Poster 24

Coarse-grained simulations of the crystallization process of short chain branched polyolefins.

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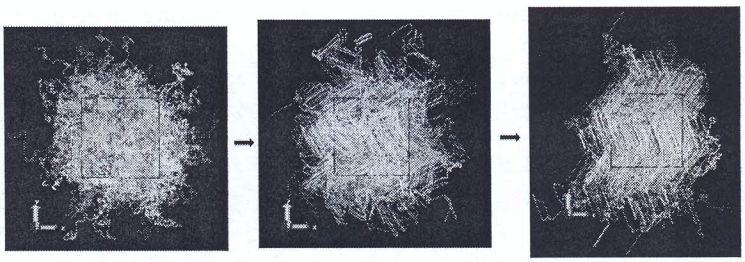
Short chain branched polyolefins (SCB-PE) are copolymers of ethylene and α-olefins, such as 1-butene or 1-hexene. The applications of these materials are versatile because the solid and melt physical properties of these plastics can be tailored by controlling the concentration and distribution of α-olefins in the copolymer. Thus, a detailed understanding of the influence of the atomistic molecular architecture on both the crystallization process and the physical properties is of great interest. Recently, atomistic[1, 2] and coarse-grained[3] computer simulations have shown to be a suitable tool for monitoring the conformation of the polymer chains at the monomer level.

In this communication, we present the development of a coarse-grained (CG) model for linear and SCB polyolefins using the Iterative Boltzmann Inversion (IBI). Afterwards, we have applied this CG model to study the crystallization process of a linear polymer (PE-00), and two ethylene/1-hexane copolymers with 1%-mol (5 butyl branches/1000C, PE-05) and 2%-mol (10 butyl branches/1000C, PE-10) of butyl branches, respectively.

The non-isothermal crystallization process has been simulated at various cooling-rates for the three CG systems. Both, the effects of the cooling-rate and the amount of SCB on the crystallinity and lamellar thickness of the semi crystalline state are discussed and compared with the available experimental data. Furthermore, the annealing at different temperatures near the melting point is also simulated. We monitor the changes in conformations, density, crystallinity and lamellar thickness as a function of the SCB. The main conclusions are: i) The CG model reproduces the decrease of crystallinity and lamellar thickness as the amount of branches increases and ii) the effects of annealing are clearly observed in the linear system but they are mitigated by the presence of the branches in the SCB models.



Melt State
(Amorphous system)

Semicrystalline state after non-isothermal crystallization
(Folding and packing of chains in crystalline domains)

Semicrystalline state after annealing
(Improving and thickening of the crystal domains)

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