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Modeling Structure Property Relations and Failure Mechanisms of PPTA Fibers using Reactive Molecular Dynamics[1] DUNDAR YILMAZ, Zirve University — Failure mechanisms of poly(p-phenylene terephthalamide (PPTA) under extreme tensile deformation has been studied using reactive potentials with molecular dynamics simulations. Amorphous PPTA systems with different molecular weights generated using an in-house developed amorphous builder. Tensile modulus of amorphous PPTA has been calculated as up to 6.7 GPa. Nitrogen and carbon vacancy defects were introduced to both crystalline and amorphous systems. The tensile modulus of defects-free crystalline PPTA calculated as 350 GPa. Introduction of 5% nitrogen vacancy defects reduced the tensile modulus to 197 GPa. PPTA fibers generated with skin core structure where skin region composed of PPTA chains in crystalline order and core region was composed of unordered PPTA chains vice versa. Relation between ratios of skin and core regions and mechanical properties of the fiber studied. Tensile load was mostly accommodated through stretching of bonds between amide group and phenyl groups. Under extreme tensile deformation PPTA chains failed at these C-N bonds.

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