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Molecular Dynamics Simulation for Vibration Analysis at Nanocomposite Plates

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Abstract : Polymer/carbon nanotube nanocomposites have a wide range of promising applications Due to their enhanced properties. In this work, free vibration analysis of single-walled carbon nanotube-reinforced composite plates is conducted in which carbon nanotubes are embedded in an amorphous polyethylene. The rule of mixture based on various types of plate model namely classical plate theory (CLPT), first-order shear deformation theory (FSDT), and higher-order shear deformation theory (HSDT) was employed to obtain fundamental frequencies of the nanocomposite plates. Generalized differential quadrature (GDQ) method was used to discretize the governing differential equations along with the simply supported and clamped boundary conditions. The material properties of the nanocomposite plates were evaluated using molecular dynamic (MD) simulation corresponding to both short-(10,10) SWCNT and long-(10,10) SWCNT composites. Then the results obtained directly from MD simulations were fitted with those calculated by the rule of mixture to extract appropriate values of carbon nanotube efficiency parameters accounting for the scale-dependent material properties. The selected numerical results are presented to address the influences of nanotube volume fraction and edge supports on the value of fundamental frequency of carbon nanotube-reinforced composite plates corresponding to both long- and short-nanotube composites.

Keywords : nanocomposites, molecular dynamics simulation, free vibration, generalized, differential quadrature (GDQ) method

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