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Segment Orientation and Optical Birefringence of Amorphous Polymers Under Tensile Deformation: Novel Computational Method applied to Different Glassy Polycarbonates UPENDRA NATARAJAN, National Chem. Lab. India, M.S. SULATHA, National Chem. Lab. India — Orientation dependent optical properties of Bisphenol A polycarbonate and two aliphatic substituted polycarbonates in glassy phase have been studied by atomistic modeling using molecular mechanics simulations under tensile deformation. Probability distributions and orientation functions show that phenylene rings and carbonate groups vectors along the main chain orient towards stretching direction following deformation. Interchain packing of rings and carbonates become ordered with strain. Efficient computational approach for calculation of optical birefringence of amorphous polymers is presented and applied to the polycarbonates in detail. Polarizability anisotropy of the polymer segments and chain as a function of deformation is calculated by combining information on the conformations and group polarizabilities, and used to estimate birefringence during deformation. Simulated and experimental values for segment orientation and bulk birefringence are in very good agreement. Effect of the optical properties of atomic groups on bulk birefringence is brought forth for the first time by molecular simulation for polymers other than polyethylene.

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