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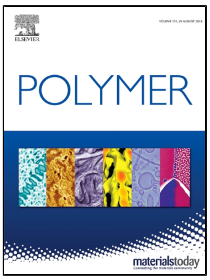

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Investigating Structure Property Relations of poly (p-phenylene terephthalamide) Fibers via Reactive Molecular Dynamics Simulations

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ABSTRACT: We modeled poly(p-phenylene terephthalamide) (PPTA) fibers in realistic size and structure and used Molecular Dynamics (MD) simulations with the ReaxFF reactive force field to investigate response to tensile deformation at extreme values. We constructed PPTA fibers in three forms: fully crystalline, fully unordered and core-shell structured with core and shell regions consisting of unordered and crystalline chains. The tensile deformation applied quasi-statically up to 15 % strain. We calculated the average tensile modulus of fully unordered and crystalline fibers as 192 GPa and 289 GPa, indicating that crystallinity significantly increases this modulus. We introduced defects in the form of nitrogen vacancies with densities up to 5 % and formulated an empirical equation to predict tensile modulus of the fiber based on defect density and crystallinity of the fiber. During the simulation, we observed domains in the crystalline region of fibers and failure of fibers started with breaking of chains located at these domain boundaries. As such, in