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Molecular engineering of high-performance elastomeric materials SHENGWEI DENG, Department of Materials Science and Engineering, Johns Hopkins University, MICHAEL FALK, Departments of Materials Science and Engineering, Mechanical Engineering, Physics and Astronomy, Johns Hopkins University
— Polyurethane is a typical elastomeric material and among the most versatile materials today. It is a linear block copolymer consisting of alternating soft and hard segments with phase separation due to thermodynamic segmental incompatibility. Inspired by the hierarchical structure of spider silk, this kind of block copolymer can be synthesized with two distinct blocks that can differ in their propensity to crystallize. Either the soft or hard segments can be amorphous or semicrystalline. Recent experiments indicate that crystallizable segments lead to higher tensile strength and that systems with crystalline hard segment exhibit better stiffness, strength and mechanical toughness. Here we implement molecular dynamics simulation to investigate the influence of block architectures on mechanical properties and molecular chain movement.

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