187a Local Dynamics of Syndiotactic Pmma Using Molecular Dynamics Simulation

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The local dynamics of syndiotactic poly(methyl methacrylate) (PMMA) have been investigated by Molecular dynamics (MD) simulations and qusielastic neutron scattering at temperatures well above the glass transition temperature. Good agreement was found between MD results and time-of-flight neutron scattering measurements as represented by the self dynamic structure factor S(q,t). Neutron experiments observed little difference between the local dynamics of the short and long PMMA chains indicating local dynamics is unaffected by the chain length. Using MD, we are able to isolate rotations of alpha- and ester methyls, and the entire carboxyl side group, which has been suggested as the origin of the beta-relaxation in PMMA. This capacity is unique to simulation as proton motion at high temperatures necessarily involves both main chain motion and rotations. We find that S(q,t) for rotation of both alpha- and ester methyls is stretched as reported from neutron data on labeled samples at low temperatures. The elastic incoherent scattering factor (EISF) is consistent with that predicted from a threefold jump rotation theory. We also investigated the molecular motions associated with the beta-relaxation by correlating it with the rotation of the entire carboxyl side group.