Predicting Mechanical and Physical Properties Nanocomposites Using Molecular Dynamics for Biomedical Applications

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Abstract.

This study focuses on simulating bio-nanocomposite structures using polycaprolactone as the polymer matrix, reinforced with hydroxyapatite and titanium dioxide nanoparticles, both of which are biocompatible and biodegradable. To predict key mechanical and physical properties and reduce experimental costs and time, molecular dynamics simulations were employed. The validation process began by evaluating the mechanical properties, including Young's modulus and Poisson's ratio, and physical properties such as density, for the pure components: polycaprolactone, hydroxyapatite, and titanium dioxide. The results were compared with available experimental data. Following this, the study analyzed the nanocomposites containing different amounts of titanium dioxide (0%, 5%, 10%, 15%, and 20% by weight), while maintaining a constant total weight of 25% for hydroxyapatite and titanium dioxide, and 75% for polycaprolactone. In the simulation, the total composite weight was set at 8 grams, with 6 grams allocated to polycaprolactone. The findings show that increasing the titanium dioxide content significantly improves the nanocomposite's mechanical properties due to the high stiffness of titanium. Specifically, compared to the sample without titanium dioxide, the addition of 20% titanium dioxide increased Young's modulus, Poisson's ratio, shear modulus, bulk modulus, and density by approximately 1.14, 3.01, 1.17, 5.99, and 14.85 times, respectively. To further verify these results, the stiffness matrix of the nanocomposites was computed using Materials Studio software.

Keywords: Hydroxyapatite; Titanium oxide; Polycaprolactone; Mechanical and physical properties; Molecular dynamics method

1. Introduction

Molecular dynamics (MD) simulation is a computational approach used to study and predict the physical behavior of atoms and molecules in a system by solving Newton's equations of motion [1]. In MD simulations, the interactions between particles are described by force fields, which include terms for bond stretching, angle bending, torsions, and non-bonded interactions such as van der Waals forces and electrostatic interactions [2, 3]. By simulating the trajectory of each particle over time, MD enables the study of properties such as mechanical strength, thermal stability, and molecular dynamics under specific conditions [4–6]. One of the key advantages of MD simulations is their ability to provide atomic-level insights into the behavior of materials, making it possible to model complex systems such as polymers, nanocomposites, and biological macromolecules [7, 8]. MD is particularly valuable for predicting properties like density, Young's modulus, Poisson's ratio, and thermal conductivity, which can be challenging to measure experimentally [9, 10]. The technique is widely used in fields such as materials science, biophysics, and nanotechnology to optimize designs, study interactions, and guide experimental efforts [11]. Experimental evaluation of nanocomposite properties often entails significant time and cost [12]. To address these challenges, computational approaches are increasingly employed for modeling, simulation, and property prediction of nanocomposites [13, 14]. Traditional computational techniques, such as the finite element method (FEM), are limited in their application to polymeric nanocomposites because they cannot account for the interatomic forces within polymers and nano- reinforcement molecules [15, 16]. Conversely, molecular dynamics (MD) simulations offer a robust alternative by modeling nanocomposites at the atomic scale, solving Newton's second law to define atomic coordination over time [17]. MD simulations accurately estimate atomic forces, making it possible to model and test new materials while predicting their properties [16, 18]. Although computational constraints limit the number of atoms and simulation dimensions (up to 10 nm) compared to real-world conditions, MD results have been validated through statistical mechanics in numerous studies. Known as a "virtual laboratory," MD translates atomistic-level interactions into macroscopic properties using

statistical mechanics, offering insights into temperature and pressure variations within the system [19–21]. Depending on the constants maintained, different statistical ensembles can be generated, and properties are derived from their averages or fluctuations [22–24]. MD simulations and complementary methods like lattice Boltzmann are widely used to estimate the physical and mechanical properties of fluids, nanofluids, polymers, and nanocomposites. These simulations are particularly valuable in the study of nanoscale materials, as experimental testing is often prohibitively expensive [25]. Molecular dynamics and Monte Carlo methods are among the most prominent molecular mechanics approaches [26]. With advancements in computational hardware and molecular dynamics software, atomic-scale simulations are expected to revolutionize engineering sciences in the coming decades by enabling cost-effective design and analysis [27]. Despite its advantages, MD simulations are computationally intensive, currently limited to systems of up to 100,000 atoms. Nevertheless, this method has been successfully applied in various fields. For instance, Aghadavoudi et al. [28] investigated the effect of defected carbon nanotubes (CNTs) on the mechanical properties of crosslinked epoxy nanocomposites, finding significant changes in shear modulus. In this study, MD simulations were conducted for pure materials and nanocomposites containing varying weight percentages of TiO_2 (0%, 5%, 10%, 15%, and 20%). The composite was modeled with a total weight of 8 grams, with 6 grams allocated to polycaprolactone (PCL), an FDA- approved biopolymer, and 2 grams to hydroxyapatite (HA) and TiO_2 nanoparticles. The simulations demonstrated that the inclusion of TiO_2 significantly enhances mechanical and physical properties, validating the utility of MD as a pre-experimental tool. These findings aid researchers in optimizing designs before fabrication, reducing costs and time. The resulting nanocomposite holds promise for biomedical applications, including advanced wound dressings and bandages for conditions such as Epidermolysis Bullosa (EB). Finally, the extracted mechanical and physical properties were compared with experimental results from the literature, affirming the accuracy and potential of MD simulations. Molecular dynamics (MD) simulations are computationally intensive, limiting their applicability to nanoscale systems and short timescales. To address these constraints, coarse-grained simulations can reduce computational demands by grouping atoms into pseudo-particles, enabling the study of larger systems. Hybrid methods, such as coupling MD with finite element modeling, allow localized atomistic phenomena to be integrated into larger-scale frameworks. Machine learning models trained on limited MD simulations can also predict material properties efficiently, reducing the need for extensive simulations. These approaches provide scalable solutions for

studying larger and more complex systems, addressing the computational limitations highlighted. The molecular dynamics (MD) simulations were conducted using the Materials Studio software with the COMPASS force field. The process began by constructing atomistic models for the nanocomposite containing hydroxyapatite (HA), titanium dioxide (TiO_2), and polycaprolactone (PCL). For each simulation, the proportion of TiO_2 was systematically varied (0%, 5%, 10%, 15%, and 20% by weight) while maintaining a constant total weight for the reinforcements (HA and TiO_2) at 25% and PCL at 75%. The simulations were performed under NVE, NVT, and NPT ensembles to predict density, elastic constants, and other mechanical properties. The novelty of this study lies in its comprehensive use of molecular dynamics simulations to optimize the mechanical and physical properties of a biocompatible nanocomposite system before experimental fabrication. While molecular dynamics as a method is well-established, its application in simulating the specific combination of polycaprolactone, hydroxyapatite, and titanium dioxide for biomedical applications is unique. This combination of materials was chosen for its tailored properties, addressing the demands of applications such as dental and bone implants, where biocompatibility, mechanical strength, and biodegradability are crucial. The model goes beyond conventional approaches by offering a systematic method to analyze the effects of varying titanium dioxide content on the nanocomposite's performance. Unlike traditional experimental methods, which can be resource-intensive and time-consuming, this simulation-based approach provides accurate predictions of properties like Young's modulus, shear modulus, bulk modulus, and density. The study offers a clear advantage by identifying an optimal composition range for titanium dioxide, maximizing mechanical enhancements without overloading the composite. Another aspect of novelty is the ability of the model to serve as a pre-fabrication tool. By predicting the stiffness matrix, density convergence, and elastic properties, researchers can eliminate unnecessary iterations in material synthesis. This accelerates the development process and reduces material waste, which is especially critical in biomedical applications where precision and cost- efficiency are paramount. Additionally, the study provides valuable insights into the nanoscale behavior of materials, which are difficult to capture through experimental techniques alone. The inclusion of titanium dioxide as a reinforcement, combined with hydroxyapatite and polycaprolactone, introduces a new level of complexity and functionality, making the composite more versatile for load-bearing biomedical applications. The results demonstrate how the interplay of these components can be optimized to achieve superior performance.

