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The Stress Analysis of Polymethyl Methacrylate (PMMA) Nanocube Using Molecular Dynamics Simulation

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ABSTRACT

Polymethyl methacrylate (PMMA) stands as a significant polymer, recognised for its unique combination of mechanical attributes, processing friendliness, and chemical stability [1]. The present study focuses on the use of molecular dynamics (MD) simulation to study the mechanical response of PMMA nanostructures to uniaxial tensile loading as an initial step to understanding the mechanisms of deformation, assessing the mechanical stability, and describing the tensile behaviour of PMMA at the nanoscale. To examine thermodynamic equilibrium, NVT—and NPT equilibria (NVT: number of particles, volume, and temperature; NPT: number of particles, pressure, and temperature) equilibrium simulations were performed along with deformation molecular configuration energy minimisation to ensure stable molecular configurations. These analyses were necessary for the advancement of PMMA to accommodate new flexible electronics, biomedical devices, and other nanotechnology systems. The nanostructures were designed in JMOL and PACKMOL software, and the simulation was executed in LAMMPS using the COMPASS force field. Structural stability was ensured by performing energy minimisation and equilibrating prior to tensile loading at 300 K and 1 atm under both NVT and NPT conditions. The findings show that PMMA nanostructures with greater aspect ratios show greater elongation under tension. The sequential stress–strain data contained separate and distinct regions of elastic and plastic deformation, which also helped to elucidate the mechanics of the material at the nanoscale and the constraints thereof. The mechanical performance of the studied PMMA nanostructures, when compared to bulk PMMA and other polymer nanostructures, was also superior and can be linked to the mechanical properties of the nanostructured morphology. This study enhances the knowledge of the PMMA in tension and provides a basis for the design and refinement of new advanced nanostructured polymeric materials. These findings should contribute to the fabrication of flexible electronics with greater durability, biomedical devices, and other applications in nanotechnology.

Keywords: *Polymethyl Methacrylate, Nanocube, Molecular Dynamics, Stress Analysis, Nanocomposites*

1. INTRODUCTION

Polymethyl methacrylate (PMMA) is an amorphous polymer known for its exceptional optical transparency, ease of manufacturing, and versatility in applications, from coatings and flexible electronics to biomedical devices [1]. The advent of nanotechnology has significantly broadened PMMA's role, especially in nanolithography, where it functions as a resist in electron beam lithography [2] and is also heavily used in nanoimprint lithography [3],[4]. Nanoimprint lithography (NIL) is a cost-effective method for mass producing micro/nanostructures, and PMMA's properties make it well-suited for this technique [5]. This capability is essential for creating nanoscale patterns and structures, which are critical in the development of advanced electronic and optical devices. As PMMA-based devices are scaled down to nanoscale dimensions, a thorough understanding of their mechanical behavior becomes crucial. However, no specific experimental challenges are mentioned, especially those related to more traditional approaches to testing. Equilibrium simulations, as stated in the abstract, are essential to promote the use of PMMA in flexible electronics, biomedical engineering, and nanotechnology. Molecular dynamics (MD) simulations are helpful because they allow atomistic insights into the modification mechanisms and stress distributions that are difficult to obtain experimentally [6].

MD simulations have been instrumental in predicting the elastic modulus of glassy polymers [7],[8]. MD simulations are crucial in estimating the mechanical properties of PMMA, which can be used as input for continuum simulations [4]. The unique mechanical properties, chemical stability, and ease of fabrication make it an excellent material for various applications, as discussed in the abstract. This study, therefore, employs MD simulations to investigate the tensile behavior of PMMA nanostructures, providing valuable guidance for the design and optimization of nanostructured polymeric materials. Understanding the deformation mechanisms, mechanical stability, and tensile behavior of PMMA at the nanoscale is essential for its applications in micro/nanotechnology [9]. This work focuses on the PMMA nanocube structure, which was chosen because of its unusual geometric properties. In contrast to other nanoscale geometries, nanocubes create isotropic confinement as well as unique edge and corner regions that serve as natural stress concentrators. These features allow the study of deformation mechanisms at the nanoscale. Furthermore,

their symmetry not only aids in computer modeling but also facilitates the analysis of anisotropic mechanical behavior in the context of uniaxial loading [10],[11].

