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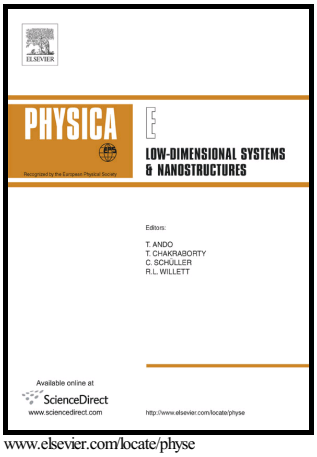

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A comparison between the mechanical and thermal properties of single-walled carbon nanotubes and boron nitride nanotubes

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ABSTRACT

Carbon nanotubes (CNTs) are semimetallic while boron nitride nanotubes (BNNTs) are wide band gap insulators. Despite the discrepancy in their electrical properties, a comparison between the mechanical and thermal properties of CNTs and BNNTs has a significant research value for their potential applications. In this work, molecular dynamics simulations are performed to systematically investigate the mechanical and thermal properties of CNTs and BNNTs. The calculated Young's modulus is about 1.1 TPa for CNTs and 0.72 TPa for BNNTs under axial compressions. The critical bucking strain and maximum stress are inversely proportional to both diameter and length-diameter ratio and CNTs are identified axially stiffer than BNNTs. Thermal conductivities of (10, 0) CNTs and (10, 0) BNNTs follow similar trends with respect to length and temperature and are lower than that of their two-dimensional counterparts, graphene nanoribbons (GNRs) and BN nanoribbons (BNNRs), respectively. As the temperature falls below 200 K (130 K) the thermal conductivity of BNNTs (BNNRs) is larger than that of CNTs (GNRs), while at higher temperature it is lower than the latter. In addition, thermal conductivities of a (10, 0) CNT and a (10, 0) BNNT are further studied and analyzed under various axial compressive strains. Low-frequency phonons which mainly come from flexure modes are believed to make dominant contribution to the thermal conductivity of CNTs and BNNTs.

Keywords:

Carbon nanotubes; boron nitride nanotubes; mechanical properties; thermal properties; molecular dynamics.