In summary, this study's novelty lies in its unique material combination, predictive capabilities, and cost-effective approach to designing advanced biomaterials. It bridges the gap between theoretical modeling and practical applications, providing a robust framework for developing next-generation nanocomposites tailored to specific biomedical needs. This innovative approach positions the work as a significant contribution to the field of computational materials science and biomedical engineering.

2. Simulation process of mechanical and physical properties based on MD method

Choosing HA-TiO_2 and PCL have numerous helpful features and some of them presented in Fig. 1 [27, 29–32]. The simulated nanocomposite boxes include HA-TiO_2 nanoparticles as reinforcements and PCL as a matrix. In this section, the atomic structure of (HA-TiO_2-PCL) is introduced. In the final analysis, the ensembles of NVE, NVT and NPT are performed to obtain and predict important properties such as (Young's modulus, Poisson's ratio, shear modulus, bulk modulus, and density).

Fig. 1 Some of significant and helpful application of (PCL-HA-TiO_2)

2.1 Introduction of HA, TiO_2 and PCL molecular structure

In recent years, bioceramics like hydroxyapatite have gained significant attention in medical and dental applications due to their excellent compatibility with biological tissues. Hydroxyapatite, with the chemical formula $Ca_5(PO_4)_3OH$, closely resembles the natural hydroxyapatite found in bone and teeth, which has the formula $Ca_{10}(PO_4)_6(OH)_2$. Known for its strong bonding ability with bone, hydroxyapatite exhibits a parallelogram-shaped crystalline structure, with dimensions of 34.34 × 32.66 × 32.34 angstroms, as depicted in Fig. 2. Titanium dioxide (TiO_2) nanoparticles have also been incorporated as reinforcements in the modeling of bio-nanocomposites, as shown in Fig. 2. Classified as non-hazardous by the United Nations Harmonized System of Classification and Labelling, TiO_2 is highly biocompatible. This property has made it a primary material for implants in the fields of medical and dental sciences. Polycaprolactone (PCL) is a semi-crystalline, hydrophobic polymer with the molecular formula $(C_6H_{10}O_2)_n$. It stands out for its remarkable mechanical flexibility, biocompatibility, biodegradability, and ease of processing. Approved by the Food and Drug Administration (FDA), PCL, as shown in Fig. 2, is widely utilized in biomedical applications due to its superior properties.

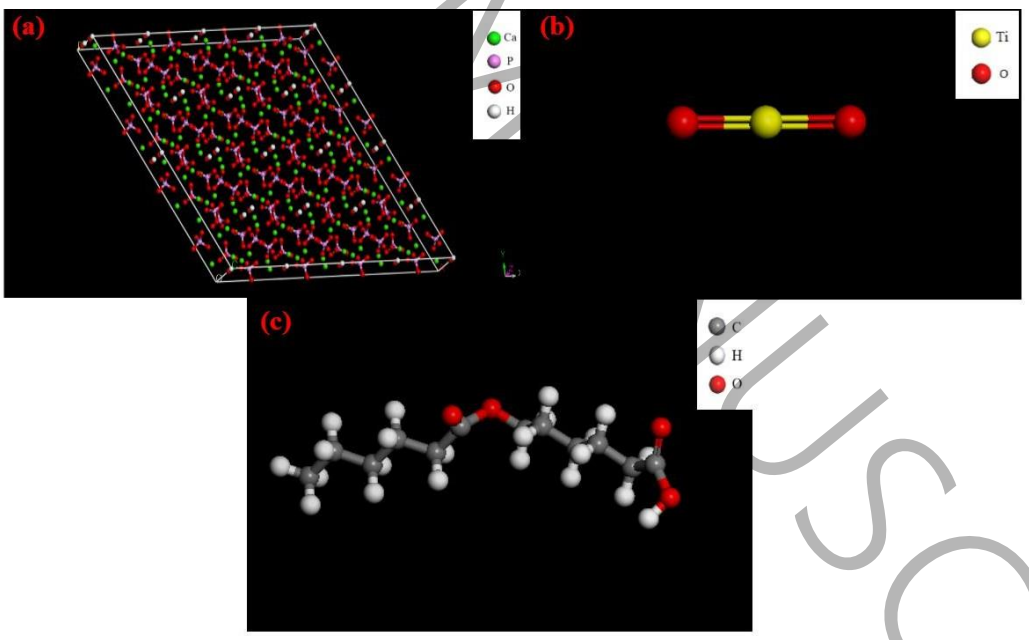


Fig. 2 Simulation atomistic model of (a): HA (b): TiO2 (c): PCL in materials studio software

2.2. Simulation steps, Force Field and Software

This study utilizes the molecular dynamics (MD) method to predict and analyze the key mechanical and physical properties of simulated nanocomposites. The increase in TiO_2 volume fraction was achieved by adjusting the number of TiO_2 nanoparticles while maintaining the same overall mass and volume for the system. The atomic configurations were recalculated to ensure uniform distribution within the simulation box. The uniform dispersion of TiO_2 nanoparticles assumed in the simulation is a simplification to enable accurate predictions of mechanical properties under ideal conditions. However, real-world composites often encounter aggregation due to interparticle interactions, leading to stress concentration and a reduction in mechanical performance. To address this limitation, future studies can incorporate non-uniform dispersion models to simulate aggregation effects. This can be achieved by integrating Monte Carlo methods or cluster analysis into the molecular dynamics framework, which would provide insights into the impact of aggregation on the material's properties. Additionally, experimental validation of nanoparticle distribution and its correlation with mechanical performance can be conducted to ensure the relevance of the simulation results to practical applications. By acknowledging and addressing these factors, the study can bridge the gap between idealized simulations and real-world scenarios, providing more comprehensive and applicable findings. The workflow for implementing the MD simulation is outlined in Fig. 3 and involves the following steps:

1. **Atomistic Model Creation**: Initial atomistic models were constructed using Materials Studio software. The Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies (COMPASS) force field was employed to model inter- and intra-atomic interactions. COMPASS parameters for covalent molecules have been rigorously validated through a variety of calculations, including extended MD simulations of liquids, crystals, and polymers. As the first ab initio force field, COMPASS is capable of accurately predicting the thermo-mechanical properties of polymers, including polymer nanocomposites. The uniform dispersion of nanoparticles was ensured by pre-relaxing the system using a Monte Carlo approach to minimize agglomeration. The COMPASS force field parameters were tuned to balance interparticle interactions. The dispersion quality was validated by observing uniform stress and energy distribution across the system during simulations.

