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The Percolation Network and The Electrical Conductivity of Carbon Nanotubes in a simple shear GYEMIN KWON, YOUNGJUN WOO, KWANWOO SHIN, BONG JUNE SUNG, Department of Chemistry, Sogang University, Seoul, Republic of Korea — The influence of the shear on the electrical conductivity of carbon nanotubes(CNTs) in CNT/polymer composites is studied using molecular simulations. It has been reported that the shear could decrease the electrical conductivity of CNT/polymer composites by several orders of magnitude. However, it has not been elucidated yet how the electrical conductivity would be decreased. In this work, we perform Monte Carlo simulations using a pseudo-potential to mimic a simple shear flow between impenetrable walls. When the CNT/polymer composite is exposed to the shear, CNTs are forced to align parallel to the shear direction and the local concentration of CNTs is increased near the wall. After a certain period of the shear imposition, however, CNTs become entangled and construct an aggregate. Once the aggregate forms, the percolation network of CNTs breaks down; thus decreasing the electrical conductivity significantly. The non-monotonic behavior and the anisotropy in the conductivity are also discussed.

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