

Abstract Submitted
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Molecular Simulation and Microstructure Characterization of Poly(p-phenylene/m-phenylene) Copolymers¹ ROBERT BUBECK, STEVEN KEINATH, Michigan Molecular Institute — Molecular simulation and characterization 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 (environs of 300°C) using variable temperature synchrotron-based WAXS. 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(p-phenylene/m-phenylene) examples. Nonetheless, entanglement molecular weights obtained by molecular modeling are useful for future experimental guidance because the level of order in the glassy phase near ambient temperature was found to be low (approx. 5%) regardless of melt processing history. The biphasic nature of the melt may also be a contributor to more difficult melt processing. Based on both the modeling and WAXS measurements, it is believed that increasing m-phenylene content might improve toughness and processibility relative to the interrogated samples.

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