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RESEARCH PAPER

Molecular Dynamics Simulation of PMMA Nanocomposites Reinforced with Ag_2O and TiO_2 Nanoparticles

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Abstract

In recent years, nanocomposites have attracted significant attention from researchers. Since experimental evaluation of their mechanical and physical properties is often costly and time-consuming, simulations are recommended as an efficient alternative for predicting these characteristics. In this study, nanocomposites composed of polymethyl methacrylate (PMMA) reinforced with biocompatible and biodegradable silver oxide (Ag_2O) and titanium oxide (TiO_2) nanoparticles were simulated. Molecular dynamics (MD) simulations were conducted using Materials Studio software to estimate the mechanical and physical properties of these nanocomposites. The study first examined the properties of pure PMMA, including Young's modulus, Poisson's ratio, and density. It then evaluated the properties of the nanocomposites at varying TiO_2 concentrations (0, 5, 10, 15, and 20 weight percent (wt%)) through MD optimization and calculation. The results showed strong agreement with experimental data for the pure material, and the predicted properties of the nanocomposites provide valuable insights prior to fabrication. These nanocomposites are proposed for biomedical applications, particularly in the treatment of trauma and infected wounds, due to the biocompatibility of PMMA, which is approved by the U.S. Food and Drug Administration (FDA).

Keywords: Polymethyl methacrylate, Silver oxide, Titanium oxide, Mechanical and physical properties, Molecular dynamic, Materials studio

1. Introduction

Due to advances in numerical methods, simulation at the atomic and molecular scale is nowadays possible [1]. Some of these methods are based on molecular mechanics [2]. The molecular dynamics method and the Monte Carlo method are the most well-known molecular mechanics-based methods [3]. In the molecular dynamics method, the equations of motion are solved to determine the direction of movement or the location of atoms and molecules. In recent years, molecular dynamics as a novel tool in the modeling of nanosystems has been the focus of researchers [4-

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6]. Molecular dynamics is a powerful tool utilized across various engineering fields such as materials, chemical, mechanical, and genetic engineering to reduce laboratory costs by simulating complex physical and chemical processes [7]. Many researchers have also used this tool to design new materials [2]. The use of this tool is rapidly expanding in engineering [8-10]. With the completion of molecular dynamics-related software and the increasing speed of computing speed in hardware, we can hope to apply atomic-scale simulations, including molecular dynamics, to all of the engineering sciences and computational methods over the next two decades and change the design [6, 11]. The main tool for conducting the simulation in this study is molecular dynamics [12]. The main reason for choosing this tool is that classical mechanics such as micromechanics theory is not a robust tool in analyzing and calculating the mechanical properties of nanocomposites and the accuracy and possibilities of this method by many researchers have been challenged [13-15], on the other hand, to conduct experimental experiments on nanostructures because of the high cost and the difficulty of implementing them at present [16]. Molecular dynamics is an experimental-theoretical method by which the properties of nanostructures can be calculated with respect to chemical constituents and force interactions between atoms [4, 17]. It is noteworthy that molecular dynamics [18], like laboratory methods, is accompanied by challenges and inaccuracies [19]. Sample selection, time to equilibrium, and the likelihood of instability during measurement can be the source of error. The limitation of the molecular dynamics method is also the computational volume constraint [20]. Molecular dynamics is currently used for systems up to 100,000 atoms [17, 21, 22]. The dimensions of the molecular dynamics simulation box are up to about 10 nm and the simulation interval is less than nanoseconds [23]. It should be noted that the molecular dynamics of individual applications also apply to practical laboratory methods [24]. For example, doing some experiments is very difficult and costly, whereas with molecular dynamics it is much easier and more cost-effective to do the experiments. These include calculating the properties of materials at temperatures near absolute zero, performing simple tensile tests on nanostructures or biological molecules, and the motion of dislocations and boundaries during metal deformation. In the field of molecular dynamics (MD), although the experimental behavior of PMMA nanocomposites reinforced with TiO_2 and Ag_2O has been previously studied, such methods are often limited in their ability to probe atomic-scale interactions and predict behavior under varied conditions. MD simulations enable precise control over nanoparticle dispersion, interfacial bonding, and external conditions such as temperature and pressure factors that are difficult to isolate experimentally. Moreover, MD allows for the exploration of nanoscale mechanical responses and interatomic force effects, providing fundamental insights into the influence of nanoparticle content and distribution on material properties [25]. This computational approach also offers a cost-effective and time-efficient alternative for pre-screening formulations before fabrication, helping to optimize composition and structure for targeted applications such as biomedical devices and wound treatment materials.

While previous experimental studies have examined the mechanical behavior of PMMA nanocomposites reinforced with TiO_2 and Ag_2O, most have focused on bulk-scale properties or averaged performance metrics without revealing nanoscale interfacial effects. Furthermore, existing MD simulations on polymer nanocomposites have primarily investigated systems with either a single nanoparticle type or different base polymers such as epoxy or polyethylene. In contrast, this study uniquely combines biocompatible PMMA with two inorganic nanoparticles Ag_2O and TiO_2 across a controlled range of concentrations [26]. By simulating their interactions at the atomic level, we aim to uncover the distinct effects of dual-phase reinforcement on density, modulus, and Poisson's ratio, offering predictive insights that are not directly observable through experimental techniques [27]. This multiscale design strategy provides a novel framework for engineering customized nanocomposites for biomedical use.

Despite extensive experimental and computational efforts to understand polymer-based nanocomposites, existing studies often focus on single-phase nanoparticle systems or lack detailed atomic-scale validation against experimental data. Most molecular dynamics (MD) simulations examine either TiO_2 or Ag_2O as isolated reinforcements, with limited exploration of their combined effects in a biocompatible polymer like PMMA. Furthermore, prior works rarely address how varying the ratio of dual nanoparticles influences the mechanical properties of the resulting nanocomposite.

