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Molecular Simulation Characterization and of Poly(pphenylene/m-phenylene) Copolymers. ROBERT BUBECK, Michigan State University, STEVEN KEINATH, Michigan Molecular Institute - Retired — Characterization and molecular simulation of the molecular structure and microstructure of poly(p-phenylene/m-phenylene) copolymers were carried out. Tensile modulus, yield stress, and entanglement molecular weight were modeled as amorphous polymers as a function of m-phenylene content. Significant biphasic character, however, was observed for two copolymers in the melt near 300°C using variable temperature synchrotron-based WAXS. The biphasic nature of the melt may be a contributor to difficulty in melt processing. Precise experimental determinations of entanglement molecular weights were frustrated by the occurrence of significant amounts of nematic mesophasic order in the rubbery and melt regimes of two commercial poly(pphenylene/m-phenylene) examples. Nonetheless, entanglement molecular weights obtained by molecular modeling can be useful for experimental guidance because the level of order in the glassy phase near ambient temperature was found to be low (5 %) regardless of melt processing history. Based on both the modeling and WAXS measurements, it is believed that increasing m-phenylene content reduces modulus, and improves toughness and processibility.

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