2. METHODOLOGY

Molecular dynamics (MD) simulations were used to examine the mechanical behavior of PMMA nanocubes. The entire workflow, as shown in Figure 1, involves model building, equilibration, and subsequent application of tensile loading using the LAMMPS simulation package. The process begins with the generation of PMMA monomers in JMOL and their assembly into the desired nanocube configuration using PACKMOL. After model building, steps are taken to perform energy minimization and equilibration to reduce any initial structural stress and achieve a configuration in which the model is stable. The nanocubes, now equilibrated, are then subjected to uniaxial tensile loading in LAMMPS, allowing detailed studies of the deformation behavior and the evolution of the stress–strain relationship.

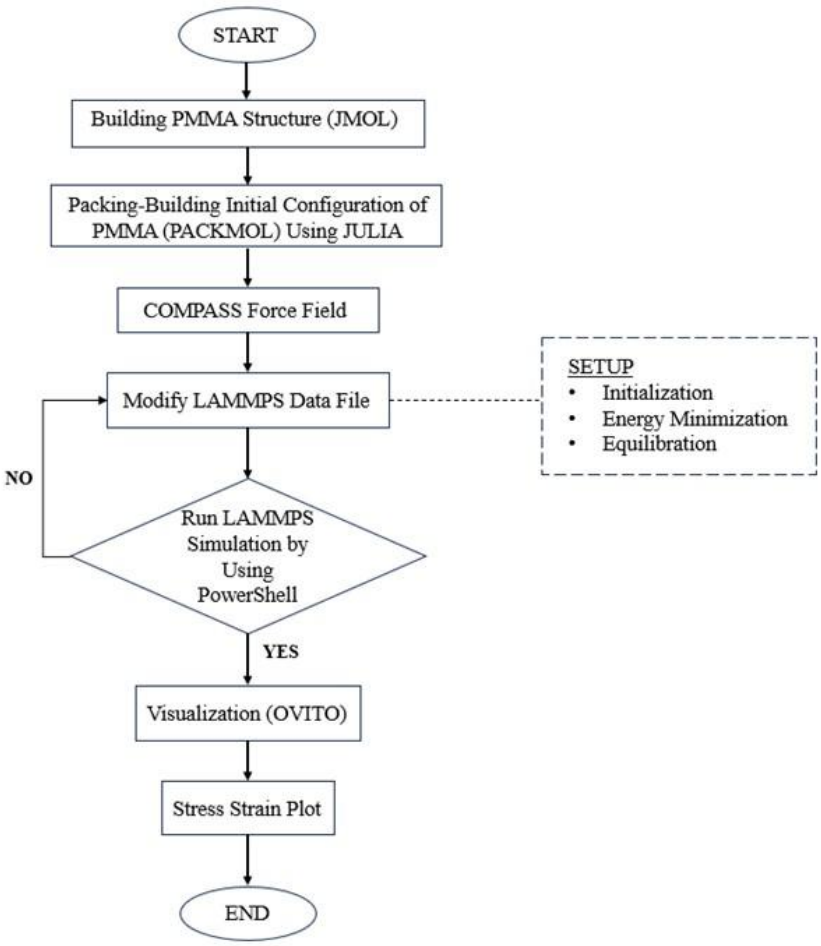

Figure 1. Flowchart illustrating the key stages in the molecular dynamics simulation.

2.1. Model Construction

Generating individual methyl methacrylate monomers is the first step in the construction of PMMA nanostructures. JMOL is an important visualization and modeling tool. It allows users to change the geometry of the molecules and serves as the building blocks of the basic PMMA building blocks [12]. Careful development of the atomic configuration of each monomer is essential to accurately model PMMA polymers. There are several important points to note. First, the elemental composition of the monomer, consisting of carbon, hydrogen, and oxygen atoms, is determined according to its chemical formula [14]. After this, the correct covalent bonds, which include single and double bonds and appropriate connections to other parts of the monomer, are added. Finally, the bond lengths and angles are adjusted to match the experimentally obtained measurements [12]. This helps to maintain realistic geometric shapes and sizes of the monomers. All of these efforts ensure that the monomers serve as a good starting point for building larger PMMA nanostructures. Figure 2 shows the structure of the PMMA monomer produced by JMOL.