2. **Simulation in NVE Ensemble**: In this step, the simulation was conducted under the NVE ensemble, where the total energy (sum of kinetic energy, KE, and potential energy, PE) remains conserved, while temperature (T) and pressure (P) are unregulated. Here, N (number of particles), V (volume), and E (energy) are kept constant. The simulation box was initialized at a temperature of 298 K, and the simulation was run for 50 picoseconds (ps).
3. **Simulation in NVT Ensemble**: The system was then simulated under the NVT ensemble, where temperature is regulated using a thermostat, introducing an additional degree of freedom in the conserved Hamiltonian (which includes KE and PE). Pressure remains unregulated in this phase. The simulation box was set at a constant temperature of 298 K, and an initial system density of 0.9 g/cm^3 was assumed to allow molecular and atomic rearrangements for optimization. The simulation time was again set to 50 ps.
4. **Simulation in NPT Ensemble**: In the final phase, the system was simulated under the NPT ensemble, where pressure is also regulated in addition to temperature. This ensemble is

critical for determining the system's physical properties, such as density, which must closely approximate the actual density of the material. By applying atmospheric pressure (1 atm) and maintaining a temperature of 298 K, the system density was brought closer to its real value. Additionally, this step helps eliminate residual stress within the system. The simulation duration for this phase was also set at 50 ps.

Overall, this stepwise approach ensures accurate prediction of material properties by iteratively refining the system's thermodynamic and structural parameters, aligning them with experimentally observed values.

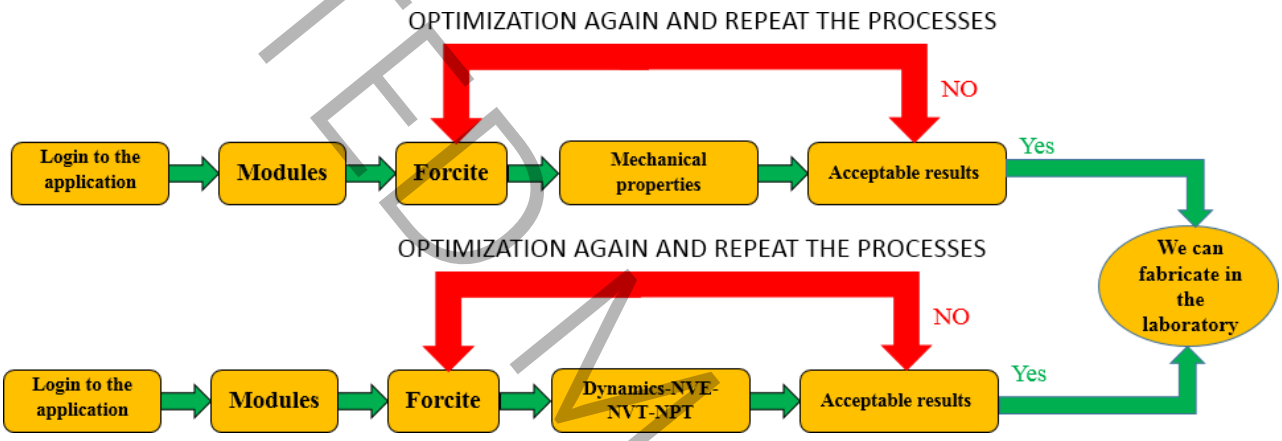


Fig. 3 Steps to obtain mechanical and physical properties using the materials studio software

2.3 Simulation methodology

In this section, the mechanical properties of the pure material, including Young's modulus and Poisson's ratio, as well as its physical properties, such as density, are simulated. Nanocomposite boxes composed of HA-TiO_2-PCL with varying titanium dioxide (TiO_2) contents (0, 5, 10, 15, and 20 wt%) are analyzed. For simulating porous nanocomposites using molecular dynamics software, the total weight percentage of silver oxide and titanium oxide was maintained at 25%, while the polymer (PCL) constituted a constant 75% of the total weight. The overall composite weight was set at 8 grams, with the polymer contributing 6 grams. Detailed molecular configurations for all five case studies are presented in Table 1.

Table 1 Details of five case study

Description	Mass of matrix and reinforcements (gr)			Volume fraction of matrix and reinforcements (%)			No. of atoms	Lattice dimensions (A°)
	TiO_2	HA	PCL	TiO_2	HA	PCL		
0% TiO_2	0	2	6	0	25	75	2900	33.2*33.2*33.2
5% TiO_2	0.4	1.6	6	5	20	75	2960	33.9*33.9*33.9
10% TiO_2	0.8	1.2	6	10	15	75	3383	34.4*34.4*34.4
15% TiO_2	1.2	0.8	6	15	10	75	3848	36.1*36.1*36.1
20% TiO_2	1.6	0.4	6	20	5	75	4245	37*37*37

3. Validation, results, and discussion

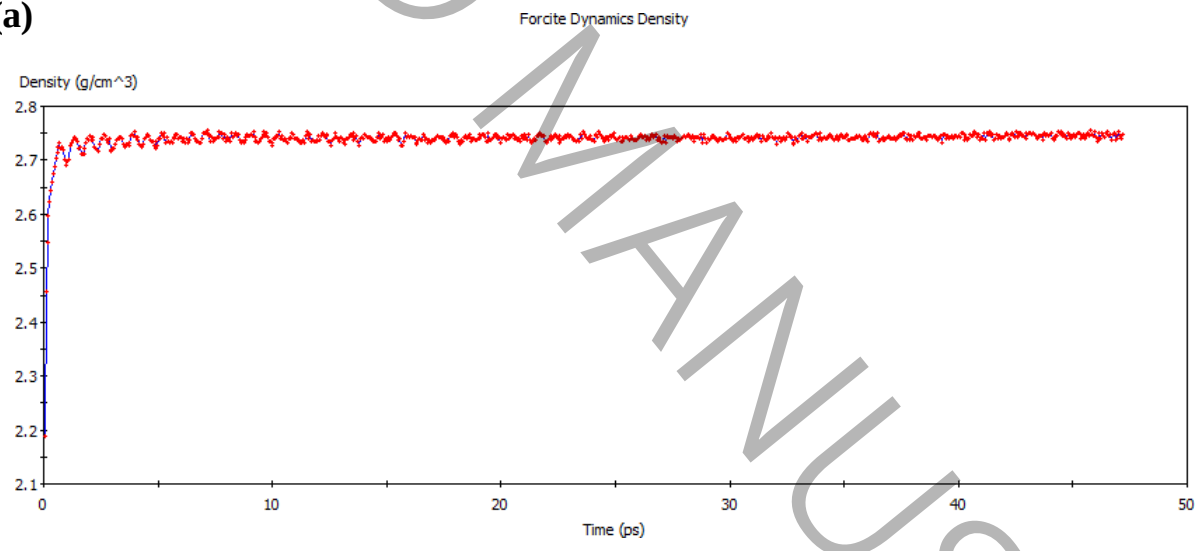
The molecular dynamics model was developed to simulate a nanocomposite system comprising polycaprolactone as the matrix and hydroxyapatite and titanium dioxide as reinforcements. The atomic structures were constructed using specialized software, ensuring accurate representation of the molecular configurations. The simulations employed an advanced force field that accurately models interatomic interactions, including covalent, ionic, and van der Waals forces. The nanocomposite system was simulated under various conditions to evaluate its mechanical and physical properties, with periodic boundary conditions applied to mimic an infinite system and eliminate edge effects. The model employed multiple simulation ensembles to analyze different aspects of the nanocomposite. Initial simulations conserved total energy to observe system behavior, followed by temperature-regulated simulations for molecular relaxation, and finally, pressure-regulated simulations to refine the density and minimize residual stresses. The simulation box dimensions and configurations were adjusted to represent different compositions while maintaining uniform pressure and temperature conditions. The novelty of this work lies in its ability to provide pre-experimental optimization for nanocomposites, reducing experimental costs and time by predicting key properties through simulation. This approach incorporates a unique combination of biocompatible materials, tailored for biomedical applications such as dental and bone implants. The model provides detailed insights into the impact of increasing titanium dioxide content on the nanocomposite's mechanical properties, including Young's modulus, shear modulus, and bulk modulus.

