Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Exploring Molecular Dimension and Trajectory of Polymer Chains Embedded in Single Crystals[1] YOULEE HONG, TOSHIKAZU MIYOSHI, University of Akron — Semicrystalline polymers are crystallized as folded chains in thin lamellae of ca. 5-20 nm from random coils in the melt and solution states.. Even though there are continuous efforts on understanding of crystallization mechanisms at molecular levels for understanding of crystallization mechanism of polymers at molecular levels, the fundamental questions - when, where, and how do semicrystalline polymers fold during crystallization?- have not been clarified due to experimental limitations. Recently, we developed a novel strategy to access chain trajectory of semi-crystalline polymers using 13C -13C double Quantum (DQ) NMR. In this work, we recently investigated determined molecular dimension as well as chain-trajectory of 13C CH3-labeled isotactic poly(1-butene) (iPB1) in form III chiral single crystals blended with nonlabeled iPB1 crystallized under low supercooling, using solid-state NMR. Comparisons of 13C -13C double quantum (DQ) NMR results at multiple sites with spin dynamics simulation revealed individual chains form the three dimensional nanoclusters via folding. This result supports proves two step process of i) cluster formation by chain-folding the prestage of crystallization. and ii) depositions of the cluster on the growth front of single crystal.

[1]National Science Foundation

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Date submitted: 13 Nov 2014 Electronic form version 1.4