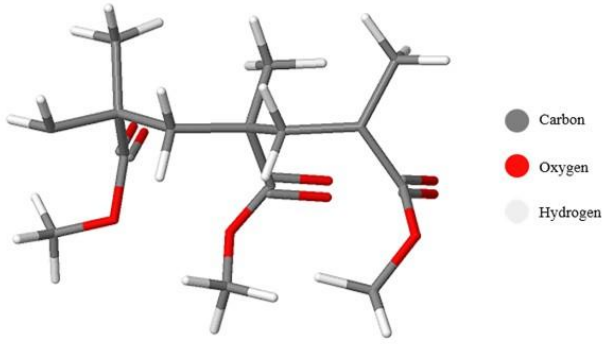

Figure 2. Structure of PMMA monomer.

Subsequently, the PACKMOL package is employed to pack these monomers into the desired nanocube configuration, specifically a cube with each side measuring 100 Å [15]. PACKMOL excels at creating initial structures for molecular dynamics simulations by efficiently packing molecules within defined regions while avoiding overlaps. Figure 3 shows the PMMA nanocube with dimensions of 100 Å x 100 Å x 100 Å.

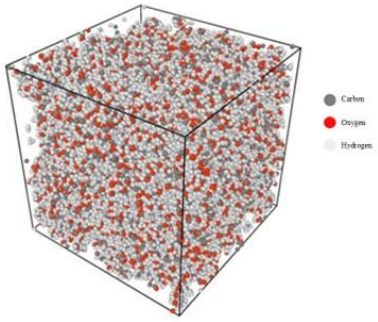

Figure 3. PMMA nanocube with dimensions of 100 Å x 100 Å x 100 Å.

The process involves defining a cubic region with dimensions of 100 Å x 100 Å x 100 Å. The coordinates of the vertices are specified to define the spatial boundaries, and a tolerance parameter is set to prevent overlap between monomers during the packing process. For systems at room temperature and pressure with coordinates in Angstroms, a distance tolerance of 2.0 Å is commonly used [15]. Following this, the number of PMMA monomers to be packed is specified, and PACKMOL then arranges these monomers randomly within the defined cubic region, ensuring that no two monomers overlap by more than the specified tolerance. The output of PACKMOL is a coordinate file containing the positions and orientations of all PMMA monomers within the nanocube, serving as the starting point for subsequent molecular dynamics simulations [16].

Intramolecular parameters govern the interactions within a single PMMA molecule, encompassing bond lengths (equilibrium distances between bonded atoms), bond angles (equilibrium angles between three bonded atoms), torsional angles or dihedrals (angles between four bonded atoms describing rotation around a bond, often modeled with a CFF-type functional form [17], and partial charges assigned to each atom to represent electrostatic interactions. Intermolecular parameters, on the other hand, define the interactions between different PMMA molecules, primarily van der Waals interactions (short-range attractive and repulsive forces between atoms, often modeled using a Lennard-Jones 9-6 potential (Sun et al., 1998) and electrostatic interactions (interactions between partial charges on different atoms). For this study, the Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies force field [18] was used. COMPASS was chosen because it is widely used in simulating polymers and soft materials. COMPASS is a many-body potential with improved non-bonded parameters. Equations 1 and 2 represent functional forms used in the COMPASS force field, which represent non-bonded and valence interactions, respectively [18]. Table 1 shows the definition of symbols for equations 1 and 2.

$$\boldsymbol{E_{non-bonded}} = \sum_{i,j} \frac{q_i q_j}{r_{ij}} + \sum_{i,j} \epsilon_{ij} [2\left(\frac{r_{ij}^o}{r_{ij}}\right)^9 - 3\left(\frac{r_{ij}^o}{r_{ij}}\right)^6] \quad (1)$$

$$\boldsymbol{E_{valence}} = \sum_{\theta} [k_2(b-b_o)^2 + k_3(b-b_o)^3 + k_4(b-b_o)^4] + \sum_{b} [k_2(b-b_o)^2 + k_3(b-b_o)^3 + k_4(b-b_o)^4] +$$