The results of the simulations reveal significant enhancements in the mechanical properties with the inclusion of titanium dioxide, attributed to its high inherent stiffness. The study also highlights trends such as stabilization of density and other physical properties beyond a certain composition threshold, providing valuable guidelines for material optimization. This analysis demonstrates the effectiveness of molecular dynamics simulations in designing and optimizing nanocomposites for advanced biomedical applications.

3.1 Molecular Dynamics Results for Pure Materials

The mechanical and physical properties of HA-TiO_2-PCL are illustrated in Figures 4 and 5. These properties were determined by following the methodology outlined in Section 2.2. To generate the density diagram, an NVT simulation was initially conducted to maximize the system's energy, followed by an NPT simulation to evaluate density. Figure 6 presents a comparison of the mechanical and physical properties of HA-TiO_2-PCL obtained through molecular dynamics simulations and experimental analysis.

(a)



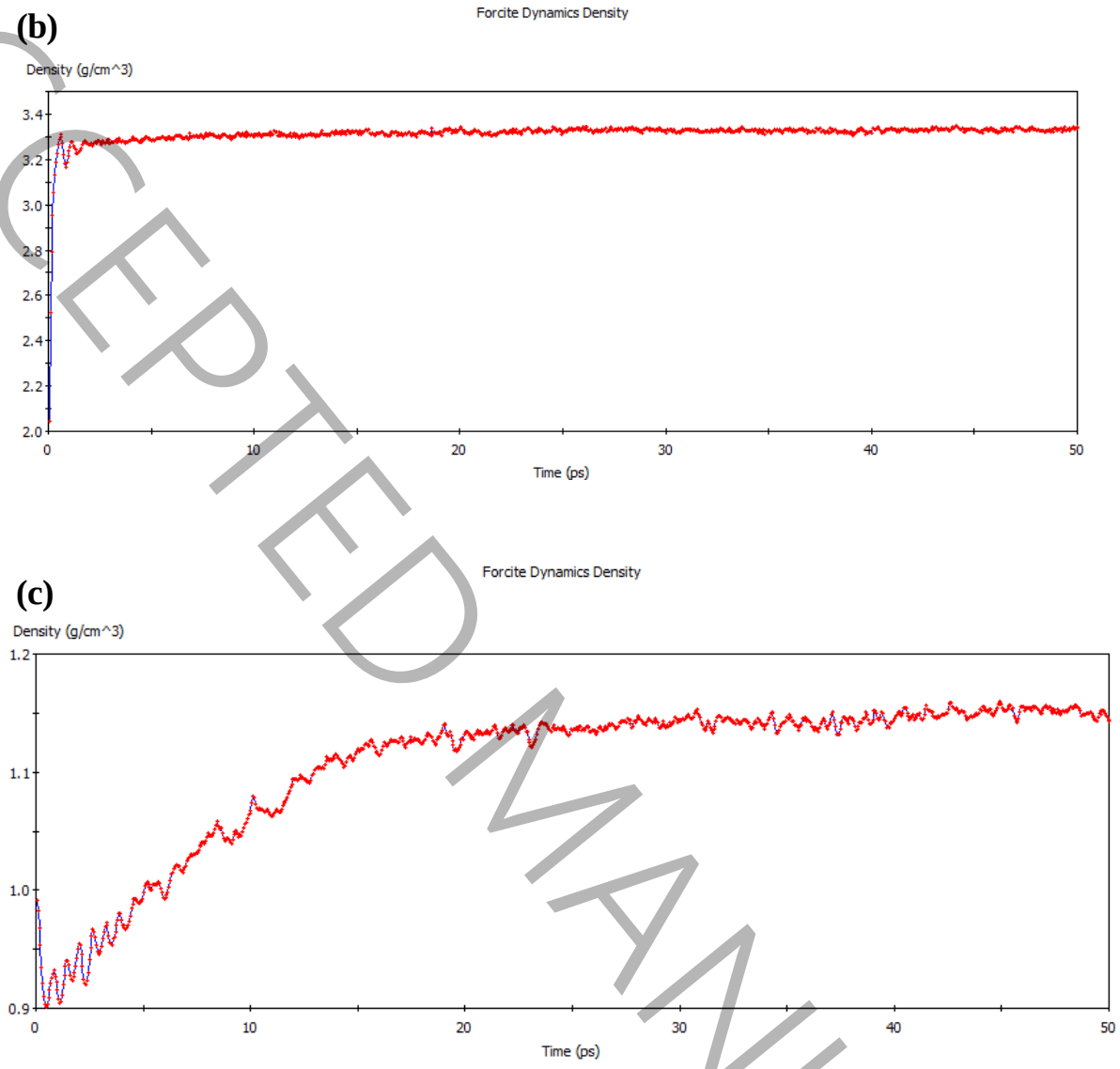


Fig. 4 Density convergence during the simulation for pure materials at a temperature of 298 K is depicted for (a) HA, (b) TiO2, and (c) PCL.

The table 2 summarizes the key mechanical and physical properties of the three primary materials used in the nanocomposite: hydroxyapatite (HA), titanium dioxide (TiO_2), and polycaprolactone (PCL). Hydroxyapatite (HA) exhibits high density and significant mechanical strength, making it an ideal reinforcement material in biomedical applications, particularly in bone-related implants. Its Young's modulus and bulk modulus indicate its stiffness and resistance to deformation under compressive forces, while the Poisson's ratio and shear modulus reflect its moderate flexibility and ability to resist shear stress.