To address these gaps, the present study develops a three-phase nanocomposite composed of PMMA, silver oxide (Ag_2O), and titanium oxide (TiO_2) using molecular dynamics simulations in Materials Studio. The novelty of this work lies in the integration of dual-phase inorganic nanoparticles with PMMA and the systematic investigation of mechanical and physical properties across five different TiO_2 concentrations (0–20 wt%). Key objectives include evaluating density, Young's modulus, shear modulus, and Poisson's ratio, and comparing simulated results against experimental benchmarks to validate the model. This study provides new insights into nanocomposite behavior at the atomic level and offers predictive guidance for future experimental design in biomedical applications.

2. Simulation Process of Mechanical Properties on Materials Studio

The simulated nanocomposite includes of (Ag_2O-TiO_2-PMMA) as introduced, consists of nano particles as reinforcements (Ag_2O/TiO_2) and one phase as a polymer field (PMMA). In this section, the atomic structure of (Ag_2O-TiO_2-PMMA) is introduced. In the final analysis, the ensembles of NVE, NVT and NPT are performed.

2.1. Silver oxide molecular structure

The development of new bacterial resistance to antibiotics is a major health issue since silver nanoparticles have antibacterial, antifungal, antiviral and protozoal properties. It is used for all touch surfaces, such as in hospitals, offices, public places, and even in residential homes. In addition to its antibacterial properties, silver nanoparticles have properties such as anti-fungal and anti-inflammatory effects, environmental compatibility, non-stimulants and non-allergens, lack of resistance to microorganisms, heat resistance, and high stability. The antibacterial properties of the particles have made it widely used in wound dressings and all other materials involved in the wound healing process. In this paper, as shown in Figure (1) Ag_2O nanoparticles have been used as reinforcements.

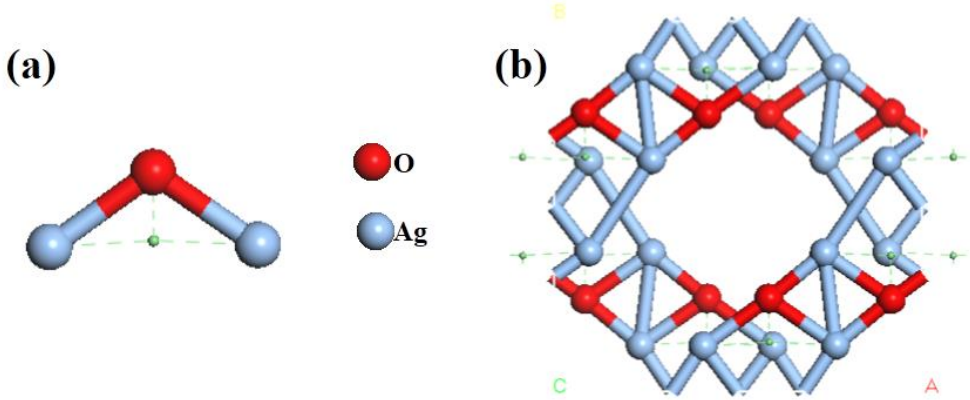


Fig 1: (a): Ag_2O molecule with single bond **(b):** Spherical crystalline Ag_2O

2.2. Titanium oxide molecular structure

Titanium oxide (TiO_2) nanoparticles, as illustrated in Figure 2, were used as reinforcement agents in the modeling of the nanocomposite. It is not classified as hazardous according to the United Nations harmonized system of classification and labeling. Today it is used as the main building for implants in medical and dental science.

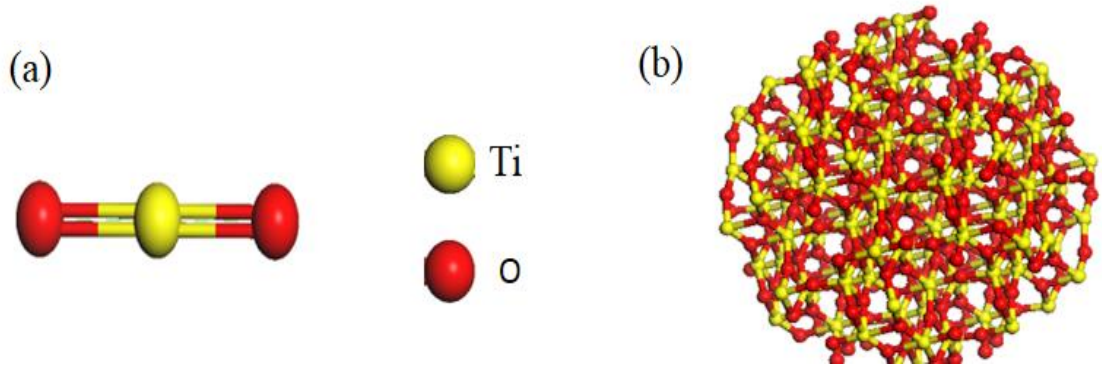


Figure (2): (a): TiO_2 molecule with dual bond **(b):** Spherical crystalline TiO_2

2.3. Polymethyl methacrylate molecular structure

Due to the above biological compatibility, poly (methyl methacrylate) is a common ingredient in modern dentistry. It is especially used in the manufacture of dental prostheses, artificial teeth and orthodontic appliances. Polymethyl methacrylate polymer as shown in figure (3) with a chemical formula ($(C_5O_2H_8)_n$) have been used as a matrix for the modeling of this nanocomposite.

