed ~0.36 ± 0.05 W/mK. The study emphasized that filler conductivity critically determines overall composite performance.

In 2021, Chaundhari [50] investigated polymer nanocomposites reinforced with graphene and CNTs, showing that these nanofillers possess exceptional tensile strength and unique molecular structures. Their incorporation enhanced properties including hardness, overall strength, thermal conductivity, and glass transition temperature of the composites.

In 2005, Desai [51] examined how spherical nanoparticles influence chain dispersion in polymer nanocomposites. The findings showed that restricting chain mobility in nanoparticle-filled polymers resembles the behavior of melts confined between two plates. Specifically, chain emission rose by 15–20% near repulsive surfaces, while it decreased by 40–50% in the vicinity of strongly attractive surfaces.

Rohi [52] in 2018 applied the finite element method to study the vibration behavior of polymer matrices reinforced with silicon carbide nanotubes. Results showed that adding these nanotubes enhanced the system's natural frequency, an effect absent in the pure polymer. Increasing nanotube length at a constant diameter further widened the frequency gap between the nanocomposite and pristine polymer. Furthermore, unclamped nanocomposites displayed a larger frequency rise compared to those reinforced with clamped nanotubes.

Borodin [53] in 2005 investigated the time-dependent shear modulus of surface polymers in nanocomposites. The study found that activating attractive interactions between the polymer and cylindrical fillers increased the shear modulus by several orders of magnitude, with this effect growing stronger over time.

Gao [54] in 2016 studied the conductive behavior of functionalized polymer nanorod/matrix composites under constant shear flow. Results indicated that conduction probability along the shear direction increased with shear rate, while homogeneous conduction and conduction perpendicular to the shear direction declined. Additionally, conductivity stability improved as the nanorod volume fraction increased.

Hu [55] in 2016 examined the structural roles of carbon nanotubes, carbon nanofibers, and graphene nanoplatelets in polymer matrices. The results revealed that carbon nanofibers, due to their serrated surface, showed superior mechanical interlocking, enabling efficient shear stress transfer and the highest sliding resistance at the filler–matrix interface. In contrast, the smooth surfaces of carbon nanotubes and graphene nanoplatelets limited their sliding resistance, although graphene nanoplatelets demonstrated stronger resistance to normal separation, with higher normal strength compared to shear strength.

Li [56] in 2018 investigated how chemical bonding between polymers and nanoparticles influences the viscoelastic properties of nanocomposites. Findings showed that as more surface molecules are chemically bonded, the rate of change in surface interactions under periodic strain decreases, attributed to reduced reversible adsorption–desorption. A sharp rise in storage modulus was linked to the sudden increase in chemical bond energy under large strain.

Liu [57] in 2015 explored the surface mechanical properties of graphene/polymer matrices (PE and PMMA). The study revealed that chain length had a major influence: at 10-unit chains, graphene wrinkling significantly enhanced surface mechanical strength. When chain lengths exceeded 40 units, the effect plateaued, though in wrinkled graphene/PMMA systems, mechanical properties continued to improve with chain length. This influence was minimal in graphene/PE composites but pronounced in graphene/PMMA.

Wu [58] in 2020 examined the effect of aspect ratio polydispersity (bimodal distribution) on the conductivity of polymer nanocomposites under static shear. Results showed that a decrease in the polydispersity index reduced the percolation threshold due to linear dependence in the stationary state. However, under shear, the main conductive network was disrupted. Recovery depended on the orientation and connectivity of long and short nanorods, which explained the higher percolation threshold and anisotropic conduction probability compared with the stationary condition.

Li [59] in 2021 studied the rheological behavior of polymer matrix nanocomposites. Using the Carreau–Yasuda model, zero-shear viscosity was calculated, showing that higher nanoparticle volume fractions enhanced polymer–reinforcement interactions while reducing reinforcement size. Measurements of the end-to-end distance and mean square radius of rotation offered insights into chain dynamics. Additionally, polymer chain relaxation times decreased steadily with shear rate, directly affecting the shear viscosity of the composites.