$$\sum_{\emptyset}[k_1(1-\cos\emptyset)+k_2(1-\cos 2\emptyset)+k_3(1-\cos 3\emptyset)]+ \quad \sum_{\theta,\emptyset}(\theta-\theta_o)[k_1\cos\emptyset+k_2\cos 2\emptyset+k_3\cos 3\emptyset]+$$

$$\sum_{\chi}k_2\chi+\sum_{b,b'}k\,(b-b_o)\,(b'-b_o')+\sum_{b,\theta}k\,(b-b_o)\,(\theta-\theta_o)+ \quad \sum_{b,\theta}k\,(\theta'-\theta_o')(\theta-\theta_o)+\sum_{\theta,\theta,\emptyset}k\,(\theta-\theta_o)(\theta'-\theta_o')cos\emptyset \qquad (2)$$

$$\sum_{b,\emptyset}(b-b_o)[k_1\cos\emptyset+k_2\cos 2\emptyset+k_3\cos 3\emptyset]\;+$$

Table 1 Definition of symbols used in equations (1) and (2)

Symbol	Description
q_i,q_j	Partial atomic charges of atom *i* and *j*
r_{ij}	Distance between atom *i* and atom *j*
r_{ij}^0	Equilibrium van der Waals separation distance between atoms *i* and *j*
ϵ_{ij}	Depth of van der Waals potential well for atom pair *i-j*
b,b_0	Bond length and its equilibrium (reference) value
θ,θ_0	Bond angle and its equilibrium (reference) value
ϕ	Torsional (dihedral) angle
χ	Out-of-plane bending angle (used for planar structures like sp^2 atoms)
k_1,k_2,k_3,k_4	Force constants for various terms (bond stretching, angle bending, torsion, etc.)
k	Cross-coupling force constant between different internal coordinates
θ′,θ_0′	Secondary angle and its equilibrium value are used in multi-angle cross-terms

The valence term includes diagonal and off-diagonal cross-coupling terms represented by the angle (θ), internal coordination of bond (b), torsion angle (ø), out-of-plane-angle(χ), and combinations of two or three internal coordinates for the cross-coupling term [18]. When implementing the COMPASS force field in software like LAMMPS, ensuring the correct definition of all these parameters is crucial. The COMPASS force field has been validated for various molecules in both isolated and condensed phases [18]. Table 2 shows the mapping of atom species from the COMPASS force field to the PMMA monomer.

Table 2 Mapping of atom species from COMPASS force field to PMMA monomer

Atom Species	COMPASS Force Field Description	Corresponding atom species in PMMA monomer
C	Sp3 carbon (tetrahedral)	Backbone carbons, methyl carbon
C	Sp2 carbon (trigonal planar)	Carbonyl carbon (C=O)
O	Carbonyl oxygen (C=O)	Carbonyl oxygen
O	Ether oxygen or Ester oxygen	Ester oxygen
H	Alkyl hydrogen (bonded to sp3 carbon)	Methyl hydrogens, backbone hydrogens

2.2. Simulation Details

The LAMMPS package was used to run simulations of molecular dynamics (MD). The interactions between atoms in the PMMA nanocube were modeled using the COMPASS force field. This force field is selected since it is specifically useful in polymer systems, as it provides a set of parameters that are able to describe both bonded and non-bonded interactions with a high degree of accuracy. The translation of the structural and simulation parameters into a LAMMPS input script with all the necessary commands was performed by the specification of the force field, atomic coordinates, time step, and simulation ensembles to be applied in equilibration and deformation. Before any mechanical loading, the system was first subjected to an energy minimization phase in order to eliminate steric overlaps as well as relieve any disfavored interatomic contacts due to the early packing step. This is done to make sure that the simulation is started in a stable and low-energy state, which increases the accuracy of future deformation studies. A normalization of the nanocube was then followed by two successive equilibration steps: (1) NVT

ensemble at constant volume to equilibrate the system thermodynamically and (2) NPT ensemble at 298 K and 1 atm to equilibrate the system both thermodynamically and pressure. In order to study the tensile behavior of the material, the tensile force was applied to the material along the z-axis with the deform command in LAMMPS. This technique is used to repeatedly scale the simulation box along the loading direction, creating a controlled strain on the nanocube. In molecular dynamics studies, the strain rate of engineering was set to 10^11 $s^{-1,}$ a standard value so that the behavior of deformation would be realistic within computationally feasible time scales...