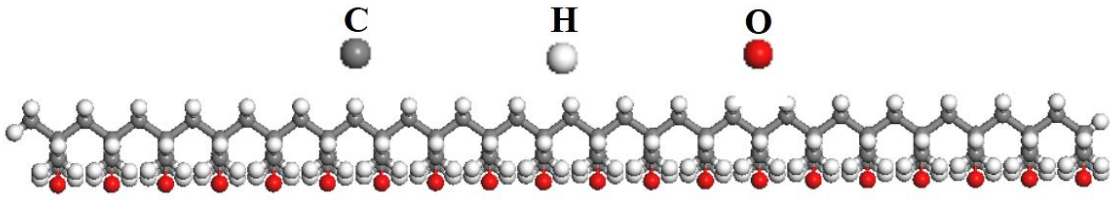


Fig 3: Poly (methyl methacrylate) polymer with 20 chains simulation

2.4. Simulation steps

In this paper, the molecular dynamics method is used to extract the mechanical and physical properties of simulated nanocomposites. The following steps have been taken to complete the molecular dynamics method:

2.4.0. Optimization Objective Function

Before performing ensemble simulations, geometry optimization was carried out to minimize the total potential energy of the nanocomposite system. The objective function in this optimization was the total energy of the system, which includes contributions from bond stretching, angle bending, torsional rotations, van der Waals interactions, and electrostatic forces. The goal was to find a stable atomic configuration corresponding to a local energy minimum, which reflects the most physically realistic structure prior to dynamic equilibration. The Forcite module in Materials Studio was used to perform this energy minimization using the COMPASS force field. The system was considered optimized when the energy convergence criteria (e.g., force and displacement thresholds) were met, ensuring that the atomic forces were minimized and the structure reached a mechanically stable equilibrium state.

2.4.1. Ensemble of NVE

At this stage, the simulation box is placed at a temperature of 298 K under NVE (constant Number of particles, Volume, and Energy). The purpose of this study is to investigate the kinetic energies and potentials of a thermodynamic isolation system. At this stage, the system is subjected to 1 atmospheric pressure under NVE. The simulation time is considered 50 ps.

2.4.2. NVT Ensemble

In this step, the simulation box is maintained at a temperature of 298 K using the NVT (constant Number of particles, Volume, and Temperature) ensemble. The primary purpose of applying the NVT ensemble is to energize the system, allowing atoms to move and gradually reach equilibrium. In other words, the NVT stage helps relax the internal stresses introduced during the initial construction of the simulation box by enabling atomic movement. An initial system density of 0.9 g/cm³ is assumed to allow sufficient molecular displacement toward a more stable configuration. The simulation time for this phase is set to 50 picoseconds (ps).

2.4.3. NPT Ensemble

Density is a key physical property in atomic-scale modeling, reflecting how closely packed atoms are in a system at equilibrium. When the molecular modeling process is properly executed, the simulated atomic density should closely match the material's actual macroscopic density. Different ensembles introduce varying conditions that influence atomic behavior; thus, tracking the convergence of properties like density over time serves as a validation of simulation accuracy. At this stage, the system is equilibrated at atmospheric pressure (1 atm) and a constant temperature of 298 K using the NPT ensemble (constant number of particles, pressure, and temperature). The goal is to adjust the system density to align with the true material density and relieve any residual stress. The NPT simulation also runs for 50 ps.

2.5. Simulation Methodology

In this section, both mechanical properties (Young's modulus and Poisson's ratio) and physical properties (density) of the pure polymer and the nanocomposite system (Ag_2O–TiO_2–PMMA) are calculated, as illustrated in Figure 4. To model the porous nanocomposite, a total of 25 wt% of nanoparticles (Ag_2O and TiO_2 combined) was incorporated, while the polymer (PMMA) content was kept constant at 75 wt%. The total mass of the composite was 8 grams, with 6 grams attributed to the PMMA matrix.