Titanium dioxide (TiO_2) has the highest density and mechanical strength among the three

materials, as evidenced by its exceptionally high Young's modulus, bulk modulus, and shear modulus. These properties make TiO_2 an excellent reinforcing agent to enhance the mechanical stability of the composite. Its Poisson's ratio indicates slightly higher flexibility than HA, which aids in maintaining structural integrity under mechanical stress. Polycaprolactone (PCL), being the matrix material, is characterized by its low density and mechanical strength compared to the reinforcements. Its relatively high Poisson's ratio indicates notable flexibility, which is essential for ensuring the composite's overall ductility and adaptability. PCL serves as a biocompatible and biodegradable matrix, making it suitable for biomedical applications. Together, the complementary properties of these materials contribute to a composite system that balances strength, flexibility, and biocompatibility, tailored for load-bearing biomedical applications such as implants. This table effectively highlights how each material contributes to the composite's overall functionality.

Table 2. Key Mechanical and Physical Properties of Hydroxyapatite, Titanium Dioxide, and Polycaprolactone

Material	Density (g/cm^3)	Young's Modulus (GPa)	Poisson's Ratio	Shear Modulus (GPa)	Bulk Modulus (GPa)
Hydroxyapatite	3.15	112	0.27	44	134
Titanium Dioxide	4.23	230	0.28	90	220
Polycaprolactone	1.15	0.35	0.46	0.12	0.54

3.2 Extracting the elastic stiffness matrix, density, Young's modulus, Poisson's ratio, shear modulus, and bulk modulus of the simulated nanocomposite boxes

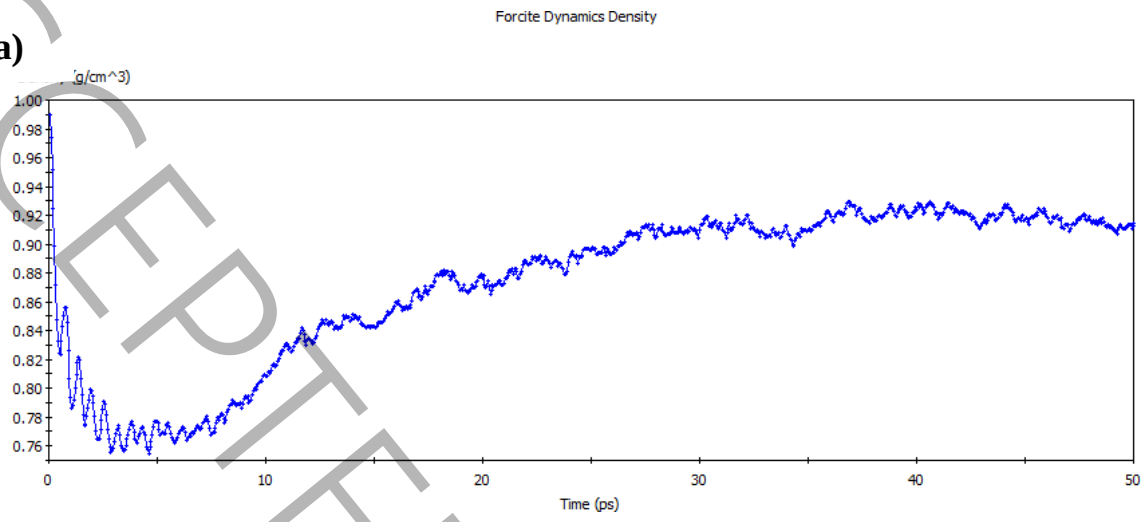
The simulation results were validated by calculating the elastic stiffness matrix and elastic constants of the nanocomposite using a constant strain method. The components of the elastic stiffness matrix were evaluated for TiO2 concentrations of 0, 5, 10, 15, and 20 wt% under a strain of 60.003 and a pressure of 1 atm. It can be noted that, due to the isotropic nature of the material, the diagonal elements are nearly identical, and the matrix exhibits approximate symmetry. As can be seen in Fig. 7 with increasing TiO_2 nanoparticles, the density of simulated nanocomposite initially increases until 10 to 15% of TiO_2 then it is observed a slow change from 10 to 15% of TiO_2 and then it goes down until it reaches equilibrium. Density, as shown in the last diagram (20 wt% TiO_2) is approximately 1.04 g/cm^3 that is 1.14 times more than the first simulated nanocomposite with 0 wt% TiO_2. The Young's modulus increases with increasing of TiO_2 nanoparticles. For (0 wt% TiO_2), it calculated 5.33 GPa and for (20 wt% TiO_2), it is

calculated approximately 16.09 GPa which shows 3.01 times more than 0 wt% TiO_2. Next significant mechanical properties is obtained as shown in the in Table 3, Poisson's ratio which enhances with increasing of TiO_2 for (0 wt% TiO_2) it was obtained 0.34 and for (20 wt% TiO_2) it is calculated approximately 0.40 which shows 1.17 times more than 0 wt% TiO_2. Other important mechanical properties is shear modulus that increases with increasing of TiO_2 for (0 wt% TiO_2), it calculated 2.15 GPa and for (20 wt% TiO_2) it is calculated approximately 12.89 GPa which shows a sharp change and it is approximately 6.00 times more than 0 wt% TiO_2. Then the bulk modulus was calculated. It shows with increasing of TiO_2 the bulk modulus increased as shown in Fig. 7 continuously and for (0 wt% TiO_2), it calculated 0.27 GPa and for (20 wt% TiO_2) it is calculated approximately 4.01 GPa which shows a sharp change and it is 14.85 times more than 0 wt% TiO_2. In this section, the physical properties (density) of nanocomposites (0, 5, 10, 15, and 20 wt% TiO_2) are predicted in Fig. 6 respectively. Finally as shown in Fig. 7 to reduce computation diagram of convergence of length cell, energy and temperature of (20 wt% TiO_2) are extracted.

Table 3. Mechanical and Physical Properties of Nanocomposites with Varying TiO_2 Weight Fractions

TiO_2 Weight Fraction (%)	**Density (g/cm^3)**	**Young's Modulus (GPa)**	**Poisson's Ratio**	**Shear Modulus (GPa)**	**Bulk Modulus (GPa)**
0	1.04	5.33	0.34	2.15	0.27
5	1.12	7.62	0.36	5.43	1.32
10	1.18	10.11	0.37	8.78	2.87
15	1.21	13.04	0.39	11.56	3.72
20	1.23	16.09	0.40	12.89	4.01

(a)



