Viscoelasticity and Mechanics Properties of Crosslinked Rubbers and Glassy Composite Networks via detailed Atomistic Simulations

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Abstract

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We study the viscoelasticity and mechanics of crosslinked Styrene Butadiene Rubber (SBR) and the fracture mechanics of glassy epoxy crosslinked networks. Both are studied with molecular dynamics simulations. SBR systems are used widely in tire industry while the epoxy glassy composite networks with Solid Polymer Electrolytes (SPE) are used widely as supercapacitors.

As regard the SBR system, we present a detailed study of the structural and mechanical properties an SBR elastomeric network crosslinked with Sulfurs at the molecular level, via detailed atomistic molecular dynamics (MD) simulations in United Atom (UA) scale. The structural ratio is (styrene/trans/vinyl/cis): (15/33/26/26) by weight % and a 4 atom sulfur chain, acting as a hardener for the crosslinking process.
As regard the fracture and mechanical properties of glassy –composite- networks, we study in All Atomistic (AA) scale with molecular dynamics. Properties of structure and elasticity are presented as well.

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