Ab initio investigation of boron nanodevices: conductances of the different geometric conformations

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Conductances of different geometric conformations of boron ribbon devices are calculated by the *ab initio* method. The I–V characteristics of three devices are rather different due to the difference in structure. The current of the hexagonal boron device is the largest and increases nonlinearly. The current of the hybrid hexagon-triangle boron device displays a large low-bias current and saturates at a value of about 5.2 μA. The current of the flat triangular boron flake exhibits a voltage gap at low bias and rises sharply with increasing voltage. The flat triangular boron device can be either conducting or insulating, depending on the field.

Keywords: boron, conductance, different geometry conformation
PACC: 7200, 7115M

1. Introduction

In the recent years, much attention has been paid to carbon systems that are regarded as possible key materials for future nanodevices. The attention originated from the observation of highly stable carbon clusters in the form of Buckminster fullerenes,[1] the subsequent observation of stable carbon nanotubes,[2] as well as the peculiar electronic structure of graphene.[3−6] However, the studies on boron demonstrated that boron was vital to the production of nanodevices. Boron is the fifth element in the periodic table and has only three valence electrons. The boron atom has some intriguing similarities to carbon, such as hardness close to that of diamond, a high melting point and a richness of chemistry next only to carbon.[7−11] The three valence electrons of boron could, in principle, form an sp^2 hybrid orbital that might lead to tubular and planar structures similar to those formed by carbon. However, boron and carbon have some differences. Bulk carbon is characterized by a 2D system (graphite) and carbon clusters feature 3D cages, while bulk boron is characterized by 3D cages and boron clusters feature 2D structures. Furthermore, the boron sheet has a huge variety of structures compared with the carbon graphite. The stable structures of the boron sheet is still an open question.

The hexagonal graphitic boron sheet was proposed. The hexagonal boron sheet is an sp^2 bonded system, but a boron atom has only three valence electrons, leading to an unstable structure.[12,13] Then the buckled triangular boron sheet was proposed[14] and the 2D triangular boron sheet was studied and used to construct boron nanotubes.[15,16] However, the buckling and large deformations show that the buckled triangular boron sheet is not very stable. Recently, the hybrid hexagon-triangle boron sheet has been proposed and found to have a most stable structure.[17]

It is interesting to explore the promising properties of boron sheets for applications in nanoscale devices due to the chemical richness of boron. In the present paper, the conductance of boron devices is investigated by the *ab initio* method. At present, most of the conductance investigations focus on the sandwich-type structure of an individual molecule material connected in between two metal electrodes.[18−21] But the bonding between the molecule and the electrode is usually ill defined and uncontrollable in current experiments,[22,23] which makes it difficult to fabricate functional electron devices with this structure. Nanoscale material systems may conduce to constructing the functional devices. We consider two-dimensional junctions formed from boron ribbon contacted by infinite metallic gold electrodes through a sulfur atom. Usually in most sandwiched devices S and Au are used as metal electrodes, which can make contacting stable. The S atom can be replaced by Cr and N atoms, such as in graphene sheets which are contacted with Cr/Au

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metal electrodes.[24] Three finite boron ribbons with hexagons, flat triangular and hybrid hexagon-triangle are selected to study their conductances. The device is divided into two different parts: an 'extended scattering' region, comprising the boron ribbon, the S atoms and part of the metallic electrodes, and the 'electrodes' which are semi-infinite on both the left- and the right-hand sides of the device.[25]

2. Calculation method

The conductances of the boron ribbon devices are calculated by using the non-equilibrium Green function method.[26] This formalism is based on the theory proposed by Datta.[27] The tight-binding Hamiltonian is used in the conductance calculations. To simplify the problem and reduce the computational cost, the calculations are performed on a boron ribbon device with finite length and finite electrode. The geometry of the device considered is in the following. The gold electrodes are oriented along the (111) direction and consist of three layers (three, seven, three), see Figs. 1(a)–1(c). The vertical distance between the S atom and the most external plane of the Au electrode is 1.90 Å (1 Å=0.1 nm) with an S–Au bond length of 2.53 Å. The other bond lengths used here are: S–B 1.97 Å, B–B 1.67 Å and Au–Au 2.885 Å.

In investigating the conductance of the boron ribbon device, the electronic transmission coefficients of the whole system are first calculated by using the non-equilibrium Green function method,[26,27]

$$T = \mathrm{Tr}(\Gamma_1 G \Gamma_2 G^+), \tag{1}$$

where Tr, the trace, is over all orbitals of the extended boron; G is the retarded Green's function matrix, which can be self-consistently evaluated from the tight-binding Hamiltonian of the scattering region and self-energies; G^+ is the advanced Green's function matrix; Γ_i, the spectral density, represents the coupling between the ith electrode and the extended region and it can be given by the imaginary part of electrode self-energy.

