When Do Semi-crystalline Polymer Fold during Crystallization?\textsuperscript{1}

TOSHIKAZU MIYOSHI, YOU-LEE HONG, 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. Lauritzen–Hoffman theory implied the crystallization process is dominated by sequential stem deposition on the growth front. Conversely, Allegra proposed a bundle model in which aggregates of 10-20 stems are produced by folding in the pre-stage of crystallization. The pre-folded chains are kinetically deposited on the growth front and thus determine the morphology at different crystallization temperatures. The folded chains preserve their own chain-folding directions, numbers, and fractions as a function of concentrations and supercooling, which would provide detailed chain-folding mechanism. We recently developed a new strategy using $^{13}$C-$^{13}$C double-quantum NMR to investigate chain-trajectory of $^{13}$C selectively labeled polymer in bulk crystals. Here, we report how re-entrance sites, fraction, and number of folded chains of *isotactic* poly(1-butene) in form III single crystals depends on supercooling conditions and solvent effects. On the basis of molecular level structures, we will discuss about chain-folding process of $i$PB1 in dilute solutions.

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