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Prediction of Optical Properties for Stretched Polymers Using Molecular Dynamics Method

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In this study prediction of birefrengence of stretched polymers was performed by molecular dynamics simulations. Polystyrene, poly[ethylene-co-norbornene] and poly[ethylene-co-tetracyclododecyne] composed of 4 polymer chains with about 50 monomers were examined by full atomistic simulations. After equilibration, the systems were subject to uniaxial elongation under constant volume. The stretching speed and temperature were reasonably determined from glass transition temperature for each polymer. Obtained results were qualitatively consistent with experimental results for commertialized polymers.