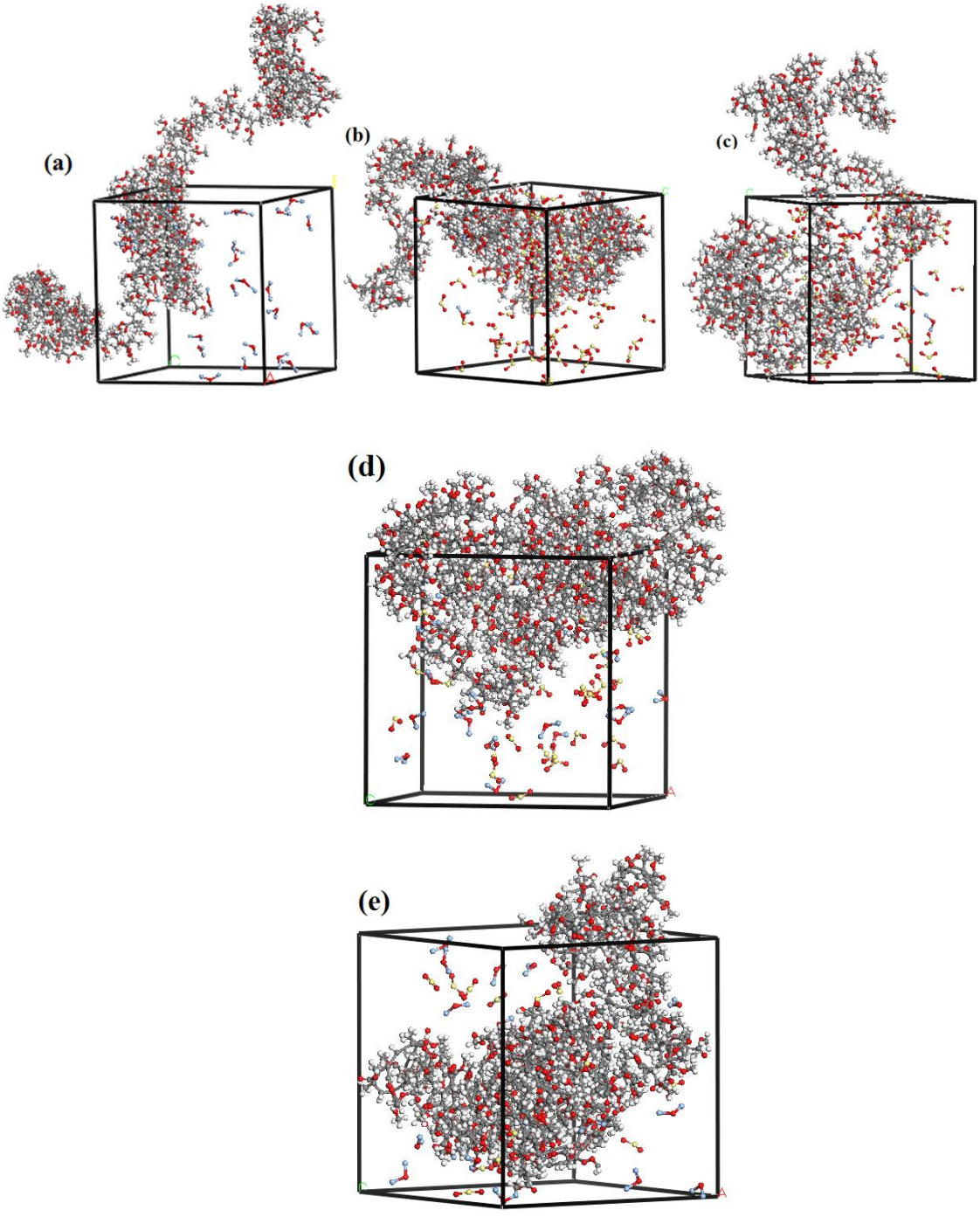


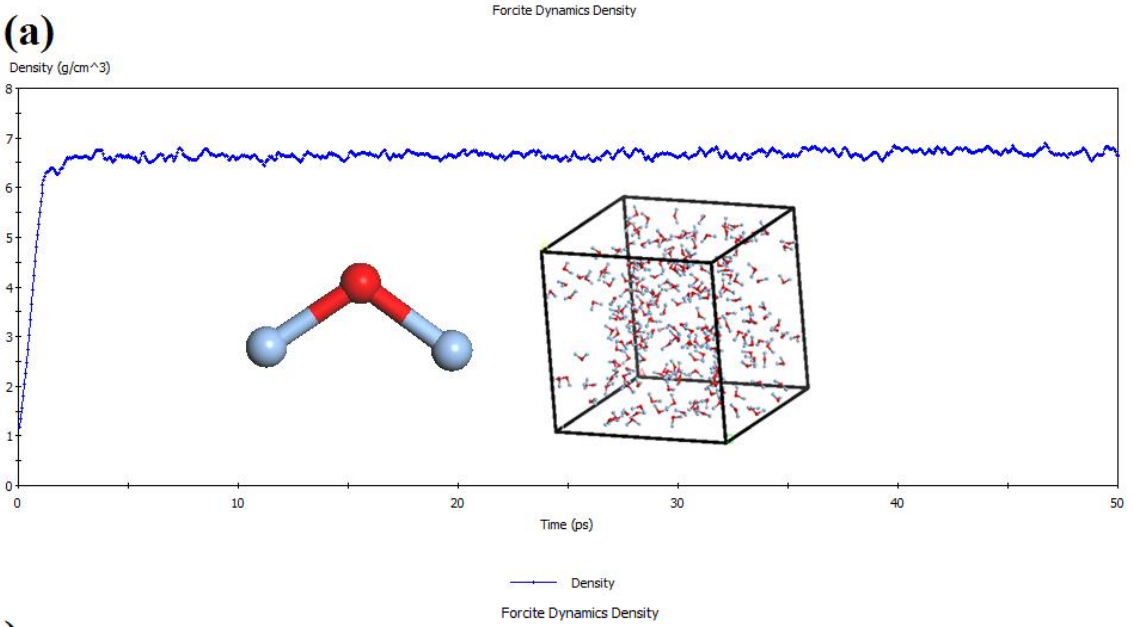
Fig 4: Simulation of nanocomposite include of **(a):** 0 wt%, **(b):** 5 wt %, **(c):** 10 wt%, **(d):** 15 wt % and **(e):** 20 wt % of TiO_2 in the Ag_2O and

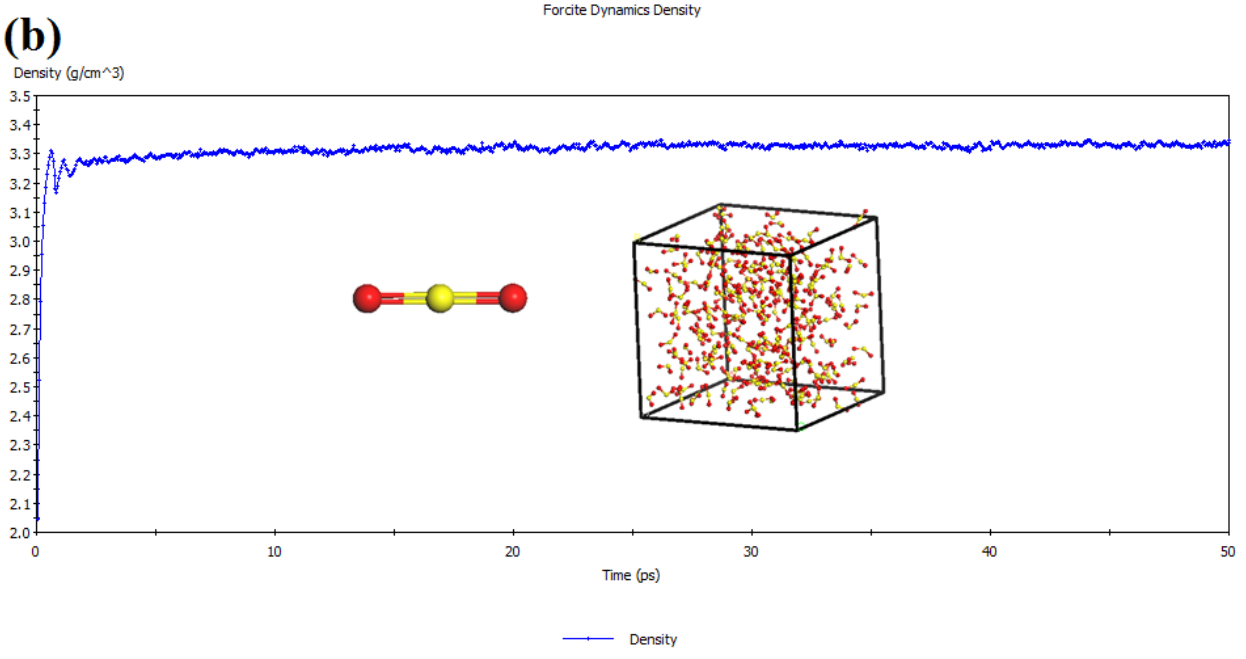
PMMA microstructure simulated in the MD software

