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Quantized Prediction of Coefficients of Thermal Expansion of 3-D CNT-Graphene Junctioned Carbon Nanostructures

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Abstract

A computational finite element analysis based on a structural molecular mechanics approach was conducted to predict effective coefficients of thermal expansion (CTE) of a novel three-dimensional carbon nanostructure, pillared graphene structure (PGS), which is constituted with several graphene sheets and single-walled carbon nanotubes. Four sets of representative unitcell models were developed atomistically having different geometric parameters of pillar length and inter-pillar distance in the PGS. Periodic boundary conditions were applied to periodic unitcell geometries to yield consistent results. Parametric study shows that both pillar length and inter-pillar distance significantly affect the effective in-plane and through-thickness CTEs. The PGS with smaller inter-pillar distance and larger pillar length yields higher in-plane CTEs, while that with larger inter-pillar distance and smaller pillar length yields higher through-thickness CTE. The calculation yields negative

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