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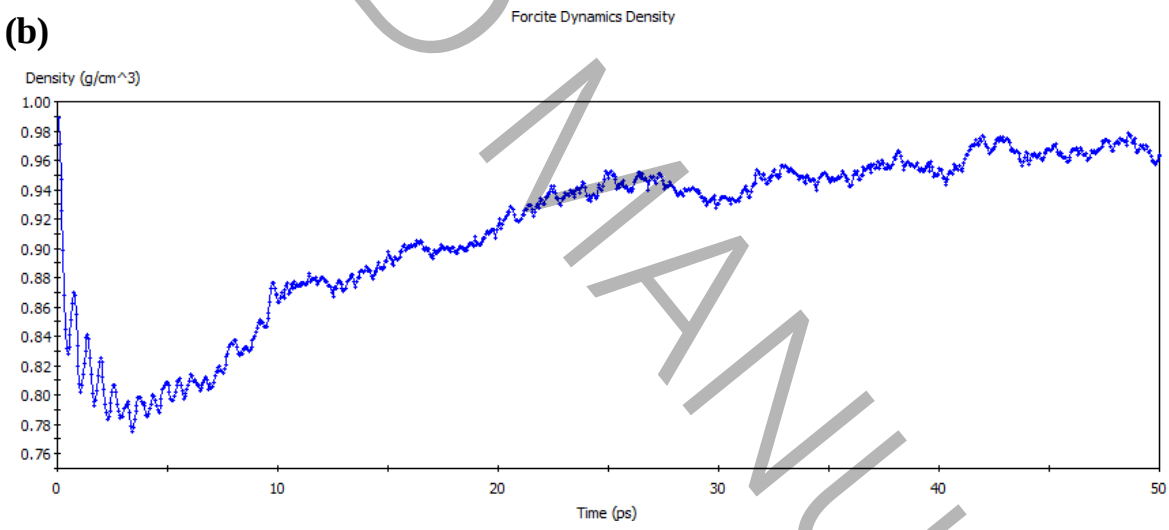

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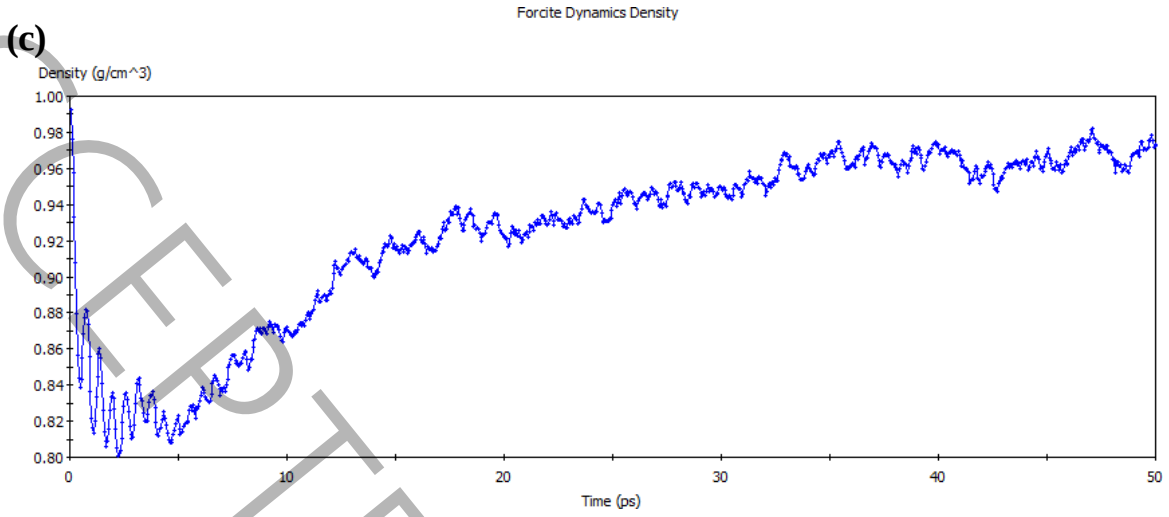

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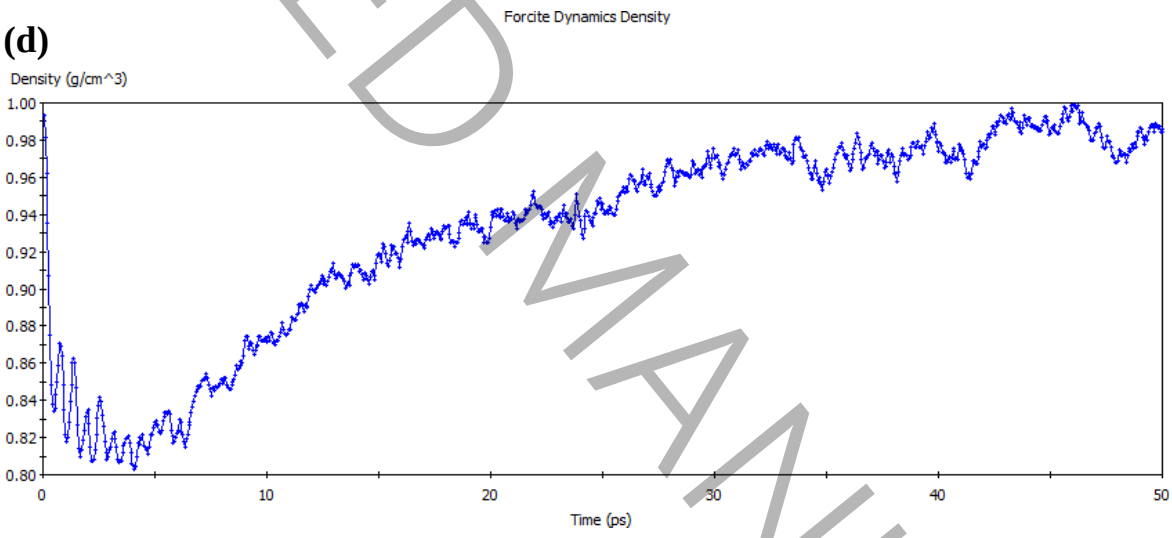