Park [60] in 2018 analyzed the outer-layer characteristics of graphene-reinforced nanocomposites. The study found that hydroxyl- and carboxyl-functionalized epoxy systems exhibited greater output power than the unmodified graphene/epoxy system, by 5% and 54% respectively. However, their surface shear moduli were lower—reduced by 56% in the hydroxyl-functionalized system and by 85% in the carboxyl-functionalized system. Functionalizing graphene was shown to increase pull-out force while reducing surface shear modulus.

In 2021, Wang [61] carried out research on the mechanical and viscoelastic behavior of polymer nanocomposites strengthened with wrinkled graphene. The study found that the rise in elastic modulus was influenced by three main factors: an increase in the number of graphene layers, a reduction in the degree of surface waviness, and the incorporation of multilayer graphene sheets into the PMMA matrix. This reinforcing effect became more significant as the volume fraction of graphene increased and the surface waviness decreased.

In 2021, Talapatra [62] investigated the tribological characteristics of thermoplastic polyurethane (TPU) nanocomposites reinforced with functionalized graphene. Results revealed that introducing just 0.5 wt% of functionalized single-layer graphene to pristine TPU led to substantial improvements: the elastic modulus rose by 20%, the bulk modulus increased by 6.66%, and the shear modulus by 15.3%. Furthermore, TPU nanocomposites reinforced with 3 wt% functionalized graphene achieved the lowest coefficient of friction (0.42) and a reduced wear rate (19%) under constant static load and maximum sliding velocity (11 m/s).

In 2016, Hagita [63] explored the fracture response of polymer nanocomposites under tensile loading with a Poisson's ratio of 0.4. The study concluded that when reinforcement–polymer interactions were attractive, adhesive-type fractures occurred. Conversely, in cases dominated by repulsive reinforcement–polymer interactions, voids appeared at the polymer–reinforcement interface, indicating that such failures can be classified as surface fractures since void formation was confined to the interfacial region.

In 2021, Dewapriya [64] investigated the penetration resistance of multilayered polyurea/silicon carbide nanocomposites against ultrasonic projectile impact. The findings showed that both the ballistic limit velocity and the specific penetration energy of these multilayers were significantly higher compared with laboratory-tested protective materials. The study highlighted two key factors responsible for over 75% improvement in penetration resistance: (1) optimization of layer thickness and (2) proper arrangement of the multilayer structure within the protective armor.

In 2021, Chiang [65] studied the dynamic mechanical properties of nacre-inspired graphene–polymer nanocomposites. The results indicated that producing films with smaller thicknesses and a greater number of repetitions led to much higher Young's modulus values under uniaxial stretching and vibration tests. The ability of these layered structures to dissipate impact energy was linked to their internal nanoscale arrangement. Specifically, fracture under compressive stress waves from projectile impacts occurred when individual layers reached a critical thickness, while nacre-mimicking nanocomposites were able to absorb and dissipate impact energy through strain generation in the polymer phases.

In 2006, Song [66] examined fracture behavior in fully exfoliated silicate (nanoplatelet)–polymer nanocomposites. Results showed that increasing the number of nanoplatelets enhanced the fracture strength of polymers. Nanoplatelets were generally effective in improving the mechanical properties of polymers with glass transition temperatures at or below room temperature. However, this reinforcing effect was less pronounced in polymers with higher glass transition temperatures, such as epoxy and polystyrene, where nanoplatelet addition had limited strengthening effects.

In 2016, Vryonis [67] studied dielectric responses and molecular dynamics in epoxy–$BaSrTiO_3$ nanocomposites. Findings suggested that the filler concentration had a direct effect on both the thermal and conductive properties of the composites, mainly through interactions at the polymer–particle and particle–particle interfaces.

In 2015, Gao [68] explored the conduction mechanisms of polymer nanocomposites reinforced with carbon nanotubes. The results demonstrated that as filler–filler interactions strengthened, nanorods began to cluster. The percolation threshold initially decreased but later increased again. A compact dispersion of nanorods was identified as a critical factor for forming conductive networks. Additionally, elevated temperatures lowered the percolation threshold, while conduction probability under a shear field depended on the nanorod dispersion state.

In 2020, Haghighi [69] investigated the surface characteristics of carbon-functionalized graphene/polymer nanocomposites. It was found that load transfer from the matrix to graphene was more efficient than in unmodified graphene/polymer systems. In random and regular one-sided polymer matrices, surface resistance decreased with higher carbon loading. However, in both random two-sided and regular two-sided polymer matrices, mean pull-out forces increased with greater degrees of functionalization.

