

ABSTRACT

Numerical Simulation Study of Elastic Behaviour of Boron – 15th Group Nanotubes

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The non-carbon nanotubes are attractive promising materials with forthcoming applications in electronic engineering, light industry and energy storage. Compounds of the elements of the 15th group of the periodic table, such as as nitrogen (N), phosphorus (P), arsenic (As) and antimony (Sb) with boron (B) are able to form 1D graphene-line nanostructures, namely, boron nitride (BN), boron phosphide (BP), boron arsenide (BAs) and boron antimonide (BSn) nanotubes (NTs). A key for the correct design and optimal functioning of innovative nanodevices and systems based on boron - 15th group NTs is understanding of the mechanical behaviour of their constituents. Amid abovementioned nanotubes, BNNTs are the most extensively studied, whereas the other have not been in the focus of research attention so far, particularly BAsNTs and BSbNTs, for which studies on their mechanical behaviour are very rare or non-existent.

In this context, the elastic properties (Young's and shear moduli, and Poisson's ratio) of singlewalled boron nitride, boron phosphide, boron arsenide and boron antimonide nanotubes (SWBNNTs, SWBPNTs, SWBAsNTs and SWBSbNTs) in a wide range of chiral indices and diameters, were studied employing the nanoscale continuum modelling (NCM) approach. The results of this comparative systematic study envisage unlocking new perspectives for the use boron – 15th group element NTs in novel devices.