Study of Polymer/Graphene Interfacial Systems through Molecular Dynamics Simulations

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Graphene nanocomposites have remarkable physical properties with important applications in many different areas. In the current work we present results, which are part of a general computational approach, based on a hierarchical simulation methodology [1], for the study of realistic polymer/graphene systems. Our primary goal is to study the effect of the graphene layers on the structural and dynamical properties of polymer systems. The work which has been accomplished up to now concerns the study of three hybrid polymer/graphene interfacial systems (polystyrene/graphene, poly(methyl methacrylate)/graphene and polyethylene/graphene) through detailed atomistic molecular dynamics (MD) simulations. [2,3,4] Various properties are being studied related to:
(a) Density profile: The time-averaged molecular density profiles, ρ(z), as a function of the distance from the graphene surfaces (z-direction) of the model films are calculated.
(b) Structural characteristics: Molecular orientation tendencies induced by the confinement are being studied by calculating the second rank order parameter and the polymer chain's conformation tensor.
(c) Mobility aspects: We study the dynamics of polymer chains, both in the level of the monomer and the chain center-of-mass, by monitoring the evolution of the mean square displacements, as well as through time auto-correlation functions of a vector along the molecule.
All above properties are examined, as a function of the distance from the substrate (Figure 1) for a series of film widths, ranging from [*2.85-14*] nm. Finally, the properties of the macromolecular chains are being compared to the properties of the corresponding bulk systems at the same temperature.
The second stage of our work involves the extension of the proposed methodology to mesoscopic description using proper coarse-grained (CG) models. This approach allows us to extend simulations in much longer systems and for much longer times.

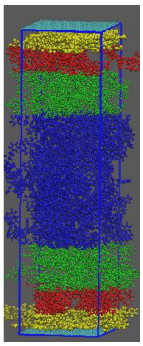

Figure 1: A snapshot of PS/graphene model system. Different colors correspond to different adsorption layers with respect to the surface.

References

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