Microscopic Insights into Compatibilized Semicrystalline Blends

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Recent work shows certain compatibilizers can enhance polyolefin blend toughness, potentially reducing the cost of mixed plastic waste recycling. While researchers have proposed several toughening mechanisms, their validation is challenging. Experiments cannot yet resolve how compatibilizers interact with crystal or amorphous domains. Employing a coarse-grained model that forms lamellae, we use molecular dynamics simulations to investigate the interfacial structure of semicrystalline polymer blends with and without compatibilizer. These simulations offer insights into how compatibilizers interact with the lamellae, including whether they co-crystallize or form trapped entanglements. Such findings could aid in compatibilizer architecture optimization.