Abstract

Ph. D. Thesis:

"Mesoscale Modeling of Carbon Black/Polymer Interfaces: Linking Atomistic and Coarse-Grained Particle-Field Representations

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The research activity, described in this Ph. D. thesis, was dedicated to the development of a novel carbon black (CB) primary particle model, with accurate morphology, to be used in coarse-grained (CG) molecular dynamics (MD) simulations. In particular, systems containing carbon black nanoparticles embedded in melts of polyethylene (PE) of varying molecular weigth (M_w), have been simulated, using a multiscale approach starting from the atomistic to the coarse-grained level. Simulations were performed either in mono and bidisperse PE melts, and in presence of either graphite or carbon black nanoparticle. The results obtained show that in bidisperse PE melts, a phase separation of the polymer takes place at the interface with the fillers, with the low M_w fraction being the most abundant one. The driving force for this phase separation has been proved to be entropical in nature, and greatly influenced by the shape and morphology of the filler (graphite or CB).

These findings can help to understand experimental results and to address improvement of the dispersion of CB fillers in polyethylene matrices.

Another part of the Ph. D. has been dedicated to the development of an all-atom model of 2-vinyl pyridine polymer, since no models were available in the literature, for the use in molecular dynamics simulations.