3. Validation, results, and discussion

3.1. Results of molecular dynamics for pure materials

The mechanical properties and density of (Ag_2O-TiO_2-PMMA) as shown in figure (5) with follow of steps were described and extracted separately. To draw the density diagram, first, the simulated NVT to maximize the energy of system and then the NPT was plotted to show the density. Table (1) has been shown the comparison of mechanical and physical properties of (Ag_2O-TiO_2-PMMA) with Molecular dynamics modeling and laboratory analysis.





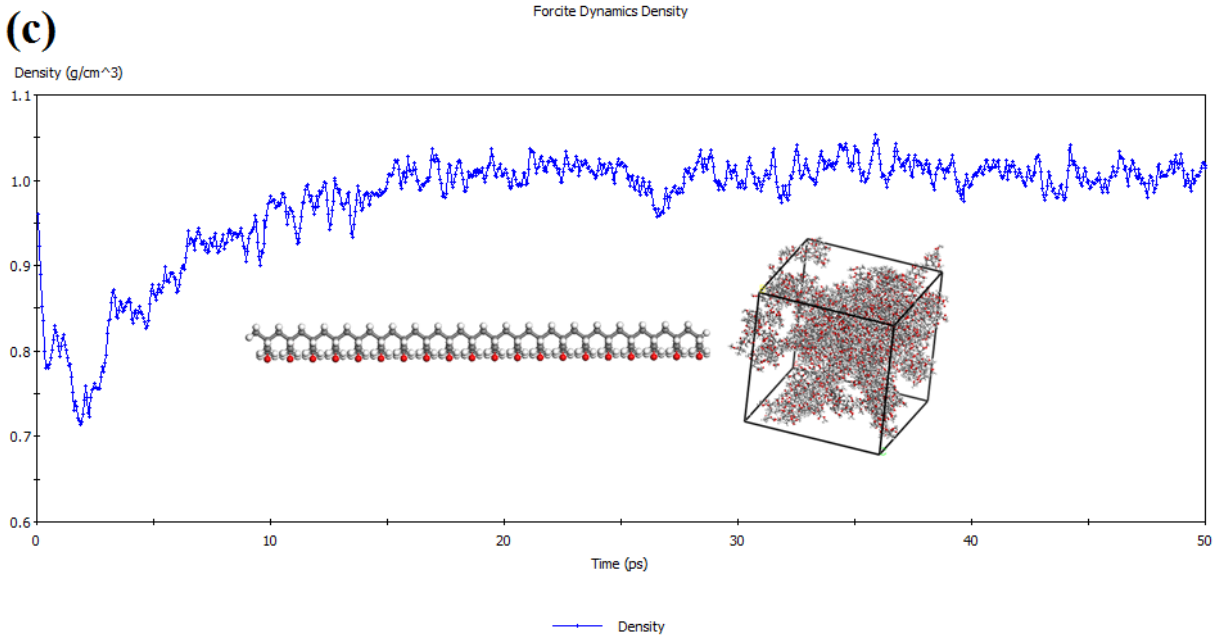


Fig 5: Diagram of density for pure materials **(a):** Ag_2O **(b):** TiO_2 **(c):** PMMA

Table 1: Comparison of mechanical and physical properties of (Ag_2O-TiO_2-PMMA) using by Molecular dynamics method with laboratory analysis

Comparison of mechanical and physical properties of (Ag_2O) using by molecular dynamics modeling with laboratory analysis			
Mechanical and physical properties	Simulation	Laboratory	percentage error between simulation and laboratory test
Density (g/cm^3)	6.70	7.20	6.94
Young modulus (GPa)	69.00	69.60	0.86
Possion ratio	0.20	0.37	45.94
Comparison of mechanical and physical properties of (TiO_2) nanoparticles using by molecular dynamics modeling with laboratory analysis			
Mechanical and physical properties	Simulation	Laboratory	percentage error between simulation and laboratory test
Density (g/cm^3)	3.20	3.97	19.39
Young modulus (GPa)	222.00	230.00	3.47
Possion ratio	0.20	0.27	25.92
Comparison of mechanical and physical properties of (PMMA) using by molecular dynamics modeling with laboratory analysis			
Mechanical and physical properties	Simulation	Laboratory	percentage error between simulation and laboratory test
Density (g/cm^3)	1.01	0.94	6.93
Young modulus (GPa)	2.50	3.00	16.00
Possion ratio	0.10	0.30	66.66

While the simulation results for Young's modulus in most materials are relatively close to experimental values, notable discrepancies exist in the predicted values for Poisson's ratio and density particularly for PMMA and TiO_2. For instance, the difference in Poisson's ratio for PMMA exceeds 65%, and density differences for TiO_2 approach 19%. These deviations highlight limitations in the MD modeling framework, especially in accurately reproducing certain nonlinear or interatomic behaviors such as lateral deformation or amorphous packing effects.

Such differences can arise due to several factors:

- The size limitations of the simulation box (nanometer scale) may not fully capture bulk behavior.
- The assumptions of isotropy and perfect bonding in the force field (COMPASS) may oversimplify real-world heterogeneities.
- Experimental measurements, especially for Poisson's ratio in polymers, often involve temperature-, time-, or strain-rate-dependent behavior that is not fully replicated under constant MD conditions.

These limitations are common in MD-based studies of polymer nanocomposites. However, despite the numerical

gaps, the trends in mechanical property evolution and qualitative agreement still provide valuable insight for materials design at the nanoscale.

