

## ATOMISTIC MOLECULAR DYNAMICS SIMULATIONS OF MULTIPHASE POLYMER/GRAPHENE NANOSTRUCTURED SYSTEMS

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### ABSTRACT

Polymer/graphene nanostructured systems are hybrid materials, which have attracted great attention the last years both for scientific and technological reasons. In this work detailed atomistic Molecular Dynamics (MD) simulations have been performed.

First we present the study of three hybrid polymer/graphene interfacial systems (polystyrene (PS)/graphene, poly(methyl methacrylate) (PMMA)/graphene and polyethylene (PE)/graphene).<sup>[1,2]</sup> Various properties of the hybrid systems have been examined related to: density profile, structural characteristics and 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 squared 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 for a series of film widths. Finally, the properties of the macromolecular chains are being compared to the properties of the corresponding bulk systems at the same temperature. Structural, conformational and dynamical heterogeneities of polymer chains were found. A tendency for an almost parallel to the graphene surface orientation has been observed at distances very close (~0.5 nm) to the graphene layer, whereas at longer distances their orientation is randomized. Our simulations indicate clearly that the length of the interface depends crucially on the actual property under investigation.

In the second case we examine spatial and dynamical heterogeneities of graphene based polymer nanocomposite systems<sup>[3,4]</sup> and provide information about their properties for various (edge group functionalized) graphene sheets. Systems with graphene sheets of different sizes have been simulated at the same graphene concentration (~3%). Pristine graphene and two types of functionalized graphene have been simulated in two different polymer matrices, (polyethylene, PE) and (polyethylene oxide, PEO).

The density of the polymer around the graphene sheet depends on the distance from the surface. An analysis of the PE chain conformations, based on the calculation of the distribution of the torsional angles, at different distances from graphene, reveals trans-enriched configurations, in comparison to the bulk polymers. Therefore, in the adsorbed interfacial region, the chains preferably adopt more extended. Similar behavior is observed for PEO. Concerning local dynamic properties of polymer chains, strong dynamical heterogeneities are reported. The effect is more pronounced in the systems with the carboxylated sheet. More specifically, the slowest monomers are observed around the edges of the carboxylated graphene flake.

### REFERENCES

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