3. RESULTS AND DISCUSSION

Minimization of energy is one of the basic steps in molecular dynamics simulations [22]. During this method, atomic coordinates are modified to make the system less energetic, and this process is repeated until all steric overlaps are resolved and the repulsive interactions are minimized [21]. The algorithm at every iteration estimates the potential energy and sustainingly moves atomic positions towards the most favorable state of the system of interest. The process is repeated until the convergence criterion is reached, which was defined as the point at which the changes in the potential energy are approaching zero, as illustrated in Figures 4 and 5. After this minimized state of the system has been achieved it was brought to equilibrium under the NVT ensemble to enable thermal relaxation to occur at constant volume and temperature. It was followed by the extension of the equilibration process under NPT ensemble at 298 K and 1 atm to set thermal and pressure equilibrium [21].

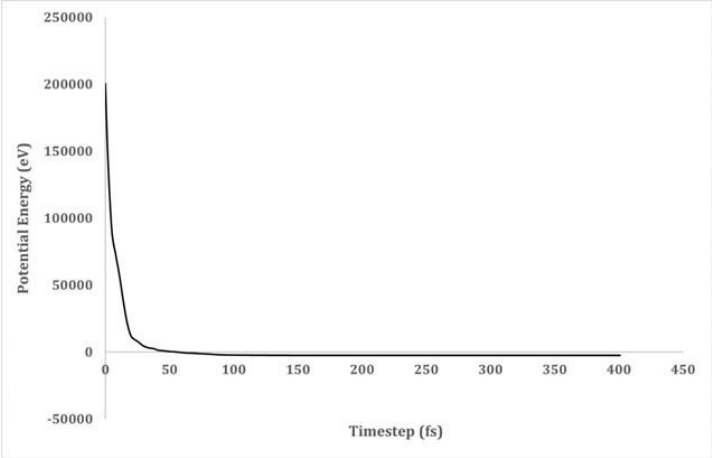

Figure 4. The full process graph of the Energy minimization process of the PMMA nanocube.

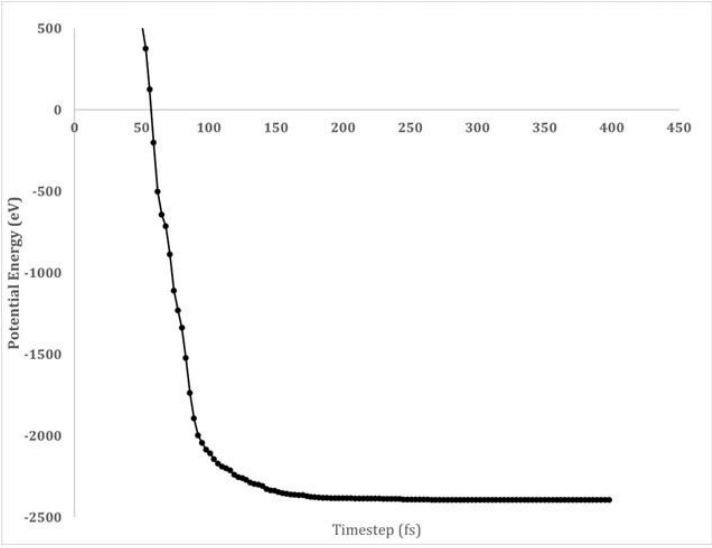

Figure 5. The details graph of **the** energy minimization process of the PMMA nanocube.

Figure 4 demonstrates that the total potential energy of PMMA nanostructure also decreases gradually until the -2393.3 eV plateau is reached. When the system reaches this stabilization, it indicates that the system has reached an energetically favorable configuration and will be ready to undergo the next step, equilibration [4]. The measured decrease of the potential energy is a consequence of the gradual rearrangement of the atoms in the PMMA nanocube

into more stable states, in effect reducing the repulsive forces between molecules and slightly increasing the attractive forces between molecular constituents [4].

