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**I. M. Danglyan[1], D. B. Hayrapetyan[2], academician E. M. Kazaryan[2]**

# Band Gap and Density of States of Multiwalled Boron Nitride Nanotubes

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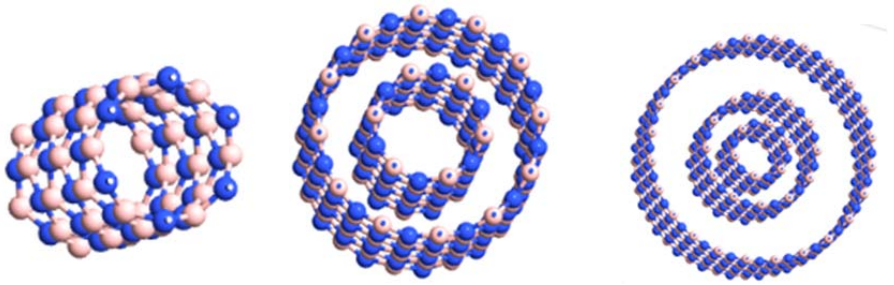
**Keywords**: *multiwalled boron nitride nanotube; band gap; density of states.*

**1. Introduction** Theoretical investigation of boron nitride nanotubes (BNNT) was firstly reported in 1994 [1,2] and successful synthesis of BNNT was done in 1995. [3]. Though the structure of BNNT is very similar to carbon nanotubes there are significant differences in their mechanical properties. Unlike carbon nanotubes large radius BNNT has constant band gap [2]. The significant difference in structure and stability has been founded with small tube size [4-5]. The BNNTs with controllable properties can be found their possible applications in the field of design and developing of optoelectronic devices of new generation. In the current paper the influence of diameter and number of walls on Multiwalled Boron Nitride Nanotubes (MW-BNNT) has been investigated in the framework of DFT generalized-gradient approximation (GGA) method.

**2. Investigation method and tool** Simulations and calculations of MW-BNNT has been done with QuantumATK software tool. Calculations has been done in the framework of DFT generalized-gradient approximation (GGA) method. In order to estimate the influence of number of walls' quantity on MW-BNNT properties, at first it has been created single-walled boron nitride nanotube with (6,0) chirality. The number of tubes have increased up to three with the same chirality indexes. The mentioned single and multiwall nanotubes have been presented in Fig. 1 a, b, c. Length of all types nanotube is 11.37Ă. The diameter of single BNNT and inner radius of multiwall BNNTs is the same and equal to 4.70 Ă. Second wall's diameter equal to 9.40 Ă. And the third one is equal to 18.80Ă.

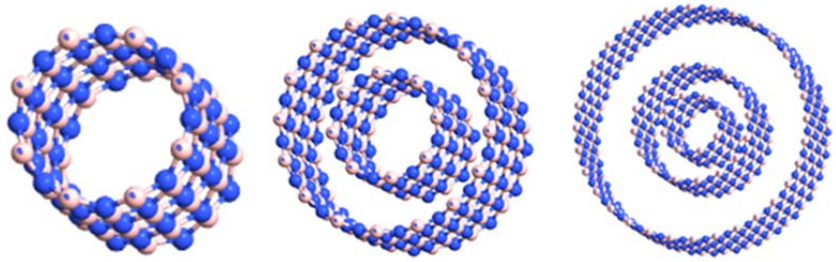
Besides the number of BNNT walls, it is interesting also to investigate the influence of the chirality number on physical properties of these structures. For this purpose, the another set of BNNTs have been chosen, namely BNNTs with



**a** **b** **c**

Fig. 1. The schematic view of single- and MW-BNNT for **a)** (6,0); **b)** (6,0) (12,0); **c)** (6,0) (12,0) (24,0). Black balls – Nitrogen atoms, white balls – Boron atoms.

these parameters: single wall BNNT with chirality indexes (8,0), double wall BNNT with chirality indexes (8,0) (16,0) and finally three wall BNNT with chirality indexes (8,0) (16,0) (32,0). The schematic views of these structures have been presented in Fig. 2 a, b, c. For all nanotubes the length has been fixed and equal to 11.37Ă. The diameter of single BNNT and inner radius of multiwall BNNTs is the same and equal to 6.27 Ă. Second wall's diameter equal to 12.53 Ă. And the third one is equal to 25.07Ă.



**a** **b** **c**

Fig. 2. The schematic view of single- and MW-BNNT **a)** (8,0) **b)** 8,0) (16,0) **c)** (8,0) (16,0) (32,0) structures.

It should be noted, that with the increase of number of atoms in the structure of nanotubes the calculation times increased non linearly. That is why the cases with more number of walls is not discussed in the current paper.

**3. Results and discussions** As we mentioned above, the numerical calculations have been done by the DFT GGA method. For all types of nanotubes the band gaps have been calculated and the results have been shown in Fig. 3. Results show that with the increase of nanotubes diameter the band gap value also increases. The band gap is changed passing from single-walled BNNT to double-walled. For the obvious the numerical results for the band gap presented in Table 1.

