

Abstract Submitted  
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**Early Stage Crystallization in Isotactic Polypropylene: Influence of Substrate-Polymer Interaction and Confinement** XIAOFENG CHEN, RAHMI OZISIK, Rensselaer Polytechnic Institute, SANAT KUMAR, Columbia University, PHILLIP CHOI, University of Alberta — Formation of helices in isotactic polypropylene was studied using on-lattice, coarse-grained, Metropolis Monte Carlo simulations. Influence of polymer-substrate interaction on polymer crystallization was studied by placing iPP chains on a flat surface. Results indicated that attractive interaction between polymer and particle plays a dominant role in the formation of helical structures. Repulsive interaction excludes polymer chains from the neighborhood of the surface and triggers crystallization transition earlier (at higher temperatures). Irrespective of the energy potential used, flat surface always influences the orientation of the helices to be parallel to the surface. Confinement effect was also investigated by changing the gallery spacing between two flat surfaces. Confinement significantly prohibits the growth of long helical structures but has no effect on the overall helicity as well as the ordering of helices.

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