Following the energy minimization step, the PMMA nanocube was equilibrated to reach structural stability to meet the target simulation conditions [22]. The equilibration process can be divided into two steps, which are usually temperature and pressure equilibration [22]. At the stage of stabilization of temperature, the system was connected to a thermal reservoir, whereby the temperature gradually increased to the desired value. This slow heating allows atoms to equilibrate their velocities and spread kinetic energy evenly all over the system so that the nanocube is brought to a thermally stable state before starting equilibration of pressure. After that, it is followed by equilibrium adjustment to the desired pressure to have the correct density in the system during the simulation [21]. This usually entails changing the size of the simulation box at constant temperature [21].

The temperature profile in the NVT equilibration phase of the molecular dynamics simulation is shown in Figure 6. As depicted in the figure, the temperature of the system levels off and oscillates around the desired temperature of 298 K, and this means that the thermal equilibrium is established. Such oscillations occur in a canonical ensemble and are caused by natural thermal motion. After a stabilization period, the temperature stabilizes and remains at an average of 298 K by 20 20-ps timestep, which shows that the thermostat used is successfully stabilizing the system at the desired temperature. This proves the validity of the NVT equilibration process and the willingness of the system to be used in the next production steps or additional simulation phases [23].

In the phase of 100 ps NPT equilibration, the simulation followed changes in temperature, volume, and energy, as it is depicted in Figure 6. Such data give a better insight into the response and stabilization of the PMMA nanocube to constant pressure and temperature conditions. The mean volume is maintained at around 11x 10^6 $Å^3$. This stability of the volume will be a sign that the system has established a state of equilibrium in which the density and the size of the simulation box as a whole will cease to vary significantly.

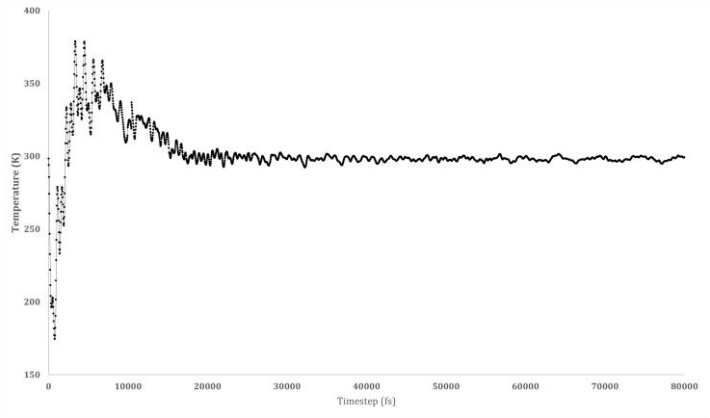

Figure 6. The PMMA nanocube's temperature vs timestep plots during the NVT equilibration phase.

Figure 7 shows the concentration of the PMMA nanocube on the course of the 100-ps NPT equilibration period. At this point, the density of the system reached a point of 0.84 $g/cm^{3,}$ which is quite much less than the accepted bulk density of 1.18-1.20 g/cm^3 [4]. This is mainly attributed to the nanoscale phenomena. Particularly, the ratio of surface to volume is large, resulting in ineffective molecular packing and extra free volume at the surface, and finite-size effects inhibit long-range chain entanglement and ordering of which are required to obtain bulk-like density. Additionally, the 100-ps short period of the simulation might not be enough to equilibrate fully and collapse internal voids. Additional knowledge on PMMA-CNT nanocomposites by Anstine et al. [7] showed that confinement at the interfaces modulates local polymer conformation and density, which is an important point to make that local polymer mobility and structural constraints at the nanoscale are the reasons why the equilibrium density is lower. These results, together, emphasize the fact that nanoscale surface effects, incomplete relaxation of the chain, and constrained polymer dynamics may inherently result in a nanostructure density in PMMA that is much lower than that of the bulk.

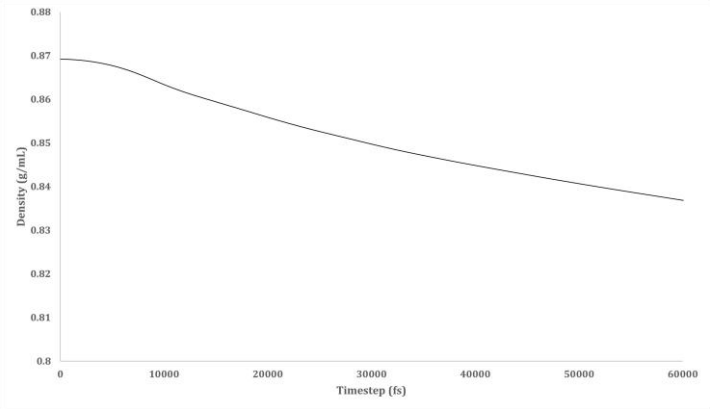

Figure 7. The PMMA nanocube's density vs timestep plots during the NPT equilibration phase.

