

The computational studies of the percolation threshold of carbon nanotube/polymer composites with various carbon nanotube molecular junctions

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The percolation behavior of carbon nano-tubes (CNTs) in polymer composites is investigated using Monte Carlo simulations and percolation theory. The percolation behavior of CNTs is crucial to electric conductivity and mechanical properties of CNT/polymer composites. It has been an issue of importance reducing the percolation threshold concentration of CNTs without a loss in electrical conductivity because one can acquire desired transparency that is an essential property for touch panel display. In this work, we investigate how the percolation threshold concentration is affected by the molecular junctions of CNTs, which can be manipulated in experiments via the electron-beam radiation. We test two types of molecular junctions : (1) X molecular junctions and (2) Y molecular junctions. We find that percolation threshold is sensitive to the types of molecular junctions and that one can achieve a lower percolation threshold concentration by mixing X-shaped CNTs with linear CNTs.

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