Topological Constraints on Chain-Folding Structure of Semicrystalline Polymer as Studied by $^{13}$C-$^{13}$C Double Quantum NMR$^1$ YOULEE HONG, TOSHIKAZU MIYOSHI, The university of akron — Chain-folding process is a prominent feature of long polymer chains during crystallization. Over the last half century, much effort has been paid to reveal the chain trajectory. Even though various chain-folding models as well as theories of crystallization at molecule levels have been proposed, they could be not reconciled due to the limited experimental evidences. Recent development of double quantum NMR with selective isotope labeling identified the chain-trajectory of $^{13}$C labeled isotactic poly(1-butene). The systematic experiments covered a wide range of parameters, i.e. kinetics, concentration, and molecular weight ($M_w$). It was demonstrated that i) adjacent re-entry site was invariant as a function of crystallization temperature ($T_c$), concentration, and $M_w$, ii) long-range order of adjacent re-entry sequence is independence of kinetics at a given concentration while it decreased with increasing the polymer concentration at a given $T_c$ due to the increased interruption between the chains, and iii) high $M_w$ chains led to the multilayer folded structures in single crystals, but the melt state induced the identical short adjacent sequences of long and short polymer over a wide range of $T_c$ due to the entanglements. The behaviors indicated that the topological restriction plays significant roles in the chain-folding process rather than the kinetics. The proposed framework to control the chain-folding structure presents a new perspective into the chain organization by either the intra- or inter-chain interaction.

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