Short-Range Order of Mesomorphic Phase of a Semi-crystalline Polymer by Solid-State NMR: Isotactic Polypropylene

SHICHEN YUAN, TOSHIKAZU MIYOSHI, Univ of Akron — Mesophase is intermediate phase between crystalline and melt state. Characterization of short-range structures of disordered mesomorphic phase without long-range order is challenging issue in polymer characterization. The short range order was considered same as α or β iPP, or neither. In this work, a new strategy using $^{13}$C-$^{13}$C through space interactions as well as molecular dynamics based on chemical shift anisotropy (CSA) re-orientation is proposed for evaluating short-range order of mesophase of isotactic-polypropylene (iPP). $^{13}$C-$^{13}$C double quantum (DQ) build up curves of $^{13}$C 15 percent CH$_3$ selectively labeled iPP and spin dynamics simulations elucidate that local packing structures in mesophase is very close to that in β phase. Moreover, exchange NMR proves that the crystalline chains perform large amplitude motions in all α, β, and mesophase. The correlation time of overall dynamics of stems in mesophase follows the same Arrhenius line with that of β phase but is largely deviated from the Arrhenius line of the α phase. Through the obtained results, it is concluded that short-range order in mesophase is exceedingly close or same to those in β phase.

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