

Structure of Polypropylene Macromolecules in the Vicinity of Fe₂O₃ Surface

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Abstract

With the expanding application of additive manufacturing processes such as Thermoplastic Fused Filament Fabrication (FFF), it is necessary to explore new classes of complex materials for production purposes. Highly-filled metal-polymer nanocomposites (MPNs) with above 50 vol% of metallic particles are a significant example of such materials which show promising results in FFF [1].

The incorporation of high concentrations of solid particles in MPNs imposes various constraints on the polymer macromolecules. Such restrictions could give rise to tremendous re-structuring of chains in the vicinity of particles surface. An attempt was made to study the structure of syndiotactic polypropylene macromolecules at the Fe₂O₃ surface utilizing detailed atomistic models. Molecular dynamics (MD) was incorporated with the Consistent Valence Forcefield (CVFF) to represent the atoms. The simulations were run for 5 ns with a time step of 1 fs. Meanwhile, the interaction energy of the chains with the surface was calculated. Moreover, the gyration radius of the chains was monitored with the distance from the surface.

The interaction energy showed attractive forces between the chains and the surface. This attraction later led to the more expansion of the chains closer to the surface compared with the chains further away in the bulk. The bead number density also approved the formation of the adjacent layer of chains on the surface. These observations provide significant backgrounds for the evaluation of the fundamental properties needed to perform multiscale modelling of such systems.

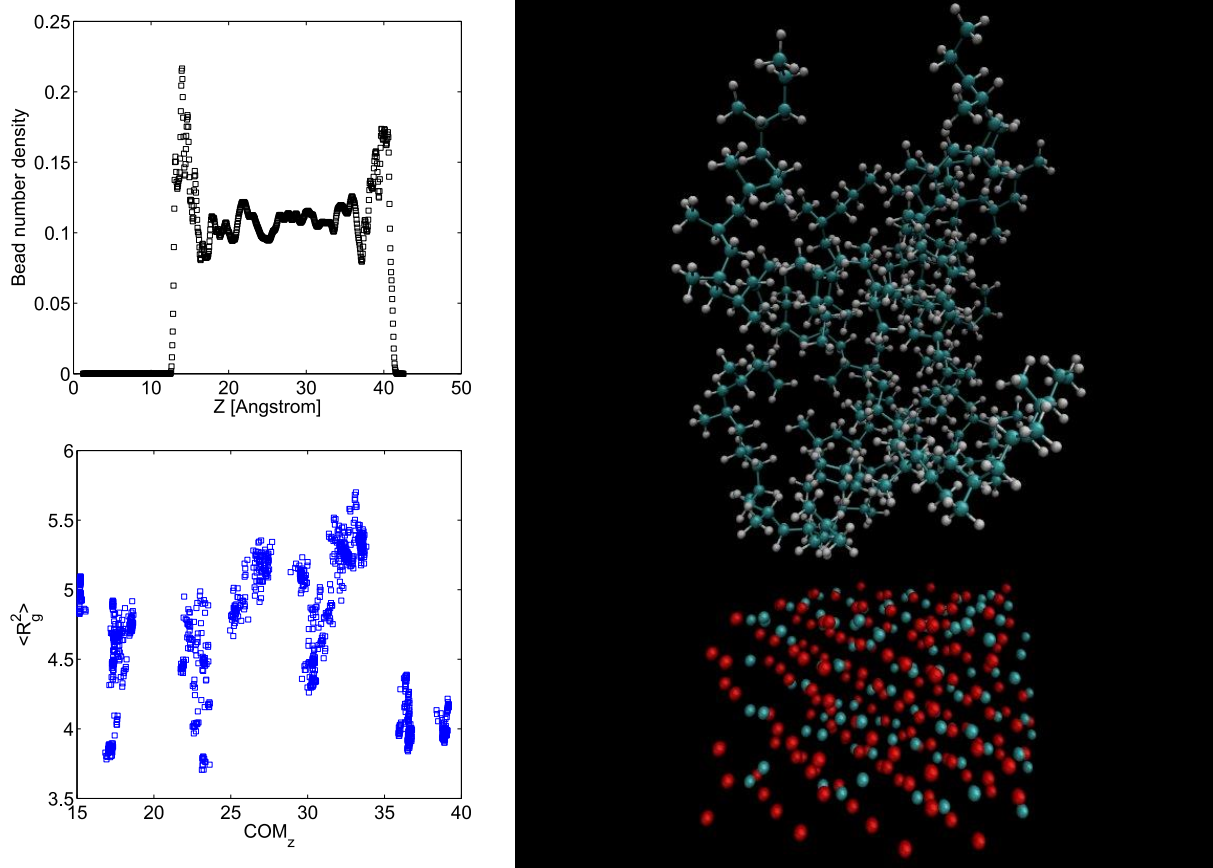


Figure 1: (top left) Bead number density in the z-direction away from the Fe_2O_3 surface; (bottom left) The average squared gyration radius as a function of the center of mass of the chain in the z-direction (COM_z); (right) Schematic representation of the polymer chains and the Fe_2O_3 surface.

Literature

- [1] Masood S., Song W.: Cyclic tests on cracked round bars as a quick tool to assess the long term behaviour of thermoplastics and elastomers, *Materials & Design*, Vol. 25, 2004, 587-594