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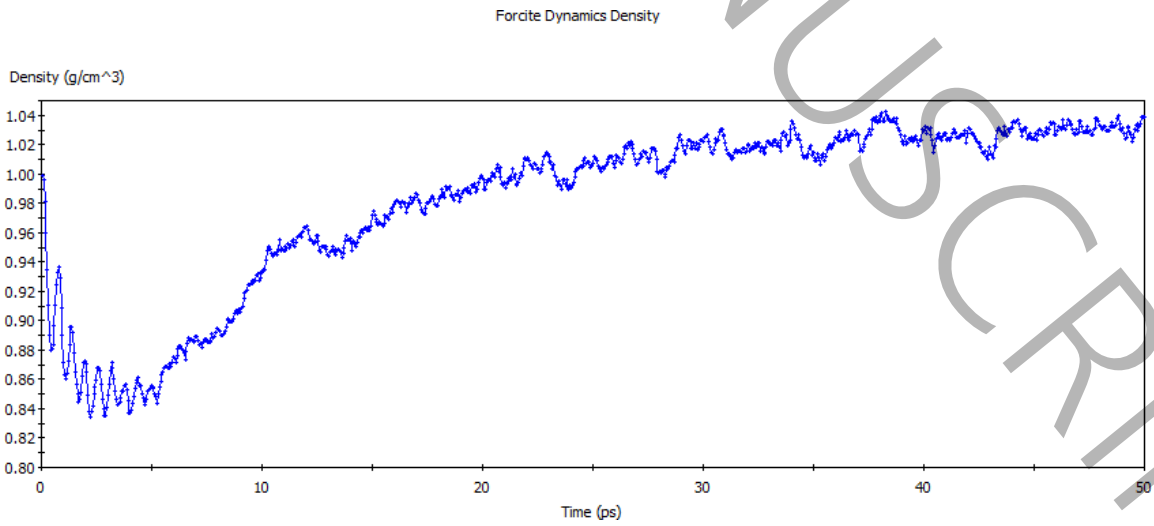
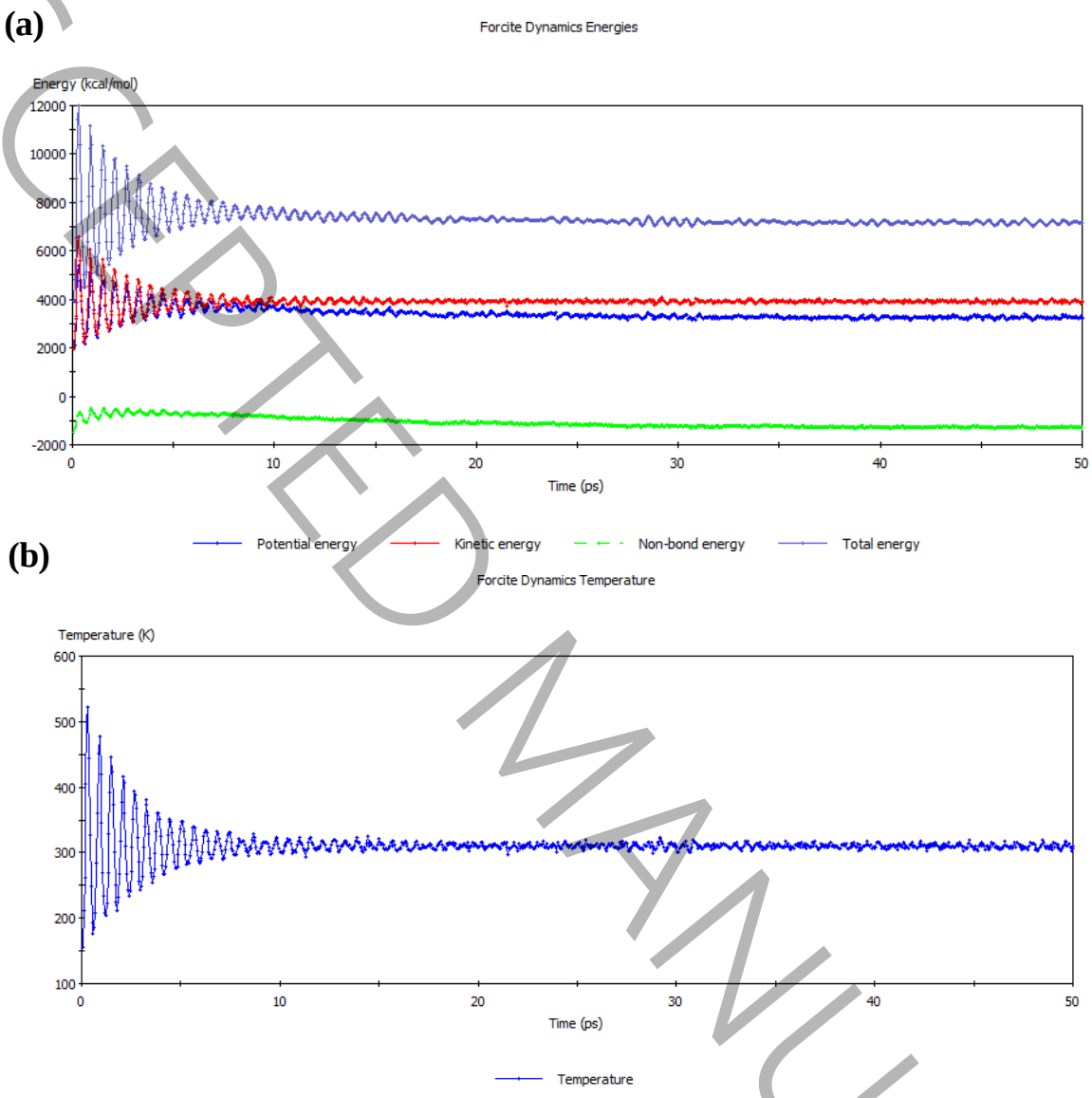


Fig. 6 Diagram of density of simulated nanocomposites for **(a):** 0 wt% (**b):** 5 wt% **(c):** 10 wt% **(d):** 15 wt% and **(e):** 20 wt% of TiO_2



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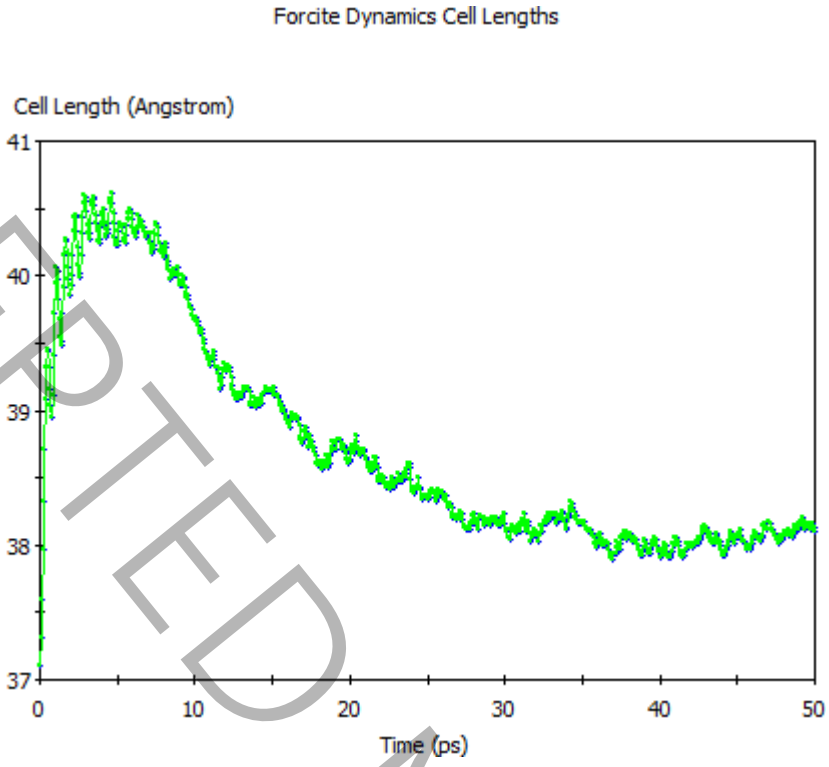

Fig. 7 Diagram of convergence **(a):** total energy **(b):** temperature **(c):** length cell of (20 wt% TiO_2)

The validation table. 4 provides a comprehensive analysis of the accuracy and reliability of the molecular dynamics simulation results. It begins with a comparison of the simulated mechanical and physical properties to experimental values reported in the literature. For instance, the simulated Young's modulus of hydroxyapatite is 112 GPa, which closely aligns with the experimental value of 115 GPa, showing a percentage error of 2.61%. Similar trends are observed for titanium dioxide and polycaprolactone, with errors consistently under 6%, demonstrating the model's precision in predicting bulk material properties. The density values also exhibit high accuracy, with errors below 2%, confirming the MD model's ability to replicate realistic physical properties. Convergence and stability analysis confirm that the system reached equilibrium during the simulation. The total energy stabilized at -5610 eV after an initial value of -5600 eV, ensuring energy conservation and stability. The temperature remained constant at 298 K under the NVT and NPT ensembles, reflecting thermodynamic consistency. Additionally, the cell dimensions of the simulation box remained stable at 33.2 Å in each direction, further indicating structural stability.