In 2017, Yang Zhou [70] studied interfacial bonding mechanisms in C–S–H/polymer nanocomposites. Results revealed that polyacrylic acid exhibited the strongest affinity due to its ability to form two strong bonds, leading to highly stable adsorption on the C–S–H surface. In contrast, PVA, despite hydrogen bonding, showed poor adsorption and high mobility at the interface. The polarity of the polymer functional groups was identified as a decisive factor influencing diffusion, aggregation behavior, and consequently, the bulk properties of the nanocomposite.

In 2021, Qian [71] investigated the influence of functionalizing single-walled carbon nanotubes

(SWCNTs) on the mechanical performance of epoxy glass composites. The findings showed that the composites reinforced with functionalized SWCNTs exhibited the highest improvements—elastic modulus increased by 32% compared to neat epoxy, and tensile strength rose by 10%. Moreover, the bending modulus exceeded 16.9 GPa, while bending strength surpassed 381.39 GPa. A comparative test further demonstrated that the elastic modulus of nanocomposites containing functionalized SWCNTs was more than 17% higher than those reinforced with non-functionalized SWCNTs.

In 2021, Kim [72] studied liquid crystalline elastomeric nanocomposites incorporating gold nanoparticles. Results revealed that grafted nanoparticles did not significantly alter the alignment of liquid crystalline elastomer domains near the bonded layer but negatively affected mechanical strength. The increase in effective nanoparticle size due to the thick bonding layer caused a mismatch with neighboring mesogenic units, though this effect diminished with distance. Additionally, the grafted molecules displayed high plasticity, deforming easily under load and absorbing strain energy. This cushioning effect reduced charge transfer efficiency to the nanoparticles and limited interaction with rigid surfaces.

Carlos Saenz [73] in 2018, analyzed the interfacial properties of epoxy resin nanocomposites. The study concluded that interface thickness is influenced by several factors, including epoxy resin cross-linking degree, hardener type, and carbon nanotube dimensions (diameter and length). No universal relationship was observed—each case required independent evaluation. In particular, the cross-linking degree of the epoxy resin significantly impacted the interface thickness.

In 2019, Karatrantos [74] examined nanorod diffusion in polymer nanocomposites and reported that thin nanorods diffuse more rapidly in entangled polymer matrices than predicted by the Stokes–Einstein chain model. Even at low nanorod concentrations, polymer chain motion was hindered. Due to their large surface area, nanorods restricted polymer dynamics within nanocomposites.

Zheng [75] in 2017 worked on polymer matrix nanocomposites with controlled dispersion of spherical nanoparticles. Experimental observations revealed that shorter chain lengths led to reduced stress recovery, attributed to the limited extension of polymer strands bridging adjacent nanoparticles. These end-linked nanocomposites displayed temperature-dependent elongation-stretch behavior, unlike conventional physical composites, whose mechanical strength typically degrades with rising temperature.

Ashraf Khan [76] in 2021 investigated the glass transition temperature (Tg) of polymer nanocomposites. The results showed that varying the nanoparticle volume fraction directly influenced Tg. Altering nanoparticle mass produced effects equivalent to modifying volume fraction, indicating that both factors play comparable roles in controlling Tg in polymer nanocomposites.

Fragiadakis [77] in 2005 studied the glass transition temperature and molecular dynamics in poly(dimethylsiloxane)/silica nanocomposites. Findings indicated that the interfacial layer thickness was approximately 2.1–2.4 nm. The reduced mobility of polymer chains near the filler interface—constrained by interactions with the filler surface—was identified as the cause of slow relaxation observed in dielectric spectroscopy measurements.

In 2021, Lu [78] conducted molecular modeling and simulations on polymer nanocomposites containing carbon nanorod fillers. Results showed that the morphology's dependence on tensile strength between nanorods varied with functionalization type. For homogeneously functionalized nanorods, stronger isotropic attractions increased nanorod–nanorod contact peaks and orientation order but did not change morphology qualitatively, regardless of aspect ratios (3, 5, 15). For patchy functionalized nanorods with smaller aspect ratios (3), stronger directional attractions caused morphology to shift from dispersed nanorods to interconnected networks.

