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Semicrystalline Polymers: A special case of polymer brushes VIKRAM KUPPA, GREGORY RUTLEDGE, Massachusetts Institute of Technology — Monte Carlo (MC) molecular simulations are employed to evaluate the interface between crystalline and amorphous polyethylene. The simulation setup mimics the interlamellar region of a semicrystalline polymer with a low effective molecular weight. All polymer chains are tethered to the crystal surface at one of their ends, thus forming tails with their other (free) ends distributed in the space between crystal lamellae. Two different systems are explored: one, in which the simulations explore a range of molecular weights due to the use of MC moves that exchange beads between different chains; and another, in which strict control of the molecular weight is exercised, thereby constraining chain lengths to a narrow window. The effects of temperature, grafting density, molecular weight distribution and the interaction between brushes on opposing crystal surfaces are investigated by examining monomer density profiles, chemical potentials and bond orientation order parameters.

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