Mechanical Properties of Carbon Nanofiber Reinforced Polymer Composites-Molecular Dynamics Approach

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Abstract : Molecular dynamics (MD) simulation has been used to study the effect of carbon nanofiber (CNF) volume fraction (Vf) and aspect ratio (l/d) on mechanical properties of CNF reinforced polypropylene (PP) composites. Materials Studio 5.5 has been used as a tool for finding the modulus and damping in composites. CNF composition in PP was varied by volume from 0 to 16%. Aspect ratio of CNF was varied from l/d=5 to l/d=100. To the best of the knowledge of the authors, till date there is no study, either experimental or analytical, which predict damping for CNF-PP composites at the nanoscale. Hence, this will be a valuable addition in the area of nanocomposites. Results show that with only 2% addition by volume of CNF in PP, E_{11} increases 748%. Increase in E_{22} is very less in comparison to the increase in E_{11}. With increase in CNF aspect ratio (l/d) till l/d=60, the longitudinal loss factor (η_{11}) decreases rapidly. Results of this study have been compared with those available in literature.

Keywords : carbon nanofiber, elasticity, mechanical properties, molecular dynamics
Conference Title : ICNNN 2016 : International Conference on Nanocomposites, Nanotubes and Nanowires
Conference Location : London, United Kingdom
Conference Dates : April 22-23, 2016