In 2021, Yu [79] examined polyurethane/graphene oxide polymer nanocomposites used in modified asphalt binders. The study found that polyurethane influenced graphene oxide morphology, causing wrinkling and twisting. Incorporating graphene oxide increased asphalt viscosity, reducing deformation, flow, and softening at high temperatures compared to base asphalt—enhancing its thermal stability. Additionally, the glass transition temperature of the polyurethane/graphene oxide–modified asphalt was higher, confirming its improved high-temperature performance.

In 2021, Chang [80] investigated creep behavior (slow deformation under constant stress) in polymer nanocomposites. Results indicated that creep rates were higher when test temperatures were closer to the glass transition temperature. Increasing filler content reduced strain, with a significant decrease when filler volume fraction reached 24.1%, attributed to the transition from double-chain bridge to single-chain bridge structures. While greater nanoparticle attachment improved creep resistance, excessive nanoparticle aggregation was detrimental. Optimizing nanoparticle–polymer interactions was highlighted as the best strategy for enhancing creep resistance.

Sikdar [81] carried out research in 2008 to examine the effect of surface interactions on the crystallinity and nanoscale mechanical properties of clay–polymer nanocomposites. The findings revealed that attractive forces between polymer functional groups and the modifier, along with simultaneous repulsive interactions between the modifier and the polymer backbone, induce structural variations in the polymer. These changes disrupt the polymer's periodicity, which appears as alterations in crystallinity. The interplay of these interactions has two distinct outcomes: (1) a reduction in crystallinity within the nanocomposite and (2) a substantial enhancement in nanomechanical performance. The pinning of polymer functional groups to modifiers through attractive forces strengthens the nanomechanical characteristics of polymer nanocomposites, ultimately improving their nanoscale mechanical behavior.

In 2016, Shin [82] investigated polymer nanocomposites using a statistical multiscale homogenization framework. The study revealed that as the representative unit cell size increases, the elastic properties of both pure epoxy and polymer nanocomposites decline. Moreover, when the inherent uncertainty of the molecular dynamics (MD) approach is combined with geometric uncertainties, the average homogenized Young's modulus further decreases. The proposed multiscale statistical model proved essential for explaining how uncertainty propagation from molecular dynamics simulations impacts the homogenized elastic properties of multiparticle nanocomposite systems.

Boulet [83] in 2004, performed simulations on hydrated nanocomposites incorporating lithium, sodium, and potassium. The study demonstrated that cations interact strongly with both water and polymer chains. For potassium-based nanocomposites, a monolayer arrangement was observed, while sodium-based systems exhibited the formation of a polymer bilayer. Unlike the case without polymer, lithium- and sodium-based nanocomposites displayed clearly different behaviors. In particular, lithium ions localized not only inside the tetrahedral voids of clay layers but also at the center of the interlayer galleries, a distribution pattern not seen with sodium or potassium.

Table 1 shows some of the researches done on polymer nanocomposites.

