From Atoms to Armor: Simulating How Polyurea Materials Absorb Shock at the Nanoscale

Polyurea is a protective polymer coating renowned for its ability to absorb and dissipate high-speed impacts, making it particularly useful in body armor and structural reinforcement applications. To explore its behavior under extreme loading, we performed molecular dynamics simulations using LAMMPS on a nanoscale model comprising more than half a million atoms. In our setup, a piston impacts the polymer at 1,000 m/s, generating a shock wave that propagates through the material.

Initially, the shock wave propagation disrupts hydrogen bond formation, resulting in the formation of nanoscale cavities (voids) during the compression phase. When the piston releases, a release wave overlaps with the reflected shock wave, resulting in the development of tensile stresses. The latter drives rapid void expansion and coalescence, a process known as spallation, which signals material failure. By tracking the spatiotemporal evolution of density and stress, and visualizing void growth directly, we gained an atomistic understanding of failure in polyurea.

These insights highlight why polyurea excels in impact protection, providing guidance for the design of next-generation coatings for defense, aerospace, and infrastructure applications.

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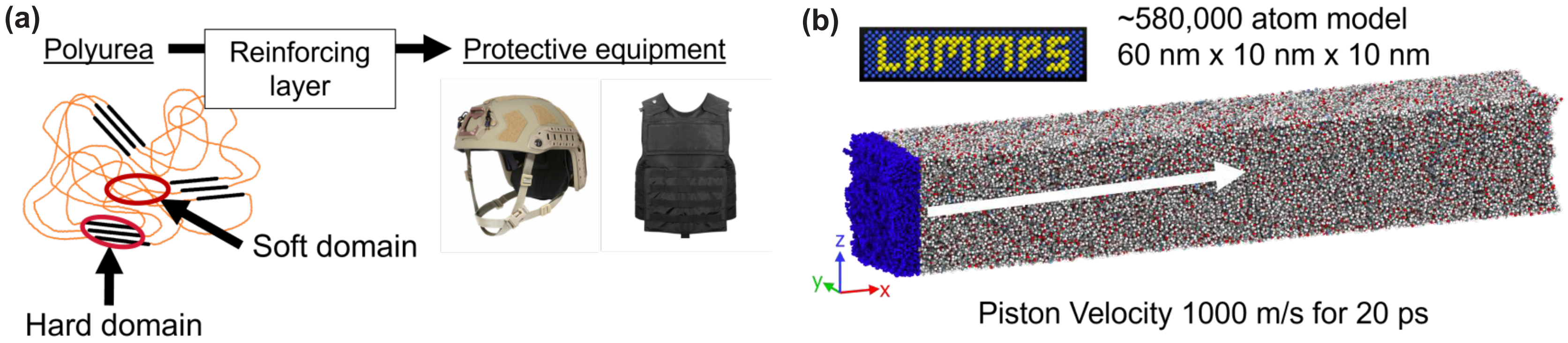
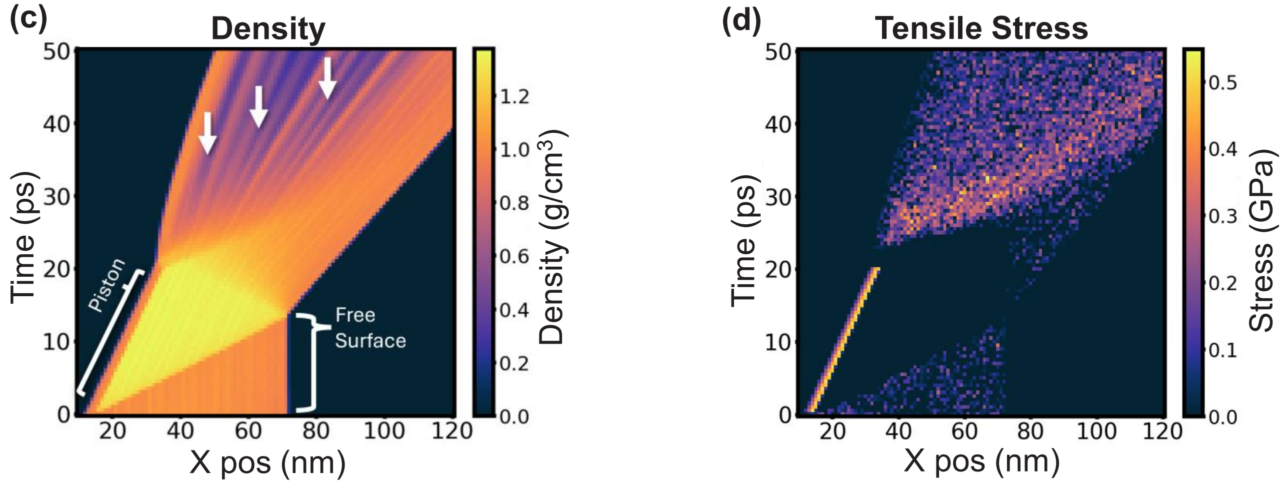
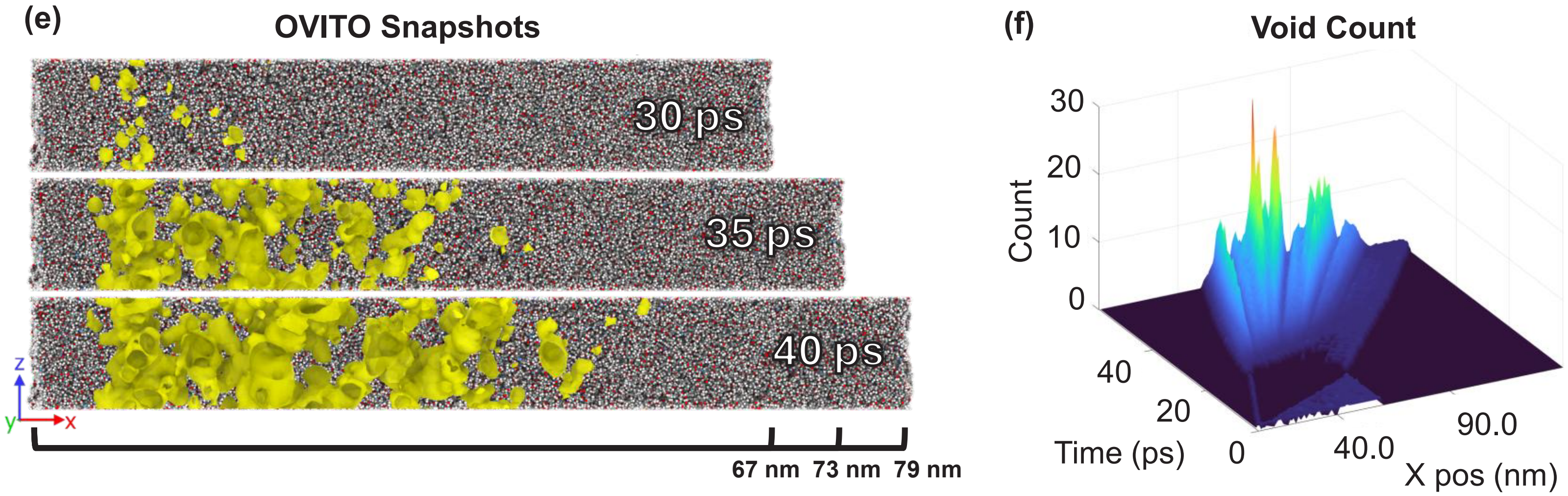


a) Flexible soft chains and rigid hard segments give polyurea its robust material properties suited for use in body armor and protective coatings. b) A piston (blue) compresses the nanoscale polyurea sample, launching a shock wave to probe impact response.



c) Spatiotemporal plot of density (g/cm^3) during compression and release. Spall planes marked with white arrows. Piston and free surface positions indicated. d) Spatiotemporal plot of tensile stress (GPa) compounding as release waves overlap.



e) OVITO snapshots showing voids nucleating (yellow) into spall planes after piston compression. f) The distribution of void count and X positional bins (nm) as time (ps) progresses.