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Structural and electronic properties of double-walled boron nitride nanocones

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ABSTRACT

First principles calculations were applied to study the structural and electronic properties of different configurations of double-walled boron nitride nanocones with a disclination angle of 60°. The analysis includes different rotation angles, distance between apexes, as well as distinct types of antiphase boundaries. The calculations indicate that the non-rotated configuration of double-walled nanocone with a defective line composed by C and N atoms, forming C-N bonds, is the most stable configuration. It was found that the yam angle, apexes distance and defective line composition present significant influence on the electronic properties of such structures. Moreover, analyzing the spin charge density, for the electronic states near the Fermi level, it was also found that the configuration with a defective line containing C atoms presents a net magnetic moment.

1. Introduction

The structural characteristics of hexagonal boron nitride (h-BN) and carbon nanomaterials have been the main subject of several scientific investigations. A special emphasis of such studies is given to the estimation, or even determination, of the structural and electronic properties of nanotubes [1,2], nanocones [3,4] and fullerenes [5,6]. The main expectation is that such nanostructures may have extraordinary electronic and mechanical properties, which can be applied to future device technologies. In particular, theoretical and experimental studies have indicated that h-BN and carbon nanocones are good candidates for cold-field electron sources. Indeed, it was found that the topology and the atomic arrangement are important factors which affect the electron emission efficiency [7,8].

Geometrically, a nanocone can be obtained using a cut and glue process, also known as Volterra process, where a slice of angle D(α) - the disclination angle, is removed from a round sheet, and the two cut sides are joined together. For boron nitride nanocones (BNNCs), with disclination angle equal to odd multiples of 60°, occurs the formation of an antiphase boundaries (APBs) composed by a defective line with non-BN bonds [9]. It was usually thought that the APBs present a greater energy cost than the lower elastic-energy cost of a disclination with smaller angles [10]. Nevertheless, this picture changes due to experimental results [4,6]. Moreover, the theoretical study of Azevedo et al. [11] demonstrated that BNNCs containing APBs can be more stable than defect-free structures. It was also shown that structures which incorporate a carbon atom at the defective line are the most stable structures, for both, boron-rich and nitrogen-rich environments.

Experimental studies indicate that the actual synthesis processes of BNNCs lead to the formation of multi-walled structures, composed by an ordered stack of nanocones [4]. Nishiwaki and Oku, using arc-melting, have concluded that the BN cone structures are stabilized by the stacking [12]. Furthermore, recent work indicates that the interaction between rotated double-walled carbon nanocones, forming Moiré patterns, have significant influence on the energy of the Fermi level and localized states [13]. On the other hand, it was systematically found that mechanical strain can strongly modify the electronic properties of graphene, graphene bilayers, ZnO and Si nanostructures [14–19]. Such observations may be a relevant point for the future development of nanomechanical sensors.

Motivated by the basic points mentioned above, in the present contribution we investigated the structural stability and the electronic properties of different configurations of double walled BN nanocones (DWBNNCs) using first principles calculations. All calculated structures present a disclination angle of 60°. In addition, the corresponding influence of the defective line in the structure properties was carefully analyzed. It was considered stacked structures with distinct rotation angles and inter-cone distances, which represents a compressive strain applied on the whole structure along the main axis. The most stable DWBNNCs configuration was found to be the non-rotated structure

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composed by two nanocones containing a line of defects which consists of C atoms bonded to N ones. Such result is partially supported by previous ab-initio calculations, which demonstrate that the incorporation of carbon at the antiphase boundary leads to highly stable BNNCs structures [11].

2. Calculations details

All calculations were carried out using the density functional theory (DFT) [20]. The generalized gradient approximation, parametrized by Perdew et al. [21], was applied for the exchange and correlation functional, as implemented in the SIESTA code [22,23]. It was assumed the norm-conservative Troullier-Martins pseudopotentials [24], in the Kleinmann-Bylander factorized form [25], and a linear combination of numeric atomic orbitals of finite range to represent a double-ζ basis set, including polarized functions and using a cutoff radius of about 15.0 Å. All the geometries were fully relaxed, until residual forces become smaller than 0.1 eV/Å. In addition, it was adopted a convergence criterion where the self-consistency is achieved when the maximum difference between the output and the input of each element of the density matrix, in a self-consistent cycle, is smaller than 10^{-4}. Furthermore, in order to estimate numerical errors, additional calculations were performed using a convergence criterion of 10^{-6}. The obtained results demonstrate that the fluctuations in the total energy calculation are smaller than 2 meV.

All structures were initially built using the geometrical cut and glue procedure, as mentioned above, with a disclination angle of 60°. Moreover, it is important to emphasize that all dangling bonds are passivated by hydrogen atoms. Therefore, such H atoms are located at the border of the nanocone base forming H-B, H-N and H-C bonds.

