

MD simulation of the influence of branch content on collapse and conformation of LLDPE chains crystallizing from highly dilute solutions.

Abu-Sharkh, Basel; Hussein, Ibelwaleed A.

Department of Chemical Engineering, Dhahran, Saudi Arabia.

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Abstract

The influence of branch content (BC) on the conformation of Ziegler-Natta linear-low d. polyethylene (ZN-LLDPE) in dil. solns. was studied by mol. dynamics simulation. Octene LLDPE with different levels of BC distributed randomly along the chain mimicking ZN-LLDPE was simulated in vacuum at 400 and 500 K. Increasing the BC decreased the chain folding and changed the conformation. The conformation undergoes a transition from lamellar to a more random coil-like structure near a BC of 40 branches/1000 backbone carbons. The findings are in agreement with exptl. results of M. Zhang et al. (2001). Extended chains with higher BC collapse faster and form more kinks than chains with lower BC with the branches acting as nucleation points for the chain collapse. At high BC, branches are obsd. to self-assemble away from the backbone.