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Influence of Confinement on Crystallization of Isotactic Polypropylene[1] XIAOFENG CHEN, RAHMI OZISIK, Rensselaer Polytechnic Institute, SANAT K. KUMAR, Columbia University — Crystallization of polymer chains in the presence of nanoparticles is an area of interest because there has been considerable progress in the synthesis of various types of nanoparticles and their use as fillers in polymeric matrices. Interactions between polymer chains and particles, effect of confinement due to nanoparticles, and shape and size of nanoparticles all play important roles in the crystallization behavior of polymers. In order to investigate these factors, computer simulations were performed on isotactic polypropylene nanocomposites. The results indicate that polymer-particle interaactions play an important role. When polymer particle interaction is strong, a high density layer near the particle surface is formed but helix formation does not take place due to the strong interaction. When interactions were not considered, particle acted as a nucleating agent for helix formation. Confinement also played an important role.

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