Fig. 1 illustrates the top and side views of the obtained relaxed structures. In Fig. 1a-c are shown the top view of single walled BNNCs, with different defective lines (APBs), composed by B-B bonds ($SWBNNC_{BB}$), C-N bonds ($SWBNNC_{CN}$) and N-N bonds ($SWBNNC_{NN}$), respectively. Fig. 1d-f show the stacked structures of the DWBNNCs, which were constructed piling two of the SWBNNCs shown in the previous Figures. It is worth to point out that such DWBNNCs were built using two BNNCs with the same type of line defects, forming the $DWBNNC_{BB}$, $DWBNNC_{CN}$ and $DWBNNC_{NN}$, respectively. Contrary, Fig. 1g shows a double walled structure consisting of a nanocone with a defective line composed by N atoms on top of a nanocone with a defective line composed by B atoms ($DWBNNC_{NNBB}$). In addition, each DWBNNC structure were finally set by the rotation of the top nanocone in respect to the other one – i.e. rotating by an yaw angle θ, as indicated in the Fig. 1d-g, which show the top view and illustrate the Moiré patterns.

3. Results and discussion

3.1. Structural stability

In order to analyze the stability of the DWBNNCs, the formation energy – i.e. the energy required to form a given structure, E_{Form}, was calculated using a thermodynamical approach based on the previous

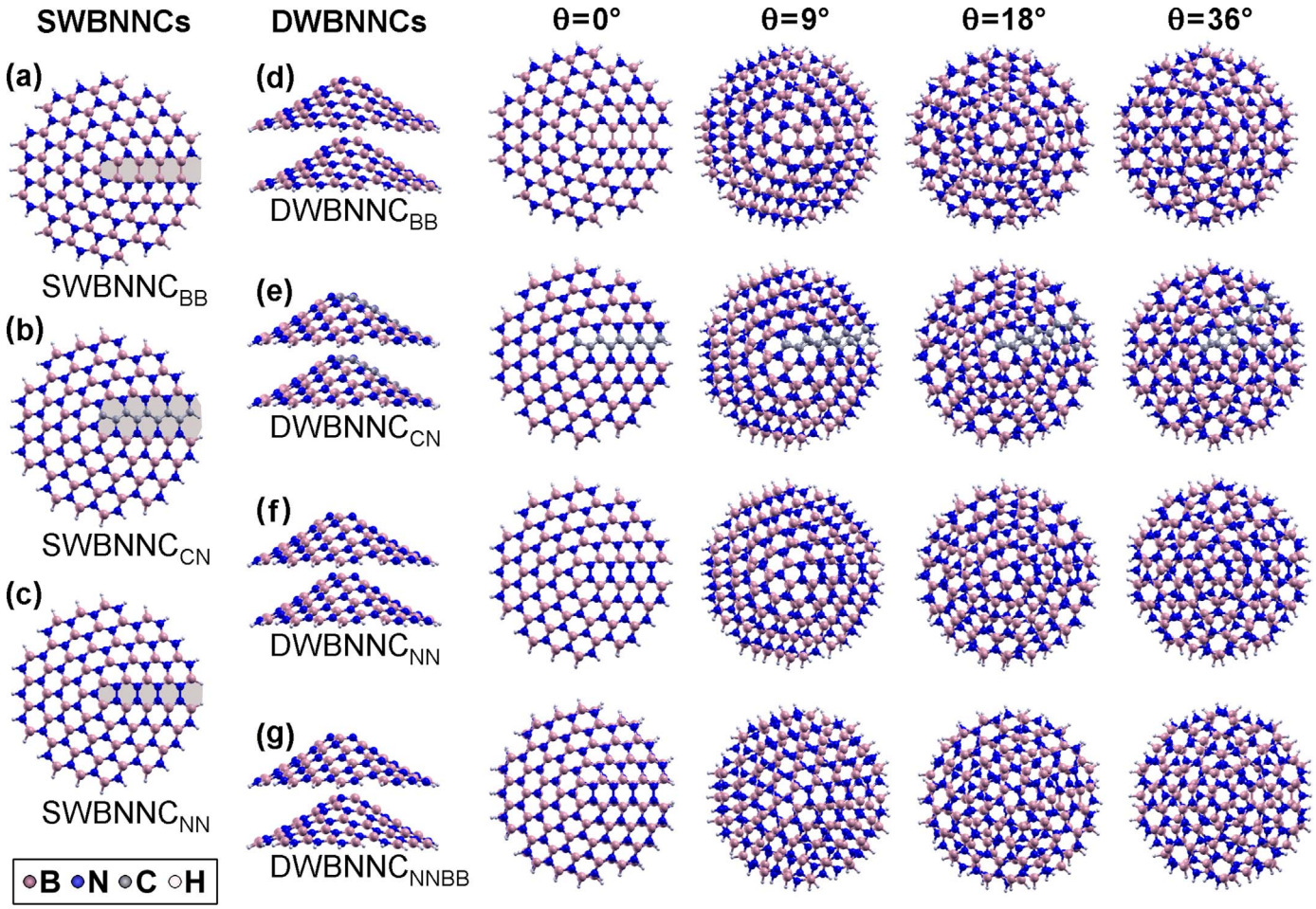

Fig. 1. Ball and stick illustration of the relaxed structures. The atomic species are indicated in the inset. The defective line composed by B-B, C-N and N-N bonds are indicated in (a), (b) and (c) by the grey areas, respectively, for the SWBNNCs. Figures (d), (e), (f) and (g) illustrate the side view of the DWBNNCs and the corresponding top view of such structures for different values of θ.