Mechanical behavior of glassy amorphous poly(ethylene oxide) under cyclic tensile loading via atomistic molecular dynamics simulations

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Abstract

The mechanical properties of a material define its response to external forces and are critical for applications in biomedical engineering, automotive, and aerospace industries. This study investigates the cyclic tensile deformation behavior of glassy amorphous polyethylene oxide (PEO) using atomistic molecular dynamics (MD) simulations, focusing on elastic and plastic deformation regimes. In the elastic regime, polymer chains exhibit reversible behavior, returning to their original conformations upon load removal. In contrast, plastic deformation, triggered by exceeding the yield stress, results in irreversible molecular rearrangements such as segmental motions and chain slippage, leading to permanent deformation. Our findings reveal the molecular mechanisms driving these behaviors, offering insights into PEO's mechanical properties and performance under repeated loading. These results provide valuable guidance for the design and application of PEO-based materials in aerospace, automotive, and food packaging industries.

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