Molecular modelling for optimum design of polymer-graphene nanocomposites

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Background

Polymer-graphene nanocomposites offer a variety of multifunctional properties that are of benefit to a range of industries (e.g. electronics or automotive). The ultimate functionality of those materials depends on the material composition and adopted processing route. It is particularly important to obtain more insight into the effects of the nanoparticle functionalisation on the local structural and functional properties of those materials across a range of conditions typical of industrial processing. Hence, the ultimate aim of this work is to develop a molecular computational model to predict most optimum surface modifications for controlled dispersion and distribution of graphene within polymers, and for enhanced end-use properties of the nanocomposites.

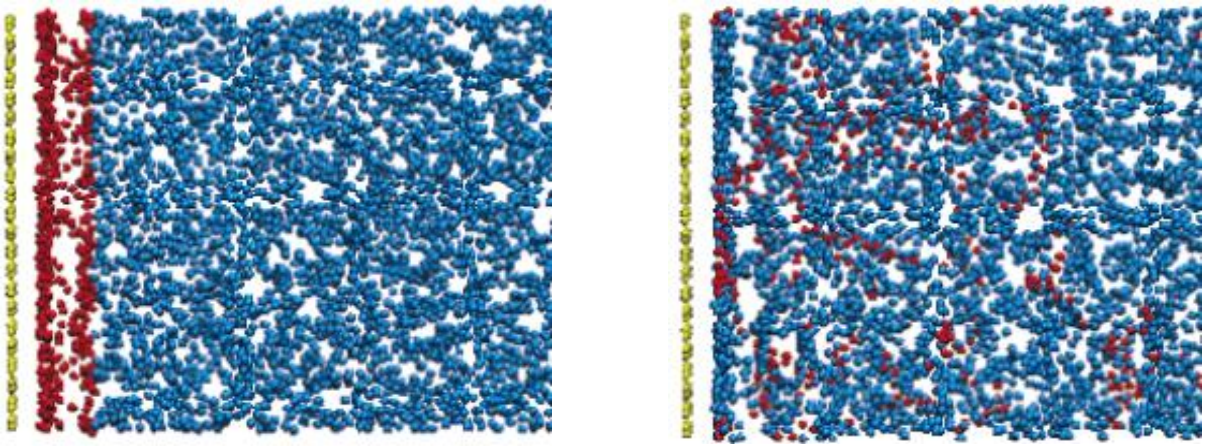

Figure 1. Segmental mobility and diffusion in the adsorbed C_{78} polyethylene (PE) melt at t=0 (left) and 10ns (right) as predicted by coarse-grained molecular dynamics simulations; graphite plane (yellow), tagged PE atoms (red); non-tagged PE atoms (blue) [*]

Programme of work

This project will involve the following work activities:

- Development of molecular models of the nanocomposites accounting for different degrees of surface modification of graphene embedded in a non-crystallising polymer and simulating these in existing codes
- Performing simulations with the developed model in the temperature-time window typical of industrial manufacturing of polymer-graphene nanocomposites
- Extracting results (e.g. polymer chains' density and conformations) and their analysis

[*] Harmandaris et al. Macromolecules 38(13): 5796-5809, 2005

- Validation with available experimental data (activities in conjunction with relevant experimentalists at IINM/WMG and the Department of Chemistry)

Possible extensions into a PhD project would include extending the model to crystallising polymers, using non-equilibrium simulation data to parameterise analytically solvable models of heat and impurity transport, and rare event simulations methods. The overall project would suit a student interested in multiscale numerical methods, software development, molecular modelling and non-equilibrium statistical mechanics.