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RIS-Monte Carlo Based Molecular Modeling of Elasticity and Photoelasticity of SBS Thermoplastic Elastomer KAPILESWAR NAYAK, Hemant Nanavati — Phase morphology and molecular conformation play an important role in dictating the physical and chemical properties of a material. SBS (Styrene-Butadiene-Styrene) thermoplastic elastomers (TPEs) exhibit two-phase morphology, and if the polystyrene content is in the range 20-30%, are modeled as polystyrene (PS) spheres in amorphous polybutadiene (PB) domain. The PB block bridges two spheres of the impenetrable PS block, where these PS spheres act as network crosslinks. The PB chain can assume a number of conformational arrangements, due to rotations about single bonds contained in the chain backbone. These conformational arrangements yield distributions of chain vector length and polarizability anisotropy, and have been determined via Rotational Isomeric States Monte Carlo (RIS-MC) simulations. The triblock nature of the SBS chains as well as the impenetrability of the PS domains have been incorporated into the RIS-MC simulations, thus incorporating the relevant primary structural aspects into the framework. The development has been extended to yield stress-elongation and birefringence-elongation relationship for TPE networks.

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