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Structure and dynamics of a model polymer nanocomposites
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We investigate the structure and the dynamics of a model polymer nanocomposite (PNC) through molecular dynamics (MD) simulations in the canonical ensemble (NVT). Several computer experiments have been carried out at different temperatures for different Lennard-Jones well-depth and filler volume fraction. We studied the real space pair correlation functions and collective scattering structure factors of the PNC melt. This structural analysis has been compared with the previous theoretical and experimental works. The reinforcement of the nanocomposite have been investigated using stress-stress autocorrelation ($\sigma_{xy}(t)$) function for different temperatures. At lower temperatures, $\sigma_{xy}(t)$ shows strong reinforcement of the nanocomposite while at higher temperatures it relaxes quite fast. Diffusion of nanoparticles in the composite has been investigated and compared with earlier works. The effect of sizes and shapes of the nanoparticles has also been investigated in this work.

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