COARSE-GRAINED MOLECULAR DYNAMICS SIMULATIONS OF POLYMER-SOLID INTERFACES IN NANOCOMPOSITES

Giuliana Giunta[1], Carsten Svaneborg[2], Ali-Karimi Varzaneh[3], Paola Carbone[1]

[1]*School of Chemical Engineering and Analytical Science, University of Manchester, UK*
[2] *Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Denmark*
[3]*Continental, Hannover, Germany*

giuliana.giunta@manchester.ac.uk

The adsorption and dynamics of polymer chains on solid surfaces play an important role in many applications, especially in polymer nanocomposites, where inorganic fillers such as carbon black are dispersed in the polymer matrix to improve composite mechanical and rheological properties. The effect that the presence of such particles has on the macroscopic properties of the material is directly linked to the polymer/filler interfacial area and the chemical nature of the particles [1]. However the molecular mechanisms by which these properties are modified are not entirely clear. This lack of understanding is mainly due to the complexity of the experimental characterization and of the material itself which often contains polymer chains with large distribution of molecular weight, particles of different sizes and geometry and different type of additives including small organic molecules which act as plasticizers [1, 2]. In this work we develop a Coarse-Grained (CG) model for graphite/PI nanocomposite, which is in this instance considered as a model for the surface of carbon-black fillers. To do that we employ the Kremer-Grest (KG) PI model developed by Svaneborg et al. [3] and implement a new efficient way to optimize the parameters for PI and graphitic surface. By performing molecular dynamics simulations we study the effect of the solid surface on the conformation of the adsorbed polymer chains (Figure 1) and the entanglement density. Finally we investigate the behaviour of the adsorbed chains in the presence of plasticizers which are added to modify the glass transition temperature of the polymer.

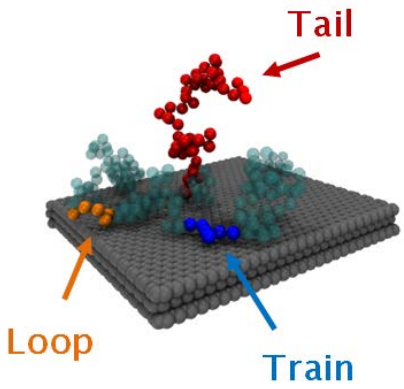

Figure 1 – Schematic representation of a polyisoprene chain adsorbed on graphite

References

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