Stress transmission in lamellar semi-crystalline polymers evaluated by molecular dynamic simulations

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Abstract

The macroscopic mechanical behavior of semi-crystalline polymers is described using concepts such as tie molecules to explain the stress is transition between crystalline lamellae through the amorphous phases. However, these particular chains are not possible to observe directly by any means. The dependence of the mechanical properties with the chain topology and entanglement has been then analyzed by a coarse-grained molecular dynamic model(1). After cooling from a melt, and isothermal treatment, semi-crystalline systems of different chain lengths and oriented lamellar structures were obtained. The different systems exhibit different entanglement densities and chains topologies. Thanks to tensile tests in the chain direction a relation between the chain topology, the entanglements and mechanical properties such as yield stress or hardening is proposed. It has been shown first that the loop chains are prevalent and play the most important role on the mechanical properties. Secondly the entanglement density is linked to the chain topology and can effectively be the descriptor of most of the mechanical properties. The link between the chain topology and the entanglement density is discussed.

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