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Chain Folding and Lamellar Thickening Behavior in Polymer Crystallization based on self-consistent field theory PING TANG, FAQIANG LIU, YULIANG YANG, Fudan University — Chain folding is a main characteristic in polymer crystallization which remains challenging in theoretical investigations, due to its spanning from the microscale of chain segment and mesoscale of entire chain trajectory in lamellae. The self-consistent field theory (SCFT) based on multi-block rod-coil chain model is employed to investigate the crystalline behavior. The chain conformation in the crystalline and amorphous regions is described with Caussian chain and rigid rods. The results indicate that lamellae thickness and the proportion of adjacent re-entry conformation depend on the combined effect of crystalline enthalpy, spatial distribution in amorphous region, and interfacial energy resulting from fold energy and conformation loss of amorphous chain at the interface. The influence of crystalline enthalpy, crystalline degree, lamellae thickness and interfacial energy on chain folding are studied. The results show that crystalline enthalpy reduces the probability of fold structure at large interfacial energy while almost no effect at small interfacial energy, indicating a synergistic effect between interfacial energy and crystalline enthalpy on the chain folding. It is also found that lamellae thickness promotes the fold structure while crystalline degree has an opposite effect. Our model demonstrates advantages in accurately describing the comprehensive features of polymer chain in polymer semi-crystal system and provided a semi-quantitative thermodynamic picture of chain folding in polymer crystallization.

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