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Chain-Folding Structures of a Semi-crystalline Polymer in Bulk and Single Crystals Elucidated by 13C–13C Double Quantum NMR[1]

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}C–^{13}C double-quantum (DQ) NMR with selectively ^{13}C isotope labeled *isotactic* poly(1-butene) form I to investigate chain-trajectory in solution and melt grown crystals at various Tcs. This new method can determine the re-entrance sites, the successive folding number (n), and the fractions (F) of chain-folding in a wide Tc range. In melt grown crystals at $Tc = 95$ °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 Tc in bulk crystals. This means chain-folding do not change in a wide Tcs.

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