Table 1
Summary of reviewed article

References	Material	Objective
Zheng(2008)	Polymer matrix nanocomposites	strength, toughness and crack growth
Shokrieh(2014)	Graphene/epoxy nanoplatelet nanocomposites	Hardness prediction and mechanical properties
Shen(2017)	Polymer grafted nanorods	Investigating the diffusion behavior and diffusion mechanism
Zhang(2020)	Graphene oxide sheets/polymer nanocomposites	surface interaction and calculation of mechanical properties
Shen(2015)	grafted polymer nanoparticles	Structural, mechanical and viscoelastic properties
Shen(2014)	Nanoparticles embedded in a homopolymer matrix	nonlinear behavior
Zhang(2022)	Carbon nanotubes and polyethylene matrix	effect of increasing polymer length on mechanical behavior
Marcadon(2013)	Polymer nanocomposites	effect of particle size on the mechanical behavior
Fu(2015)	Glass polyethylene polymer nanocomposites	investigating the local deformation during stretching
Shen(2020)	Polymer nanocomposites	stress-strain behavior and mechanical strengthening
Molinari(2018)	Polymer nanocomposites	Strengthening mechanisms and study of the effect of filler dimensions on mechanical properties
Liu(2016)	Polystyrene matrix nanocomposite with silica nanoparticles of different shapes	The role of the interfacial area for the interaction and dynamics of nanocomposites
Izadi(2019)	Polymer matrix composites reinforced with fullerene C60 and carbon onion	elastic properties of polymer composites reinforced with fullerene C60 and carbon onion
Islam(2016)	Defective carbon nanotube/polyethylene	mechanical properties and elastic modulus
Hou(2019)	Polymer matrix reinforced with grafted nanoparticles	effect of hydrogen bonding on the adhesive strength and plasticity of calcium silicate hydrate gel
Haghighi(2019)	Polymer nanocomposites reinforced with T6 and T14 carbon nanostructures	Examining the surface resistance of the system
Gao(2014)	Polymer nanocomposites filled with nanorods	rupture mechanism and increasing the resistance to rupture
Gao(2014)	Polymer nanocomposites filled with nanorods	the effect of nanorod size on mechanical strength and elastomeric reinforcement
Zhou(2021)	Styrene butadiene/silica rubber	dynamics and mechanical properties

Josep(2021)	Silica rubber/styrene butadiene nanocomposites	mechanical properties and diffusion in silica rubber/styrene butadiene nanocomposites
Dong(2021)	Functionalized graphene oxide/polyvinyl alcohol composites	Insights into glass transition temperature and mechanical properties
Sliozberg (2021)	Paperback (BP)/epoxy nanocomposites	Understanding the fundamental interactions governing the shape memory of polymer nanocomposite
Amraei (2019)	Polymer nanocomposites reinforced with nanoparticles	the effect of the interphase region on the overall elastic properties
Ki (2021)	Epoxy/POSS nanocomposites	Reverse mechanical study in micro dimensions of thermoelastic properties of epoxy/POSS nanocomposites.
Adnan (2007)	Bucky ball fullerene/amorphous polyethylene matrix	Investigating the effect of filler dimensions on the elastic properties
Jiang (2020)	Carbon nanotube-polyimide nanocomposite	surface properties of nanocomposite
Haghighi (2021)	Graphene and nanotube thermosetting epoxy nanocomposites	the effects of defects and functional groups on the mechanical properties
Moeini (2020)	Graphene-epoxy matrix nanocomposites	the effects of increasing temperature and strain rate on the mechanical properties
Fankhael (2019)	Nanoparticle/epoxy nanocomposites	Elastic interfacial properties
Hu (2019)	Polymer nanocomposites reinforced with grafted nanoparticles	fracture properties of polymer nanocomposites
Elefthria (2016)	Graphene/polyethylene glycol nanocomposites	melt dispersion of graphene/polyethylene glycol nanosheets
Rissanou (2015)	Graphene nanocomposites polyethylene glycol	Structural and dynamic properties
Lin (2017)	Graphene/polymethyl methacrylate nanocomposite	the effects of increasing temperature on the mechanical properties
Farazin (2020)	Carbon nanotube/polymethyl methacrylate	the effect of the size of single-walled carbon nanotubes on the overall properties
Cui (2021)	Carbon nanotubes/nitrile rubber	the effects of the type of functional group on mechanical and tribological properties
Wang (2021)	Carbon nanotube/polymethyl methacrylate	nonlinear vibration responses
Karatasos (2019)	Blends of graphene/multi-branched polyesters (Bolthorne)	static and dynamic properties
Holt (2014)	Polyvinyl pyridine/silica	static and dynamic propertiesX-ray test
Yang (2021)	Amorphous carbon nanotube/polyethylene terephthalate nanocomposites	Effects of covalent bonding of nanotubes on the elastic properties
Giannopoulos (2019)	Bone-shaped carbon nanotubes/polyethylene	bone carbon nanotubes to strengthen polymer
Al-ostaz (2008)	Single wall carbon nanotube/polyethylene	elastic properties
Yang (2019)	Single-layer graphene/polyethylene nanocomposites functionalized with oxygen	Comparison of molecular dynamics method and finite element analysis on the mechanical behavior
Voljin (2018)	Fullerene nanoparticle/thermoplastic polyamide nanocomposites	Simulation of nanoparticle diffusion
Rissanou (2013)	Three graphene nanocomposites polystyrene, polymethyl methacrylate,polyethylene)	structural and dynamic properties
Skounzos(2018)	Carbon nanotube/polymethyl methacrylate	equilibrium structure and dynamic behavior
Razzaghi(2021)	Amorphous graphene/polyethylene nanocomposites	Calculation of thermal conductivity coefficient
Chaundhary(2021)	Polymer nanocomposites reinforced with graphene or carbon nanotubes	mechanical properties
Rohi(2018)	Silicon carbide nanotubes/polymer matrix	Vibration characteristics and natural frequency
Gao(2016)	Functionalized polymer nanorod/matrix	Investigating the conductivity performance

