# THE STRESS ANALYSIS OF POLYMETHYLMETHACRYLATE (PMMA) NANOCUBE USING MOLECULAR DYNAMICS SIMULATION

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**Abstract**

Polymethyl methacrylate is a widely used polymer valued for its mechanical properties, chemical stability, and ease of fabrication. This study investigates the mechanical behavior of PMMA nanostructures under uniaxial tensile loading using molecular dynamics (MD) simulations. The objectives include understanding deformation mechanisms, mechanical stability, and tensile response at the nanoscale. PMMA nanostructures were constructed with JMOL and PACKMOL software, and simulations were performed using the COMPASS force field within the LAMMPS framework. Energy minimization and equilibration under NVT and NPT ensembles at 300 K and 1 atm ensured stable molecular configurations before mechanical loading. The effects of temperature and pressure variations on structural stability were also examined.Results show that PMMA nanostructures with high aspect ratios exhibit significant elongation under tensile stress. Stress-strain analysis reveals distinct elastic and plastic deformation phases, providing insights into nanoscale mechanical properties and limitations. Comparison with generic polymer nanostructures and bulk PMMA highlights enhanced mechanical performance due to nanoscale structuring. These findings deepen the understanding of PMMA's tensile behavior at the nanoscale and offer guidance for designing optimized nanostructured polymeric materials. The study's outcomes have potential applications in developing more durable flexible electronics, improved biomedical devices, and advanced nanotechnology.

Keywords: Molecular dynamics, Nanocube, Nanostructures, Polymethyl methacrylate, Stress-strain analysis