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Local Dynamics of Acid- and Ion-containing Copolymer Melts. KAREN WINEY, ROBERT MIDDLETON, University of Pennsylvania, JACOB TARVER, MADHUSUDAN TYAGI, CHRISTOPHER SOLES, NIST, AMALIE FRISCHKNECHT, Sandia National Laboratory — Interest in acid- and ion-containing polymers arises in part from applications as single-ion conductors for selectively transporting a counter ion for battery applications. Structurally, the low dielectric constant of organic polymers and strong ionic interactions leads to ionic aggregation. Here the polymer backbone motion was investigated through quasi-elastic neutron scattering measurements (QENS) and compared with fully atomistic molecular dynamic simulations of precise poly(ethylene-acrylic acid) copolymers and their ionomers (pxAA-y%Li). The effect of carbon spacer length (x=9, 15, 21) between the acid groups and the degree of neutralization (y) with Li on PE backbone dynamics were considered. Systematic slowing in chain dynamics were observed with increasing neutralization where polymer dynamics appear constrained due to anchoring effects. Simulations provide complementary viewpoints indicating a gradient in chain dynamics as a distance away from acid groups. These results indicate that the addition of pendant acid groups inhibit typical PE backbone motion and the neutralized forms strongly suppress the fraction of mobile PE chain.

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