3.2. Diagram of Radial Distribution Function

One of the key parameters used to assess the equilibrium state of a system in molecular dynamics simulations is the radial distribution function (RDF). RDF provides insight into the spatial distribution of atoms by describing how atomic density varies as a function of distance from a reference particle. It quantitatively represents mass distribution within the system at the atomic scale and is defined by Equation (1).

$$g(r) = \frac{\rho(r)}{\rho} = \frac{\langle N(r \pm \frac{\Delta r}{2}) \rangle}{\Omega(r \pm \frac{\Delta r}{2})} \frac{1}{\rho}, \tag{1}$$

In this respect $\frac{\rho(r)}{\rho}$ the density of the number of atoms in the shell to the radius (r) in volume of $\Omega(r \pm \frac{\Delta r}{2})$ and ρ is the density of the number of atoms in the total volume of the system. For solids, the RDF at distances as shown in figure (6) must converge to the value of 1. And it is a measure of the equilibrium of a solid atom's system.

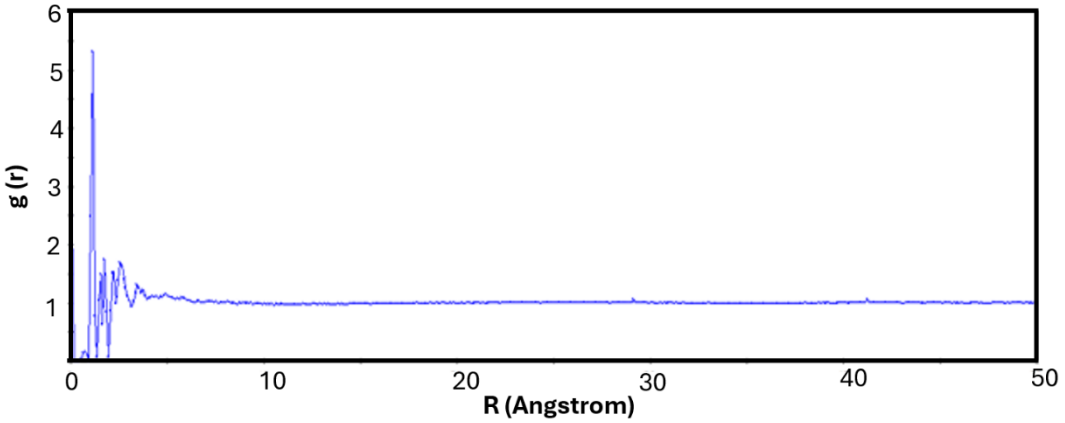


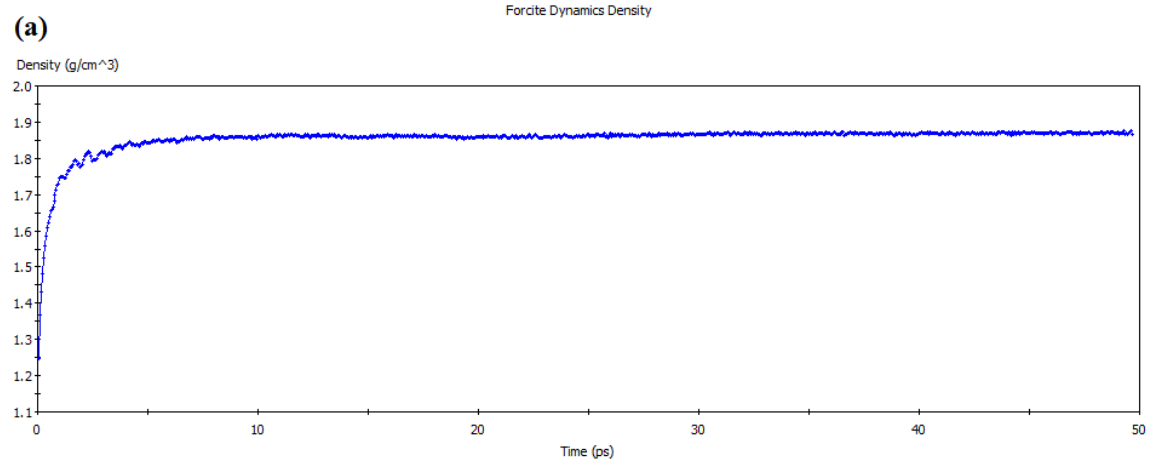
Fig 6: Diagram of the radial distribution of atoms and their convergence to the number 1

3.3. Extraction of Physical and Mechanical Properties of the Simulated Nanocomposite

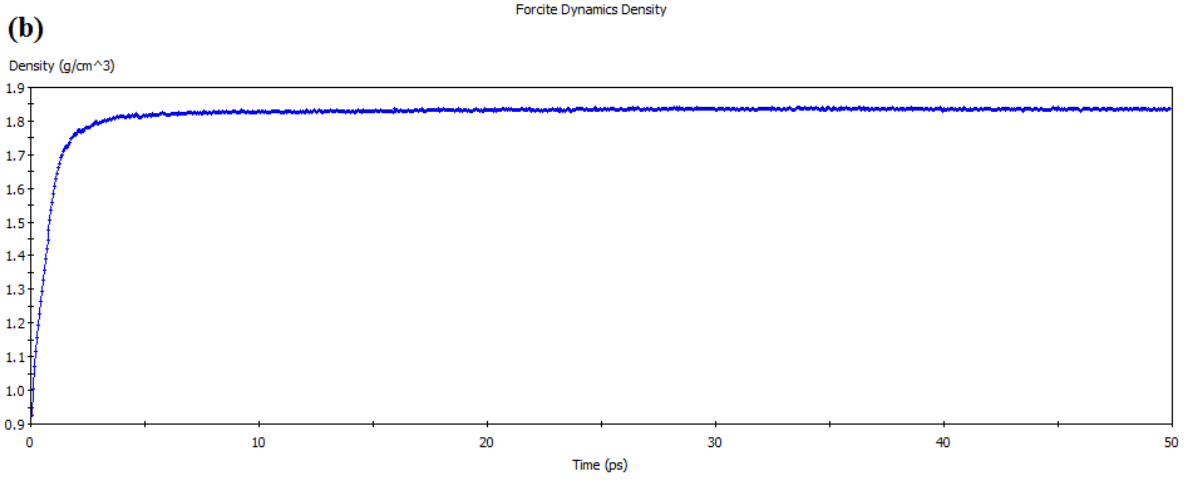
The primary objective of this study is to extract and simulate the physical and mechanical properties of a three-phase nanocomposite using molecular dynamics (MD). However, direct simulation of nanoscale composites using MD tools is often limited by computational constraints. For accurate modeling, the molecular structure of the nanocomposite must ensure that interatomic distances reflect those found in real materials. Achieving this level of precision typically requires a simulation box on the order of 100 nm, which exceeds the capabilities of most current MD simulation platforms.

