Integrated Computational Design of Tunable 3D CNT/Graphene Hybrid Nanomaterials

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Carbon nanotubes (CNTs) have received great attention due to their exceptional multi-functional properties (thermal, electrical, and mechanical properties). However, CNTs exhibit superior properties only along the axial direction due to the presence of strong covalent bonding in the carbon plane; they exhibit poor properties in the transverse direction since there are only weak van der Waals interactions among individual nanotubes. Therefore, the CNTs are essentially one-dimensional (1D) nanomaterials and their applications have been somewhat limited. A novel carbon nanomaterial has been proposed recently: the three-dimensional carbon nanotube/graphene hybrid (3D CNT/Graphene). The 3D CNT/Graphene is consisted of vertically aligned carbon nanotube pillars interconnected by horizontal graphene layers. This unique hybrid architecture would possess desirable transport and mechanical properties in the transverse directions (along the graphene planes) while maintaining the excellent properties in the axial directions (along the nanotubes). Unlike conventional materials whose microstructures are relatively “fixed”, these new 3D nanomaterials are highly “tunable” from the structure standpoint. Through this project, an Integrated Computational Material Engineering (ICME) approach was used to design and optimize the 3D CNT/Graphene hybrids. Various representative models of the 3D CNT/Graphene have been constructed and analyzed by using the finite element method. Results show that the axial modulus of the 3D CNT/Graphene increases exponentially with respect to the graphene thickness while the transverse modulus remains constant. The optimal design of 3D CNT/Graphene requires a minimum normalized thickness of g/t>5, where g and t are the thickness of horizontal graphene and vertical nanotube, respectively.