Chain-Folding Structures of a Semi-crystalline Polymer in Bulk and Single Crystals Elucidated by 13C–13C Double Quantum NMR

YOU-LEE HONG, TOSHIKAZU MIYOSHI, The University of Akron — Semi-crystalline polymers are crystallized as folded chains in thin lamellae of ca. 5-20 nm from random coils in the melt and solution states. However, understanding of detailed chain-folding structure and crystallization mechanism are still challenging issue due to various experimental limitations. We recently developed a new strategy using \(^{13}\text{C}–^{13}\text{C}\) double-quantum (DQ) NMR with selectively \(^{13}\text{C}\) isotope labeled isotactic poly(1-butene) form I to investigate chain-trajectory in solution and melt grown crystals at various \(T_c\)s. This new method can determine the re-entrance sites, the successive folding number \((n)\), and the fractions \((F)\) of chain-folding in a wide \(T_c\) range. In melt grown crystals at \(T_c = 95^\circ\text{C}\), a comparison of experimental and simulated DQ efficiency determined that the polymer chains alternatively change chain-folding directions and the stems tightly pack via intramolecular interactions, and the fraction \((F)\) of adjacent re-entry structure ranges from 70\% at \(n = 4\) to 100\% at mixed structures of \(n = 1\) and 2. Furthermore, DQ efficiency is independent of \(T_c\) in bulk crystals. This means chain-folding do not change in a wide \(T_c\)s.

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