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Atomistic modeling of bio-based polymeric fibers IN-CHUL YEH, B. CHRISTOPHER RINDERSPACHER, JAN W. ANDZELM, Macromolecular Science and Technology Branch, U.S. Army Research Laboratory, LASHONDA T. CURETON, JOHN LA SCALA, Coatings, Corrosion, and Engineered Polymers Branch, U.S. Army Research Laboratory — We performed molecular dynamics simulations on the amorphous phase of two bio-based polymers, poly (butylene furanamide) and poly (hexamethylene furanamide). Simulations of corresponding petroleum-based polymers, nylon 4, 6 and nylon 6, 6, were also performed. Glass transition temperatures estimated from a series of simulations were in good agreement with experimental measurements. Stress-strain relationships under uniaxial deformation were also analyzed. Bio-based polymers show higher glass transition temperatures and comparable yield points despite having overall weaker hydrogen bonds compared with their counterparts nylons. This result suggests that the furan ring plays an important role in the thermodynamic and mechanical properties of bio-based polymers.

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