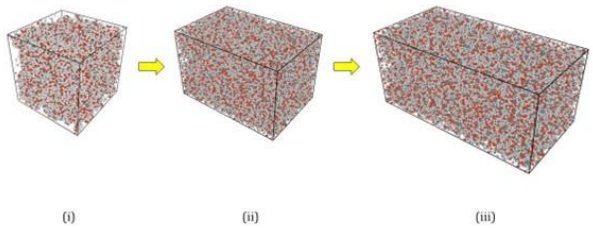

Figure 8. Illustrates the PMMA nanocube being pulled under uniaxial stress at i) 0 ps, ii) 50 ps, and iii) 100 ps.

Figure 8 is used to demonstrate that the nanocube PMMA is pulled in uniaxial stress at i) 0 ps, iii) 100 ps, and iii) 50 ps. The first linear area is the elastic deformation of material in which the stress is proportional to the strain. The slope of this area is the Young's modulus, and this is a measure of the stiffness of the material. The strain-strain curve becomes non-linear as the strain increases, which means that the material starts exhibiting plastic deformation. A characteristic of the non-linear region is that there is a slow increase of stress with increasing strain, which culminates in a certain maximum value of stress, which is termed tensile strength. The behavior that was observed is consistent with previously known mechanical behavior of PMMA at the nanoscale [4]. The results show that PMMA has a mechanical behavior transformation at the nanoscale with solid-like mechanical behavior, and fluid-like mechanical behavior [24].

Figure 9 illustrates the tensile stress-strain curves of nanocubes of PMMA of different sizes. The stress-strain curves of the PMMA nanocubes exhibit an early linear elasticity stage and a subsequent non-linear stage, and this is in agreement with the behavior of polymeric materials.

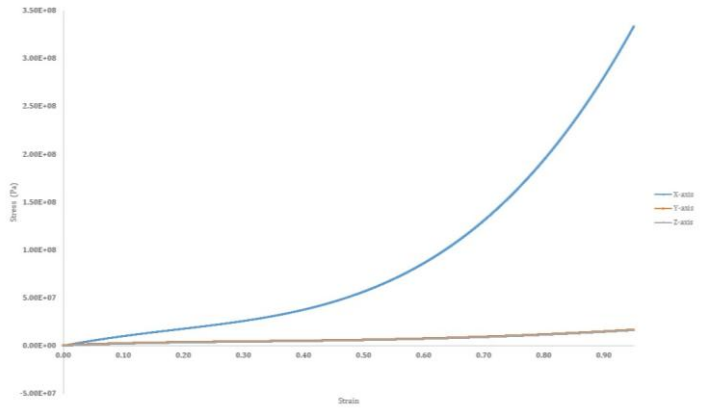

Figure 9. The stress-strain curves of PMMA nanocubes with various sizes under tensile loading.

The curve that is seen in the X-direction when carrying out the uniaxial tensile simulation in comparison with the Y and Z directions is due to the direct outcome of the applied load and the resultant behavior of the material under these particular conditions. The exponential rates of the stress-strain curve in the X-direction are a clear indication of this behavior, which means that there is nonlinear deformation with the strain rate [25]. Conversely, the trend of no external loads acting on the Y and Z directions indicates that there are very low responses of stress. The very mild, almost planar tendencies in these directions may be attributed to Poisson's effect, whereby a longitudinal strain on the material results in a slight lateral strain and, in consequence, to slight compressive stresses in perpendicular directions to the exerted force [26]. However, these stresses are significantly lower than those that are found along the X-axis, which highlights the predominant deformation behavior in that direction. Taken together, these observations indicate that PMMA changes its solid-like to more fluid-like response with deformation at the nanoscale [27].