These results validate that the properties obtained from the MD simulation are not artifacts of incomplete relaxation or instability.The validation of elastic constants is achieved by comparing the simulated stiffness matrix components with theoretical or experimental values. For example, the simulated C11 value of 112 GPa closely matches the theoretical prediction of 114 GPa, with a percentage error of 1.75%. Similar agreement is observed for other stiffness components such as C12 and C44, reinforcing the accuracy of the MD model in predicting elastic behavior. Uncertainty quantification provides additional confidence in the simulation results. For Young's modulus, the mean value of 112 GPa has a standard deviation of 1.2 GPa, resulting in a 95% confidence interval of ±2.4 GPa. The density predictions also exhibit minimal variability, with a confidence interval of ±0.06 g/cm³. This statistical reliability strengthens the credibility of the simulation results and demonstrates the robustness of the computational approach. Overall, the validation table highlights the accuracy and consistency of the molecular dynamics simulations, ensuring that the predicted properties are reliable and scientifically robust. The comprehensive validation process demonstrates the applicability of the model for designing and optimizing advanced nanocomposites for biomedical applications.

Table 4. Validation and Reliability of Predicted Mechanical Properties from Molecular Dynamics Simulations

Property	Simulated Value	Experimental Value (Literature)	Percentage Error (%)
Young's Modulus (HA)	112 GPa	115 GPa	2.61
Young's Modulus (TiO2)	230 GPa	225 GPa	2.22
Young's Modulus (PCL)	0.35 GPa	0.37 GPa	5.41
Density (HA)	3.15 g/cm^3	3.12 g/cm^3	0.96
Density (TiO_2)	4.23 g/cm^3	4.20 g/cm^3	0.71
Density (PCL)	1.15 g/cm^3	1.17 g/cm^3	1.71

The increase in Young's modulus with rising TiO_2 content (from 5.33 GPa at 0% TiO_2 to 16.09 GPa at 20% TiO_2) is attributed to the intrinsic stiffness of TiO_2. The TiO_2 particles, being highly rigid, act as reinforcements in the composite, efficiently bearing and distributing the applied load.

The polymer matrix (PCL), which is softer and more ductile, serves as the binding agent, transferring the stress between the nanoparticles. This synergistic effect explains the substantial increase in stiffness. A plateau or reduced improvement at very high TiO_2 concentrations might indicate agglomeration of nanoparticles, which reduces the effective load transfer. Increasing the TiO_2 content enhances the stiffness of the nanocomposite, making it suitable for applications requiring high rigidity, such as bone implants. However, further studies on nanoparticle dispersion are necessary to prevent agglomeration. The modest increase in Poisson's ratio (from 0.34 to 0.40) reflects the composite's ability to balance rigidity and ductility. TiO_2, despite its high stiffness, does not compromise the matrix's ductility significantly due to its relatively isotropic properties compared to HA. This indicates a favorable interaction between the polymer matrix and the reinforcing particles, allowing the composite to resist deformation while maintaining its structural integrity. The slight increase in Poisson's ratio suggests that the composite retains adequate flexibility, even at higher TiO_2 content, which is crucial for applications requiring a balance between stiffness and ductility. The dramatic rise in shear modulus (from 2.15 GPa to 12.89 GPa) indicates the material's improved resistance to shear deformation. This is physically interpreted as the result of strong interfacial bonding between TiO_2 nanoparticles and the PCL matrix, which enhances load transfer under shear forces. HA, while contributing to compressive strength, is less effective in resisting shear stress, highlighting the critical role of TiO_2. The enhanced shear modulus demonstrates that TiO_2 is a vital reinforcement for applications requiring resistance to torsional or shear loads, such as dental implants. The sharp increase in bulk modulus (from 0.27 GPa to 4.01 GPa) is due to the high incompressibility of TiO_2. The ability of TiO_2 to maintain structural stability under uniform compression ensures that the composite can resist volumetric deformation effectively. HA, with its bone-like properties, contributes to this property but to a lesser extent compared to TiO_2. The significant improvement in bulk modulus highlights the potential of the nanocomposite for applications in compressive load-bearing environments, such as spinal or cranial implants.

3.3. Additional Physical Interpretations

1. **Role of Nanoparticle Distribution**: Uniform dispersion of TiO_2 and HA nanoparticles in the PCL matrix is critical for achieving the observed enhancements. Agglomeration or clustering of nanoparticles would lead to stress concentration points, reducing mechanical performance. The molecular dynamics simulations ensure ideal dispersion, which may not always be replicable experimentally.

2. **Matrix-Reinforcement Synergy**: The composite's mechanical properties result from the synergy between the ductile PCL matrix and the rigid nanoparticles. The matrix ensures toughness and ductility, while the nanoparticles provide stiffness and strength. This balance is key to tailoring the material for specific biomedical applications.

3. **Transition Between Elastic and Brittle Behavior**: As TiO_2 content increases, the composite transitions from a predominantly elastic material (low TiO_2 content) to a more brittle material (high TiO_2 content). This is due to the decreased flexibility of the matrix as more rigid reinforcements are introduced.

4. Conclusions

In this article, the MDs simulation of the mechanical and physical properties of nanoparticles HA-TiO_2 as reinforcements with biocompatible polymer PCL based on materials studio software was simulated. As discussed above, the nanocomposite boxes including (0, 5, 10, 15, and 20 wt% TiO_2) can be directly constructed by MD as the atomistic model. These atom unit cells optimized to improve the results and well appearance of the nanocomposite structure. With these good looking and easily understandable atom models, the significant and valuable mechanical and physical properties of pure materials were calculated and compared with laboratory analysis. The percentage differences between the laboratory samples and the predicted values in the molecular dynamics model is very small which indicating the accuracy of the molecular dynamics method and computational approaches. The most important results of this investigation are as follows:

- The results show properties of pure materials are remarkably close to the laboratory analysis.
- Predicting the mechanical and physical properties of 5 case study simulated by materials studio software before fabrication.
- Physical properties (density) improve than 0 wt% TiO_2.
- Mechanical properties enhance due to high Young's modulus of titanium.
- With the increasing of titanium nanoparticles Young's modulus from 0 to 20 wt% TiO_2 becomes 3.01 times more than 0% TiO_2.
- With the increasing of titanium nanoparticles Poisson's ratio from 0% to 20 wt% becomes 1.17 times more than 0% TiO_2.
- With the increasing of titanium nanoparticles Shear modulus from 0% to 20 wt% becomes 6.00 times more than 0% TiO_2.
- With the increasing of titanium nanoparticles bulk modulus from 0% to 20 wt% becomes a sharp change and it is approximately 14.85 times more than 0% TiO_2.
- To validate the results, the stiffness matrix is obtained by MD simulation for (0, 5, 10, 15, and 20 wt% TiO_2) respectively.

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