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Molecular dynamics simulation of phase transition of boron nitride single walled nanotube

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Abstract

The melting of zigzag, armchair and chiral single walled boron nitride nanotubes (SWBNs) investigated using molecular dynamics (MD) simulation based on Tersoff-like many body potential. The MD simulation has been employed in the constant pressure, constant temperature (NPT) ensemble. The temperature and pressure of the system were controlled by Nose-Hoover thermostat and Berendsen barostat, respectively. We have computed the variation of the melting temperature with the radius of BN nanotube. The results show that the melting temperature of nanotubes increase with increasing in the size of radii, but this dependence is not the same for the various chiral angle of nanotubes. The relation of the melting point with radius for three types of nanotubes i.e. zigzag, armchair and chiral obtained. Moreover, our results show that the melting temperature of nanotubes approach a constant value at larger radii.

Keywords: molecular dynamics simulation, melting temperature, boron nitride nanotube, Tersoff-like potential

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