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Modelling poly(p-phenylene teraphthalamide) at Extreme Tensile Loading using Reactive Potentials[1] DUNDAR YILMAZ, Zirve University — Aromatic polyamides classified as rigid-rod polymers due to orientation of their monomers. Because of their excellent mechanical and thermal properties, aramids are widely used in the industry. For example DuPont's brand Kevlar, for its commercial aromatic polyamide polymer, due to wide usage of this polymer in ballistic applications, habitually used as a nickname for bulletproof vests. In order to engineer these ballistic fabrics, material properties of aramid fibers should be studied. In this work we focused on the poly(p-phenylene teraphthalamide) PPTA fiber, known as brand name Kevlar. We employed Reactive potentials to simulate PPTA polymer under tensile loading. We first simulated both amorphous and crystalline phases of PPTA. We also introduced defects with varying densities. We further analysed the recorded atomic positions data to understand how tensile load distributed and failure mechanisms at extreme tensile loads.

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