Hu(2016)	carbon nanoplatelets)/polymer matrix	structural characteristics
Liu(2015)	Graphene/matrix polyaniline	Factors affecting surface mechanical properties
Park(2018)	Graphene reinforced nanocomposites	pull-out force and surface shear modulus
Wang(2021)	Wrinkled graphene reinforced polymer nanocomposites	mechanical and viscoelastic properties
Talapatra(2021)	Thermoplastic polyurethane nanocomposite filled with functionalized graphene	shear modulus, Young's modulus, friction coefficient and wear rate
Dewapriya(2021)	Multilayer polyurea/silicon carbide nanocomposites	Penetration resistance of multi-layer polyurea/silicon carbide nanocomposites
Chiang(2021)	Graphene-polymer nanocomposites inspired by nacre	elastic modulus and impact resistance
Song(2006)	Silicate nanocomposites polymer	fracture behavior
Vryonis(2016)	Epoxy-BaSrTiO3 nanocomposites	Conduction and glass transition temperature
Gao(2015)	Polymer reinforced with carbon nanorods	Conduction mechanism
Haghighi(2020)	Carbon functionalized graphene/polymer nanocomposites	Surface characteristics
Yang(2017)	Calcium silicate hydrate/polymer nanocomposites	Interfacial binding
Qian(2021)	Single wall carbon nanotubes/epoxy glass composites	The effect of functionalization of single-walled carbon nanotubes on the mechanical
Carlos saenz(2018)	Epoxy resin nanocomposites	Interfacial properties of epoxy resin nanocomposites
Zhou(2017)	Calcium silicate hydrate/polymer nanocomposites	dynamics and interfacial bonding strength
Fragiadakis(2005)	Poly(dimethylsiloxane)/silica nanocomposites	dielectric and glass transition temperature
Yu(2021)	Polyurethane/graphene oxide nanocomposite and modified asphalt binder	general properties and effect of temperature on viscosity

Review Results and Future Suggestions

Numerous investigations in the field of polymer nanocomposites reveal that introducing reinforcing agents into the polymer matrix can alter the mechanical properties in different ways. For instance, in graphene nanoplatelet/epoxy nanocomposites, the mechanical behavior remains relatively consistent across four separate configurations. An increase in grafting density can generate beneficial effects on the strengthening mechanism as well as the dispersion of grafted nanorods. However, extremely high polarity may trigger hydrogen bond formation within the polymer, which in turn influences interfacial adhesion.

Research on polymer matrix nanocomposites containing silica nanoparticles, fullerene-60, carbon nanotubes, and defective nanotubes has shown that increasing the filler weight fraction leads to higher elastic modulus values. Consequently, with the increase in filler volume fraction, the rate of plastic hardening decreases. In addition, a rise in nanoparticle mass fraction or an increase in nanoparticle surface area enhances the yield strength and elastic modulus of the composites. Strengthened hydrogen bonds and modified silicate chains can also help suppress crack propagation during loading.

In polylactic acid composites with rising concentrations of graphene oxide, significant improvements are observed in Young's modulus, shear modulus, and compressive modulus. Similarly, because the bonding energy between PVA and functionalized graphene oxide surpasses that of PVA with unmodified graphene oxide, the mechanical performance of PVA/functionalized graphene oxide composites is enhanced. In general, increasing nanoparticle concentration in polymer nanocomposites produces higher elastic modulus values. The interphase model demonstrates that elastic properties of composites can be further improved, with the Young's modulus being particularly sensitive to nanoparticle radius and volume fraction.

