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Molecular Dynamics Simulation for Buckling Analysis at Nanocomposite Beams

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Abstract : In the present study we have investigated axial buckling characteristics of nanocomposite beams reinforced by single-walled carbon nanotubes (SWCNTs). Various types of beam theories including Euler-Bernoulli beam theory, Timoshenko beam theory and Reddy beam theory were used to analyze the buckling behavior of carbon nanotube-reinforced composite beams. Generalized differential quadrature (GDQ) method was utilized to discretize the governing differential equations along with four commonly used boundary conditions. The material properties of the nanocomposite beams were obtained using molecular dynamic (MD) simulation corresponding to both short-(10,10) SWCNT and long-(10,10) SWCNT composites which were embedded by amorphous polyethylene matrix. Then the results obtained directly from MD simulations were matched with those calculated by the mixture rule to extract appropriate values of carbon nanotube efficiency parameters accounting for the scale-dependent material properties. The selected numerical results were presented to indicate the influences of nanotube volume fractions and end supports on the critical axial buckling loads of nanocomposite beams relevant to long- and short-nanotube composites.

Keywords : nanocomposites, molecular dynamics simulation, axial buckling, generalized differential quadrature (GDQ)
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