To address this limitation, this study employs molecular dynamics to simulate the mechanical behavior of nanocomposites using scaled molecular models. The mechanical and physical properties of the individual components (one-phase models) were discussed in the previous section. In the current section, the predicted properties of the three-phase nanocomposites are presented in Table 2 and illustrated in Figure 7.

(a)


Forcite Dynamics Density
Density (g/cm^3)
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
0
10
20
30
40
50
Time (ps)

(b)


Forcite Dynamics Density
Density (g/cm^3)
1.9
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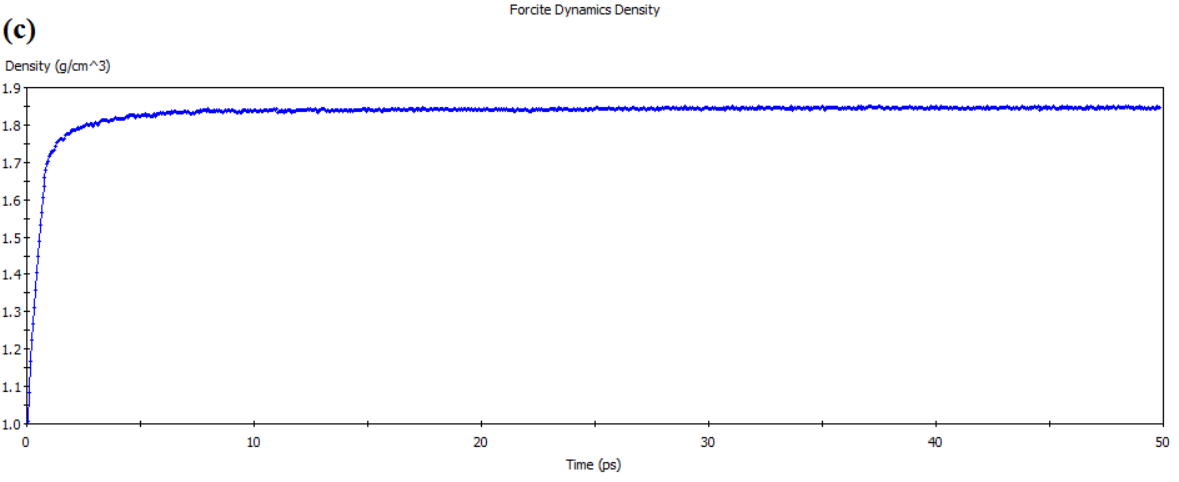
Time (ps)

(c)


Forcite Dynamics Density
Density (g/cm^3)
1.9
1.8
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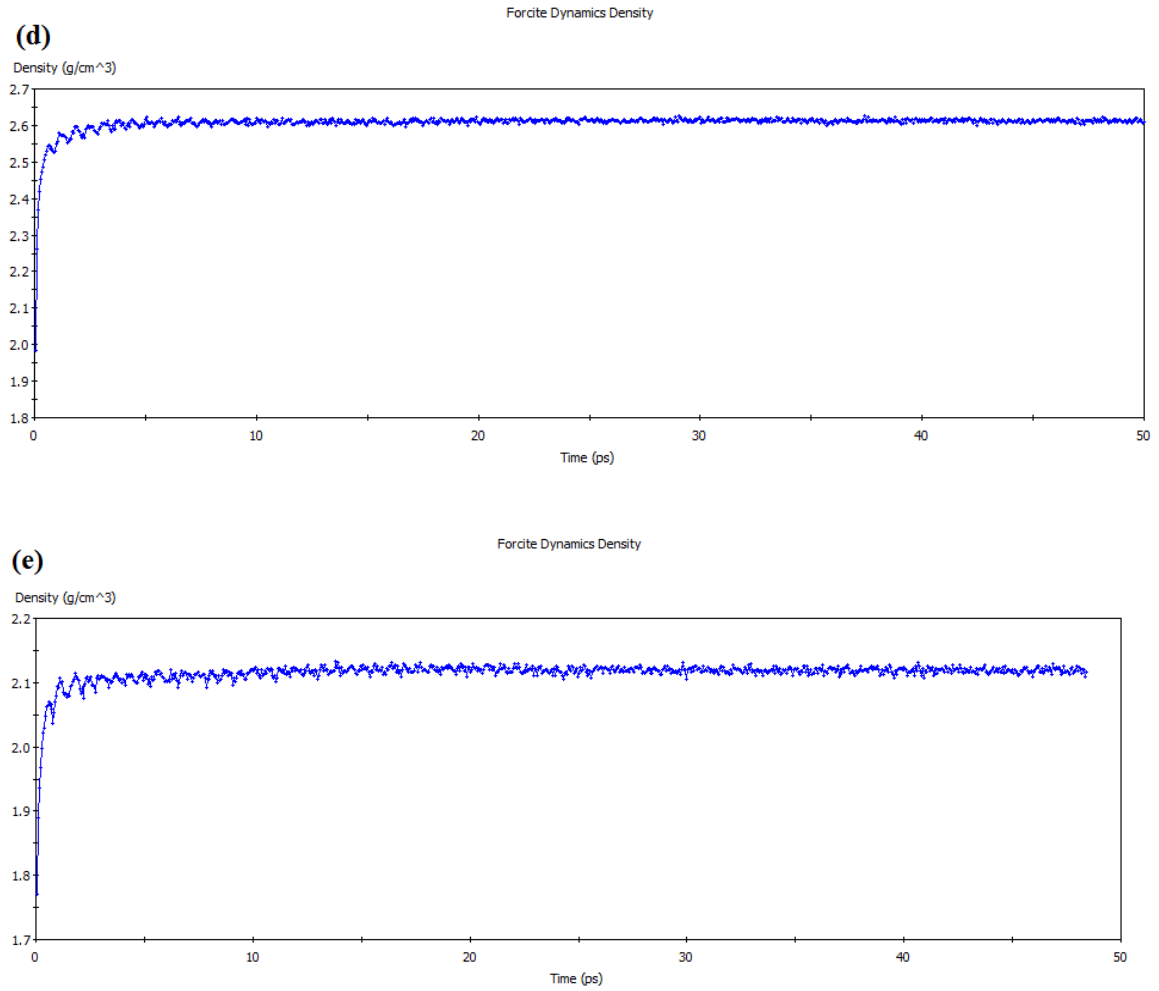