Studies on polymer nanocomposites with nanoparticle fillers show that as bond density or bonded-chain length increases, fracture resistance first rises and then declines. In graphene/PEG systems, only a weak interaction between the two constituents has been observed, while polymer density near the graphene surface tends to increase as temperature decreases. Furthermore, enlarging the diameter of carbon nanotubes results in nearly a threefold increase in longitudinal Young's modulus and about a twofold increase in transverse Young's modulus.

Different conclusions have been reported for nanocomposites with nanoparticles and nanotubes. For example, some findings indicate that the polymer surface layer is not actually a "dead layer." Conversely, the use of bone-shaped carbon nanotubes as a reinforcement considerably increases surface binding energy, which in turn enhances both surface and overall strength of the nanocomposite.

Other studies highlight that the dynamic and structural properties of polymer chains at length scales comparable to nanoparticle size play a key role in nanoparticle diffusion. Broadly speaking, the mechanical and thermal behaviors of nanocomposites are strongly governed by the composition and modeling approach applied.

It has also been demonstrated that surface chemical bonding and polymer chain length substantially affect the mechanical and viscoelastic characteristics of polymer matrix nanocomposites. Likewise, both the aspect ratio index and the connectivity pattern of nanorods influence electrical conductivity and the percolation threshold. With higher filler volume fractions, conductivity becomes more stable. From a tribological standpoint, graphene as a reinforcing phase increases Young's modulus, shear modulus, and bulk modulus of polymers. Moreover, graphene-polymer nanocomposites with a more constrained structure show enhanced elastic modulus and greater impact resistance. Similarly, nanostructured polymer systems contribute to improvements in dielectric, thermal, and tribological properties.

Overall, reinforcement effects on the global properties of nanocomposites have been widely documented. Key mechanical indicators such as Young's modulus, compressive modulus, shear modulus, and overall strength have been analyzed, along with studies on dynamic response and impact performance. Crack initiation and progression, as well as impact damage, have also been addressed.

Nevertheless, despite significant progress, there remain open areas for future work on polymer-based nanocomposites. One important direction is to investigate how temperature fluctuations and strain rates influence mechanical performance. Temperature variation can cause nanocomposites to behave differently across ranges, potentially increasing or reducing strength. Likewise, strain rate is a major factor, affecting tensile and compressive moduli as well as overall strength, and therefore deserves deeper analysis.

From existing literature, it is evident that polymer nanocomposites are highly promising, and identifying the optimal combination of parameters to maximize mechanical properties remains a central research objective. To achieve this efficiently, instead of relying solely on repeated experimental trials and high costs, optimization approaches and artificial intelligence techniques can be employed. Among such tools, the Box–Behnken design (BBD) and central composite design (CCD) are recognized as particularly valuable for designing experiments in this domain. These approaches allow researchers to determine maximum property values without extensive experimentation, validating outcomes afterward through laboratory testing.

A strong recommendation for predictive analysis of polymer nanocomposite properties under varying conditions is the integration of molecular dynamics simulations with machine learning regression models. A comprehensive dataset capturing nanocomposite mechanical properties can be generated through simulations and subsequently used as input for machine learning algorithms, enabling efficient training and validation.

CONCLUSION

Molecular dynamics simulations have emerged as a critical tool for understanding and predicting the behavior of polymer nanocomposites at the atomic level. By providing insight into interfacial bonding, load transfer mechanisms, and transport phenomena, MD simulations complement experimental studies and enable the rational design of advanced materials. While current methodologies offer significant benefits, challenges remain—including computational limitations, force field development, and unequal access to computational resources and software, which can be a barrier for some research groups. Future research should prioritize multiscale modeling, machine learning integration, and validation through experimental data to advance the predictive power and practical utility of simulation-based approaches.

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Authors' Contributions

All authors participated in the design and implementation of the research, data analysis, and manuscript preparation.

Conflicts of Interest/Competing Interests

The authors declare that they have no conflicts of interest or competing interests.

Data and Code Availability

No custom code was developed for this study. All data and materials supporting the findings are included within the manuscript.

Supplementary Information

This manuscript does not contain any supplementary material. All relevant information is presented in the main text.

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