Dynamical Aspects of Percolation Networks of Carbon Nanotubes in Polymer Composites  
GYEMIN KWON, BONG JUNE SUNG, Department of Chemistry, Sogang University, Korea — Carbon nanotubes (CNTs) form a percolating network easily in polymer nanocomposites due to their high aspect ratios, thus improving both electrical and mechanical properties of composites. However, poor dispersion of CNTs has been a stumbling block to their application in industry. Therefore, extensive studies on the structure and thermodynamics of CNTs have been carried out to enhance the dispersion of CNTs in composites and find optimal conditions for better electrical and mechanical properties. But little attention has been paid to the dynamic aspects of percolation networks of CNTs, which should be also a critical factor to determine physical properties of composites. In this study, we investigate the 1st order survival rate, the assortative coefficients, and the bond connectivity time correlation function of percolation networks by using molecular dynamics simulations. We find that the CNT network dynamics becomes significantly slow and the CNT networks become dynamically stable as the concentration of CNTs increases beyond the percolation threshold concentration. We also investigate the effect of intermolecular interaction between CNTs and polymers on the dynamic behaviors of CNT networks.

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