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Effects of Dimensionality and Flexibility of Conductive Fillers in Nanocomposites on Percolating Network Formation and Electrical Conductivity SEULKI KWON, HYUN WOO CHO, BONG JUNE SUNG, Department of Chemistry, Sogang University, Seoul 121-742, Republic of Korea — We conduct extensive langevin dynamics(LD) simulation to explore how the dimensionality and flexibility of conductive fillers in polymer nanocomposites influence their percolation network formation and electrical conductivity. The percolation network formation of nanoparticles in polymer matrices is critical to obtaining desired properties of polymer nanocomposites. Some nanofillers such as carbon nanotubes(CNTs) and graphene nanosheets, are so flexible that they become either wavy or crumpled. Such a variability in nanofiller conformation brings a change to the percolation network, but has been often ignored in the theoretical and computational investigation. We consider three kinds of nanofillers of different dimensionality : zero-dimensional(0D) nanospheres, one-dimensional(1D) nanorods, and two-dimensional(2D) nanoplates. We estimate the percolation network concentration(φ_c) and electrical conductivity with careful finite-size scaling. When the sizes of nanofillers are comparable, the dimensionality of nanofillers influences on φ_c and electrical conductivity of nanocomposites significantly. The effect of flexibility of nanofillers is less significant than that of dimensionality.

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