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Buckling behaviors of metal nanowires encapsulating carbon nanotubes by considering surface/interface effects from a refined beam model

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Abstract

We develop a refined beam model to describe the buckling characteristics of hollow metal nanowires encapsulating carbon nanotubes (NWs@CNTs), where the interfacial van der Waals (vdW) interaction, interfacial shear stress as well as surface effect are taken into consideration. The analytical expressions for cohesive energies of the vdW interaction between carbon nanotubes (CNTs) and hollow nanowires are obtained through continuum modeling. The interfacial shear coefficients for NWs@CNTs with CNTs of different diameters and nanowires of different lattice orientations are derived by molecular dynamics simulations. The surface effects of nanowires are addressed by a function of the bulk surface energy density and surface relaxation parameter. The present results show that all the aforementioned three factors play key roles in the buckling behaviors of NWs@CNTs. In particular, the competition between CNTs and

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