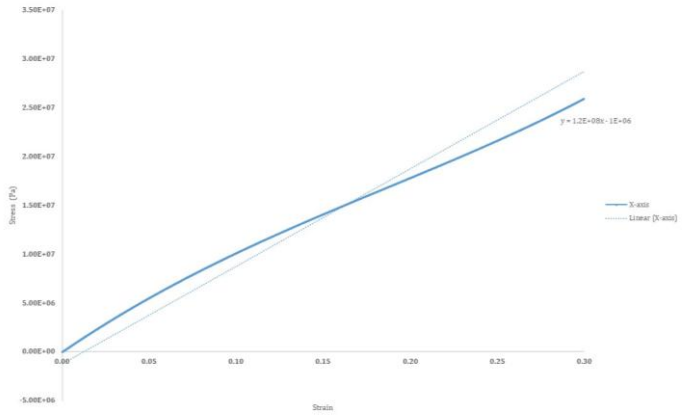

Figure 10. The stress-strain curve of the PMMA nanocube along the x-axis.

In Figure 10, the elastic region of the PMMA nanocube is loaded in tensile in the x-direction. Based on the trendline gradient, the Young's modulus is calculated to be around 0.12 GPa at 100 Å x 100 Å x 100 Å in the form of a nanocube, which is lower than the bulk PMMA modulus in (Anstine et al. 2.4-3.25 GPa) [7]. This significant decrease is a symptom of the strong impact of nanoscale effects on mechanical behaviour. The size of the object gets smaller, the ratio of surface/volume grows considerably, and a greater part of the atoms on the surface exist, but fewer of them have neighboring atoms. Interatomic forces on these atoms are weaker than in the bulk phase, giving them a softer mechanical response and a resultant decrease in stiffness. Moreover, it is also the case that the atomic coordination of the substance and the alterations on the local bonding environment at the nano-scale also lead to the observed reduction in the Young's modulus.

It has also been found that the nonlinear dependence of the reduction of the modulus of Young on decreasing size is also observed in other organic thin films and nanostructured materials, which supports the fact that PMMA demonstrates the softening of elastic behavior at the nanoscale [28]. The trend reveals the shortcomings of the classical, continuum-based definitions of the Young modulus for systems at an atomic scale. Bulk mechanics assumptions, including uniformly distributed stresses and insignificant surface effects, are no longer valid at such dimensions, leading to atomic potentials, surface reconstructions, and interfacial phenomena being the dominant factors in influencing mechanical response. All these factors explain why the Young's modulus of the nanocubes of PMMA is far lower than it is in the bulk samples of the material [7].

4. CONCLUSION

Simulations based on molecular dynamics were conducted in which the tensile behavior of PMMA nanocubes was investigated, and the mechanical response of the nanocubes at the nanoscale was better understood. The simulations gave important information on the deformation of PMMA under uniaxial tension, and specifically, the distribution of stress and structural changes during the loading condition. The simulations have been analyzed, and it is evident that the mechanical character of PMMA has undergone a clear transition as it first exhibits more of a solid-like behavior when acting as a bulk, but as its dimensions are lowered to the nanoscale, it starts to behave more like a fluid. This change is accompanied by a significant reduction in Young modulus, which is a softening effect, which increases with the smaller the size. This can be explained by the increasing influence of the surface effects and the weakening of the atomic coordination of surface atoms in smaller sizes. The results also show that the Young's modulus of PMMA nanocubes is significantly less than that of PMMA in bulk, both partly because the surface-volume ratio is higher and partly because the interatomic bonding forces are weaker at the nanoscale. The results stem directly from the condition of the process and the mechanical properties. Mechanical properties of PMMA on the nanoscale are important to possible applications in nanotechnology, where the behavior of a material in the nanoscale can be dramatically different than that of the same material on a large scale. Due to its

ubiquitous chemical usage and easily defined behaviour, PMMA is often of interest as the target polymer in thermal nanoimprint lithography systems, and the knowledge obtained here can be used especially well to streamline nanoscale manufacturing processes.

The molecular dynamics simulation and analysis of the present work provide a deep insight into the mechanical behavior of PMMA nanocubes under stretching force, and it is important to know the material behavior in nanotechnology, which is dependent on size. The development of the work in the future might be aimed at investigating the impact of various loading conditions, temperatures, and chemical variations on the mechanical behavior of PMMA nanocubes.

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