

Abstract Submitted
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Nascent Crystallization and Nascent Morphology XIAOZHEN YANG, Institute of Chemistry, CAS — It was found that recognition of nascent morphology enables us to control the ultimate property of the polymerized product. The nascent morphology is at mesoscale, its formation regarding to detailed mechanism is at molecular level. Molecular dynamics simulation of growing chain organization on catalyst surface was performed by modifying the codes for normal NVT ensemble into the giant canonical ensemble. We found that a growing chain as simulated from 10 bond length to 1010 bonds undergoes novel behaviors through stages of the nucleation and the crystal growth on the surface. 64 chains growing in a 8×8 matrix was also examined. Variation of the catalyst density distribution was found correlative to the different nascent morphologies.

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