It should be noted that increasing number of walls from 2 to 3 the number of walls has insignificant impact on band gap. In our opinion the small variation in the band gap values connected to the accuracy of DFT GGA method and it

can be taken as the same for 2 and 3 walls nanotubes. It is clear from the Figure 3 that density of states increased and it is more obvious in DOS analyze.

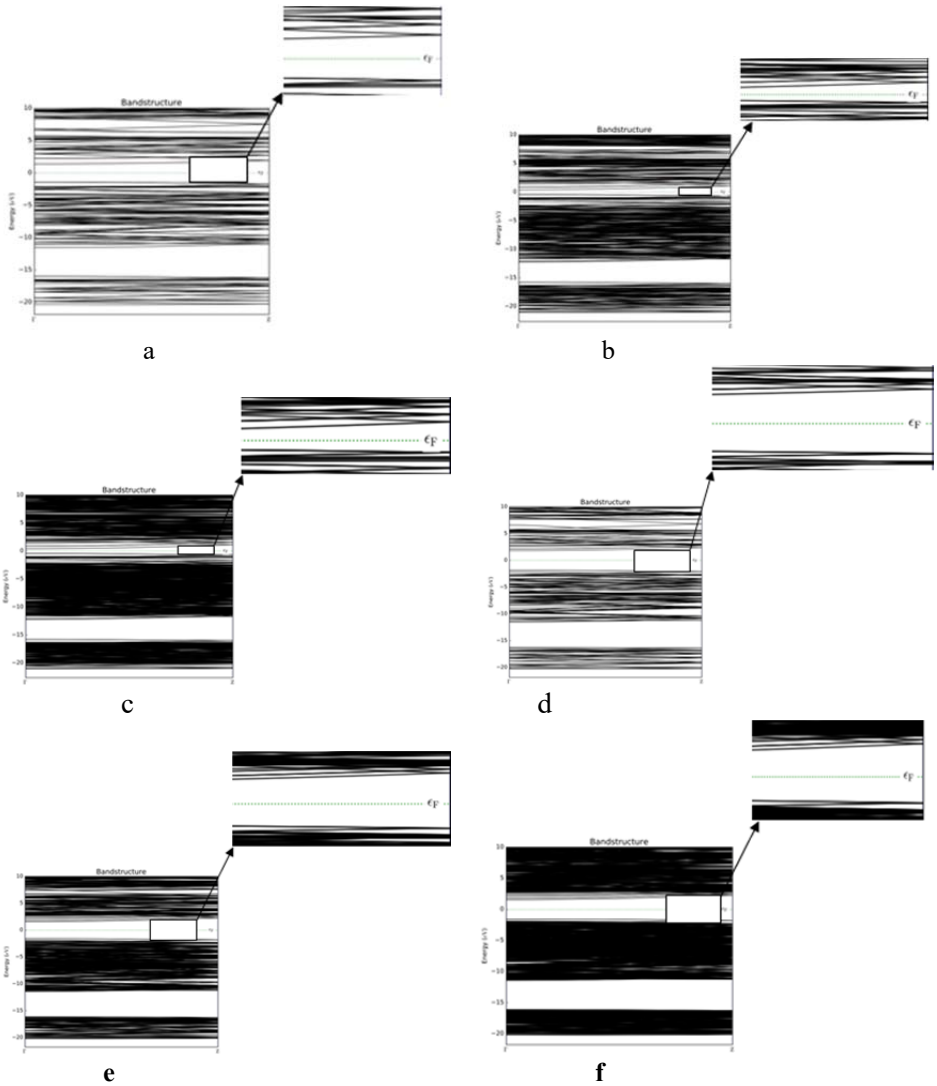



Fig. 3. Band structure of **a)** (6,0) **b)** (6,0) (12,0) **c)** (6,0) (12,0) (24,0) **d)** (8,0) **e)** (8,0) (16,0) **f)** (8,0) (16,0) (32,0) MW-BNNT

**Table 1. Values of band gaps for different nanotubes.**

| Chiralitry index | Band Gap (eV) |
|---|---|
| 1. (6,0) BN | 2.8241 |
| 2. (6,0) (12,0) BN | 0.8582 |
| 3. (6,0) (12,0) (24,0) BN | 0.8589 |
| 4. (8,0) BN | 3.6597 |
| 5. (8,0) (16,0) BN | 3.1272 |
| 6. (8,0) (16,0) (24,0) BN | 3.1277 |

