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Dispersion/Aggregation of polymer grafted nanorods in a polymer matrix studied by Dissipative Particle Dynamics JOAO MAIA, SHAGHAYEGH KHANI, Case Western Reserve University — Nanorods are incorporated into polymer matrices for fabricating composite materials with enhanced physical and mechanical properties.The final macroscopic properties of the composites are directly related to the dispersion and organization of the nanoparticles in the matrix. For instance, a significant improvement in the mechanical properties of the nanorod-polymer composites is observed upon formation of a percolating network. One way of controlling the assembly of nanorods in the polymer medium is adjusting the chemical interactions which is done through grafting polymer chains on the surface of the rods. The recent developments in the computational techniques have paved the road for further understanding of the controlled dispersion and aggregation of nanorods in polymer matrices. In this study, Dissipative Particle Dynamics (DPD) is employed in order to investigate the effect of enthalpic and entopic variables on the phase behavior of the abovementioned nanocomposites. In DPD, the interaction parameter between the components of the systems can be mapped onto the Flory-Huggins χ-parameter via well-known Groot-Warren expression. This works studies the effect of the enthalpic and entropic variables on phase transitions. The main goal is to provide a phase diagram than can be used to guide the experiments in designing new materials.

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