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Modeling of block copolymer/nanoparticle nano-composites

MARCO PINNA, University of Central Lancashire, Preston, UK, IGNACIO PAGONABARRAGA, University of Barcelona, Spain, ANDREI ZVELINDOVSKY, University of Central Lancashire, Preston, UK — We develop a coarse grained simulation technique to study dynamics in soft nano-composites. The system consists of block copolymer melt with embedded nano-size particles. The time evolution of the system is described by a hybrid method combining a field based simulation for block copolymer component and a particle based method for nano-colloids. The block copolymer is modelled by cell dynamics simulation technique, and nano-particles are modelled as soft particles with prescribed density profile. A cross interaction term is controlling the interplay of dynamics of both components. The influence of nano-particles on block copolymer morphology is investigated.

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