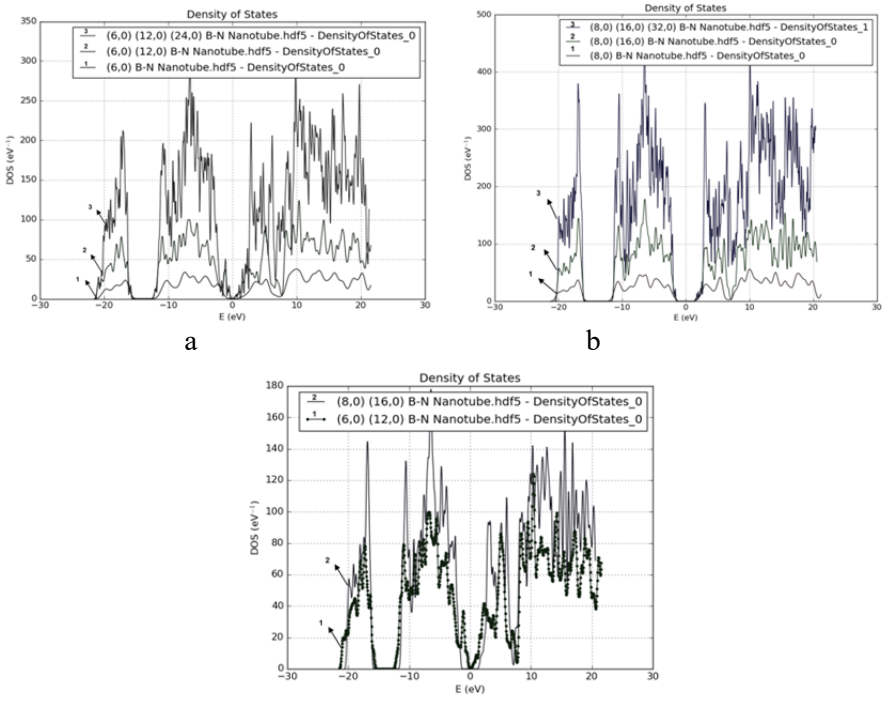



Fig. 4. DOS comparisons of **a)** (6,0); (6,0) (12,0); (6,0) (12,0) (24,0); b) (8,0); (8,0) (16,0); (8,0) (16,0) (32,0); c) (6,0) (12,0); (8,0) (16,0) zigzag MW-BNNT.

The DOS analyze of BNNT has been demonstrated in Fig. 4. Fig. 4 a presented the comparison of DOS for the first set of nanotubes, namely BNNTs with these chirality indexes (6,0); (6,0) (12,0); (6,0) (12,0) (24,0). It shows that the DOS increases when increases with number of walls. Fig. 4 b presented the same comparison for the second set of nanotubes, namely BNNTs with these chirality indexes (8,0); (8,0) (16,0); (8,0) (16,0) (32,0).

In the Fig. 4 c the comparison has been done for the nanotubes with the same structure (two walls) but with different chirality indexes. With the increase of chirality index, the band gap increase significantly.

**Conclusion.** In summary, DFT GGA method has been used to estimate the band gap dependence of MW-BN nanotube on number of walls and diameter for zigzag structure. It has been found that number of walls starting from two is not influence on bandgap but increases the density of states significantly. Keeping number of walls of nanotube constant and increasing the diameter of nanotubes brings significantly band gap gain and increases the density of states.

[1]Synopsys Armenian
[2]Russian-Armenian University
e-mail: irena.danaglyan@synopsys.cc

**I. M. Danglyan, D. B. Hayrapetyan, academician E. M. Kazaryan**

## Band gap and density of states of Multiwalled Boron Nitride Nanotubes

The structure, stability of the zigzag single-walled and multiwalled Boron Nitride nanotubes have been investigated in the framework of generalized-gradient approximation (GGA) density functional theory (DFT). Results show that number of walls starting from two have not impact on band gap but increase density of states significantly

**Ի. Մ. Դանգլյան, Դ. Բ. Հայրապետյան, ակադեմիկոս Է. Մ. Ղազարյան**

## Բորի նիտրիդի բազմաշերտ նանոխողովակի արգելված գոտին և վիճակների խտությունը

Միաշերտ և բազմաշերտ զիգզագ կառուցվածքԻով բորի նիտրիդի նանոխողովակի կառուցվածքը և կայունությունը ուսումնասիրվել են խտության ֆունկցիոնալի տեսության ընդհանուր գրադիենտի մոտավորության շրջանակներում։ Արդյունքները ցույց են տալիս, որ շերտերի քանակը, սկսած երկրորդից, չի ազդում արգելված գոտու էներգիայի վրա, բայց զգալի փոխում է վիճակների խտությունը։

**И. М. Данглян, Д. Б. Айрапетян, академик Э. М. Казарян**

## Запрещенная зона и плотность состояний многослойной нанотрубки нитрида бора

Структура и стабильность однослойных и многослойных зигзагных нанотрубок из нитрида бора исследована в рамках теории функционала плотности в обобщенном градиентном приближении (GGA). Результаты показывают, что число слоев, начиная со второго слоя, не влияет на ширину запрещенной зоны, но значительно увеличивает плотность состояний.

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