Interfacial Properties of Linear-Cyclic Polymer Blends

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Dynamics of polymers in the melt state is strongly influenced by molecular architecture [1-4] and it is a subject of both industrial and fundamental interest in polymer physics and rheology. Theoretical and computational studies of pure (CPs) and linear (LPs) polymers have been intensively performed in the last decades, however linear-cyclic polymer blends (LCBs) have not been scrutinized to the same depth so far. These polymer systems are important because most experimental data on pure CPs are ´´contaminated´´ by the presence of LPs (mainly due to limitations in the purification methods), and the dynamics of LCBs is extremely sensitive to the concentration of LPs. Moreover, blending polymers with different molecular topologies could also be relevant to control interfacial segregation so to avoid macroscopic phase segregation of the polymer film, and providing optimal mechanical properties for a number of polymeric materials used for industrial applications [5,6]. In our brief presentation, we will show some results of a systematic study of bead-spring models of LCBs by means of molecular dynamics simulations. These results are also obtained by changing the nature of the interface and considering the adsorption of the system on a solid substrate (flat wall). We will discuss our findings in the light of theoretical evidences suggesting that cyclic chains segregate to the surface by maximizing the conformational entropy of the system [7], and experimental results providing evidence of the contrary, i.e. cyclic chains are depleted at the film surface [8].

References

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