Fig 7: Diagram of density for (**a):** 0 wt% (**b):** 5 wt% (**c):** 10 wt% (**d):** 15 wt% and (**e):** 20 wt% of TiO_2

Figure 7 illustrates the variation in nanocomposite density as a function of TiO_2 concentration (0 wt% to 20 wt%), while keeping the PMMA matrix constant at 75 wt% and adjusting the Ag_2O content accordingly. The general trend shows an increase in density with rising TiO_2 content up to 15 wt%, which is expected due to the higher intrinsic density of TiO_2 compared to both PMMA and Ag_2O. However, a slight decrease in density at 20 wt% TiO_2 is observed, which may result from packing inefficiencies or local structural distortions at higher nanoparticle loading. This nonlinear behavior highlights the complex interplay between filler content, particle dispersion, and matrix-filler interfacial interactions. The density peak at 15 wt% suggests an optimal filler ratio for maximizing material compactness before aggregation effects begin to dominate. Such insights are difficult to obtain experimentally, underscoring the strength of MD simulations in probing atomistic packing and structural evolution.

Table 2: Predicting the mechanical and physical properties of simulated nanocomposite

Ag_2O (25%) +TiO_2 (0%) +PMMA (75%)			
Density (g/cm^3)	Young modulus (GPa)	Shear modulus (GPa)	Possion ratio
1.85	9.80	3.77	0.3
Ag_2O (20%) +TiO_2 (5%) +PMMA (75%)			
Density (g/cm^3)	Young modulus (GPa)	Shear modulus (GPa)	Possion ratio
1.80	3.36	10.00	0.20
Ag_2O (15%) +TiO_2 (10%) +PMMA (75%)			
Density (g/cm^3)	Young modulus (GPa)	Shear modulus (GPa)	Possion ratio
1.80	80.71	19.71	0.18
Ag_2O (10%) +TiO_2 (15%) +PMMA (75%)			
Density (g/cm^3)	Young modulus (GPa)	Shear modulus (GPa)	Possion ratio
2.60	169.00	36.86	0.17
Ag_2O (5%) +TiO_2 (20%) +PMMA (75%)			

Density (g/cm^3)	Young modulus (GPa)	Shear modulus (GPa)	Possion ratio
2.10	148.07	1.20	0.24

Compared to prior molecular dynamics studies, which often examine a single nanoparticle in isolation or lack validation against experimental benchmarks, this study integrates dual-nanoparticle reinforcement and compares simulation results with real-world experimental data for Ag_2O, TiO_2, and PMMA. This validation step enhances the reliability of the predictions. Furthermore, by modeling five different TiO_2 weight fractions while keeping the PMMA matrix constant, we provide a systematic understanding of how varying nanoparticle ratios impact mechanical performance. These findings help bridge the gap between computational design and practical material development particularly for biomedical applications where tuning mechanical and physical properties is crucial for implant compatibility, wound dressing durability, or drug delivery functionality.

4. Conclusions

This study employed molecular dynamics (MD) simulations to investigate the mechanical and physical properties of PMMA-based nanocomposites reinforced with silver oxide (Ag_2O) and titanium oxide (TiO_2) nanoparticles. Five different TiO_2 concentrations (0 wt% to 20 wt%) were modeled while maintaining the overall nanoparticle content at 25 wt% and the PMMA matrix at 75 wt%.

The simulation results revealed the following key findings:

- Density increased with TiO_2 content up to 15 wt%, peaking at 2.60 g/cm³, before slightly decreasing at 20 wt%, indicating a saturation point for effective nanoparticle packing.
- Young's modulus rose sharply with increased TiO_2 content, reaching a maximum of 169 GPa at 15 wt% TiO_2, suggesting significant reinforcement potential.
- Shear modulus followed a similar trend, confirming the strengthening role of dual-phase nanoparticles.
- Poisson's ratio showed inconsistent behavior, with some values (e.g., 0.70) exceeding the theoretical physical limits, indicating possible numerical instability or miscalculation that requires further refinement.

Although discrepancies were observed between simulated and experimental data particularly for Poisson's ratio and density the general trends in property enhancement and qualitative agreement support the validity of MD simulations for preliminary material screening.

Overall, this work demonstrates that MD simulations can provide valuable insight into the nanoscale mechanics of biocompatible polymer nanocomposites, enabling more informed design prior to fabrication. Future studies should focus on refining boundary conditions, increasing simulation box size, and using advanced force fields to improve quantitative accuracy.

Informed Consent Statement

Not applicable.

Data Availability Statement

Not applicable.

Conflicts of Interest

The authors declare no conflict of interest.

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