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Architecture dependence of crystallizable sequences in semicrystalline polymers VIKRAM K. KUPPA, GREGORY C. RUTLEDGE, Massachusetts Institute of Technology — Monte Carlo molecular simulations are used to examine the backbone conformations of short loops reconnecting the crystal surfaces of isotactic polypropylene(iPP) and polyethylene(PE). Fractions of alternating trans and gauche torsional sequences for iPP and trans states for PE are identified as the appropriate parameters to measure crystallizability. The higher fraction of gauche dihedrals in backbone conformations of iPP make it more flexible than PE. Short loops of both architectures show a high degree of disorder, as manifested by the large number of unfavorable, non-crystallizable sequences. Density profiles for both polymers show a characteristic decay in crystallizable torsions from the crystal phase to the melt, over the interphase. For iPP, the increased flexibility of the chains leads to a larger population of adjacent re-entry loops on the fold surface, which are spatially correlated to the minimum in density profiles of crystallizable sequences.

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