Effect of atom vacancies on elastic and electronic properties of transversely isotropic boron nitride nanotubes: A comprehensive computational study

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Abstract

Molecular dynamics (MD) simulations were carried out with a three-body Tersoff potential force field to predict the transversely isotropic elastic properties of pristine and defected BNNTs. This is accomplished by imposing uniaxial tension, twisting moment, in-plane shear and in-plane biaxial tension to the BNNTs. Effects of various factors such as chirality and diameter of BNNTs, vacancy concentration, and distribution of vacancy pores along the length and circumference of BNNTs were critically examined. This study reveals that the elastic coefficients of BNNTs decrease as their diameter increase, except axial Young's modulus. Young's modulus of BNNT increases with the diameter and reaches its maximum value when the tube diameter is ~14 Å and then it starts decreasing. We also found that the axial Young's modulus of a BNNT increases as its aspect ratio increases and stabilizes at a particular value of aspect ratio (L/D~15). The vacancies greatly affect the elastic properties of BNNTs; for instance, the vacancy concentration of 2% in (10,10) BNNT reduce its axial Young's, shear, plane strain bulk and in-plane shear moduli by 14%, 25%, 14% and 18%, respectevely. Furthermore, we studied the electronic properties of pristine and defective BNNTs under four transversely isotropic loading conditions using the strain effective method. The results reveal that the electronic properties of BNNTs can be altered via different routes: loadings conditions, diameter and vacancy concentration. This fundamental study highlights the critical role played by vacancy defected BNNTs in determining their elastic and electronic properties as they are vastly being used in multifarious applications such as nano-electronic devices and reinforcements in multifunctional nanocomposites.

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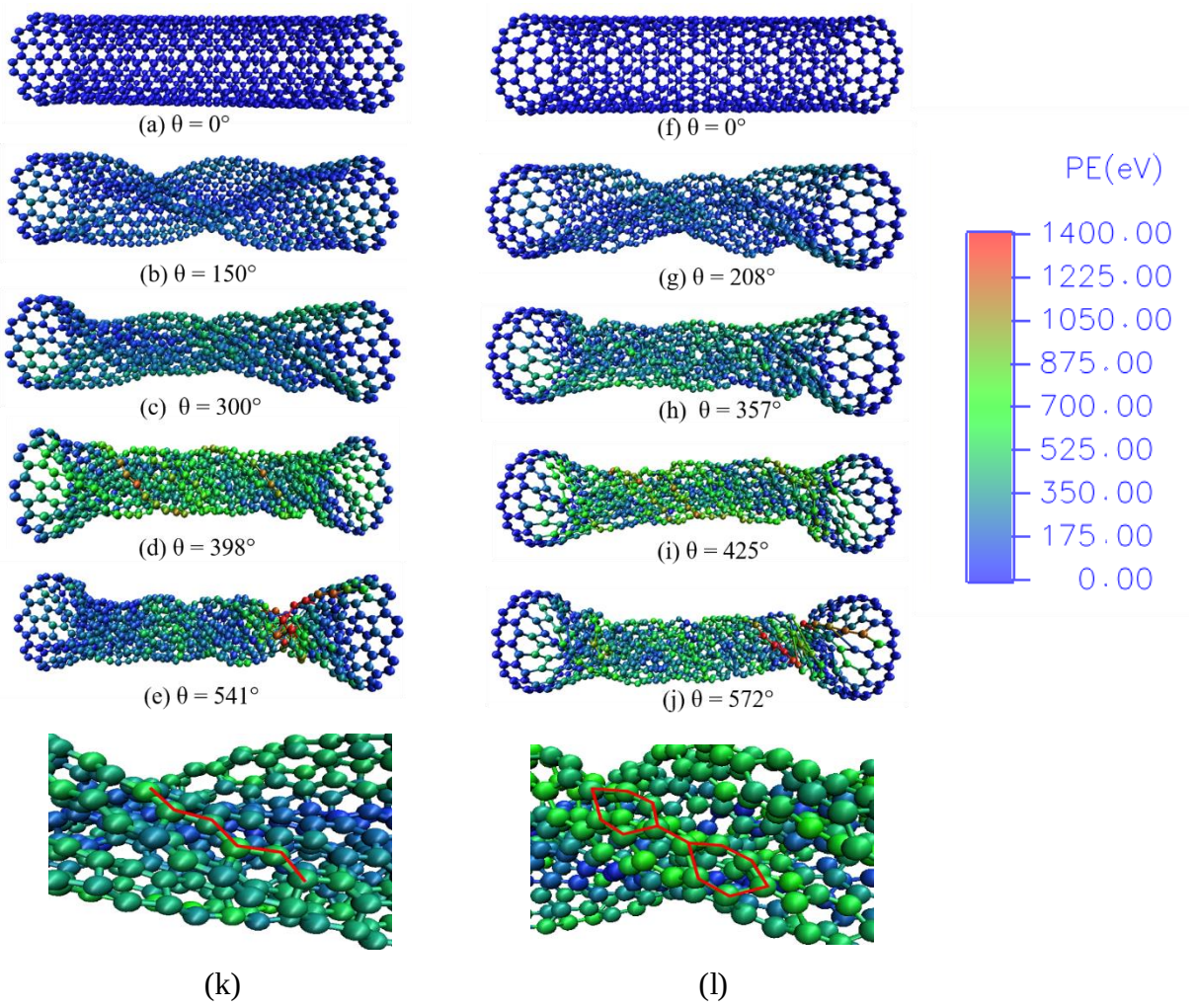

Fig. Snapshot of failure of (10, 10) and (0, 17) BNNTs under torsional deformation.