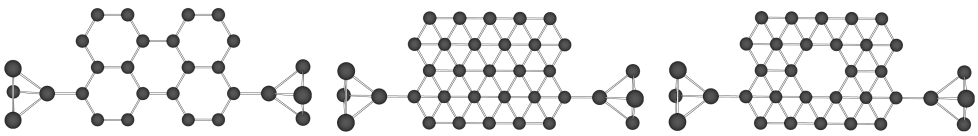
The terminal current is

$$I = \frac{2e}{h} \int_{-\infty}^{+\infty} \mathrm{d}E T(E, V)[f(E - \mu_1) - f(E - \mu_2)], \tag{2}$$

where $f(E)$ is the Fermi function with electrochemical potentials μ_1 and μ_2. The details of the calculation method can be found in Ref. [28].

3. Results and discussion

The conductance formalism is used to investigate the transport properties of three geometric conformation boron ribbon devices consisting of 20 boron atoms, 27 boron atoms and 26 boron atoms, separately (see Figs. 1(a)–1(c)). The details of the transport behaviour of the three devices are displayed in Figs. 2(a)–2(c) and Figs. 3(a)–3(c) by the densities of states (DOSs) and the transmission coefficients, each as a function of the injection energy of the electron. The peaks of DOS indicate not only the positions of the renormalized boron ribbon levels of the extended states, but also the broadening of the boron ribbon levels due to the presence of the electrodes and bias. The conductance characteristics are shown in Figs. 4(a)–4(c). The Fermi level of the gold (111) is chosen to be −9.5 eV.[28] Notice that this value of E_{F} differs from the work function of Au (111) in Ref. [29] (−5.31 eV) because the Hückel energy level is 4–5 eV lower than the correct value relative to the value in vacuum.[28]



(a) (b) (c)

Fig. 1. Geometries of the devices investigated in this work. A boron ribbon is contacted to two finite Au electrodes with structures of (a) hexagonal boron, (b) flat triangular boron, (c) hybrid hexagon-triangle boron.

It can be seen from Figs. 2(a)–2(c) that there are some differences. First, the positions and heights of the peaks in the DOS for the three structural boron ribbons are different from each other. Second, the numbers of the peaks in the DOS Fermi level are different, and their corresponding gaps are also different from each other.

The largest gap of the peak is observed on the hexagonal boron ribbon device, and the second largest gap is seen from the hybrid hexagon-triangle boron ribbon device. Third, the largest DOS at the Fermi level exists in the figure of the hexagonal boron ribbon device, which will affect the conductance significantly. The DOS at the Fermi level in Fig. 2(c) is a little larger than that in Fig. 2(b).

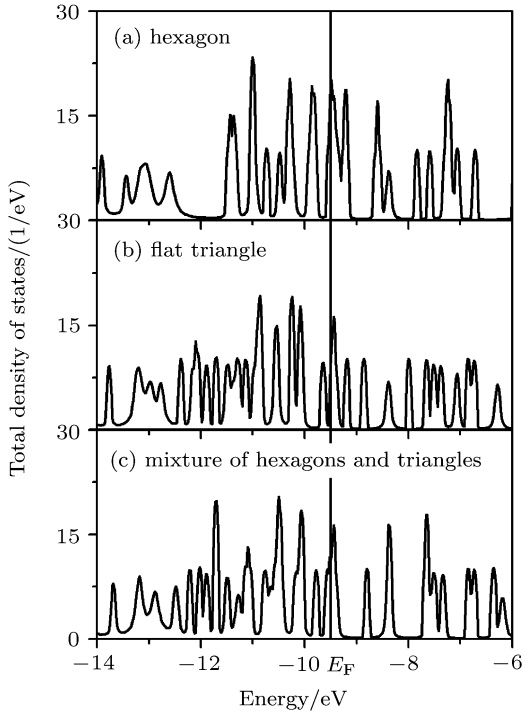


Fig. 2. Total densities of states for boron ribbon devices with structures of (a) hexagonal boron, (b) flat triangular boron, (c) hybrid hexagon-triangle boron.

As expected, in Figs. 3(a)–3(c), the positions of peaks in the transmission coefficients are correlated well with those of the peaks in the DOSs for three types of boron ribbons. The height of the peak in transmission, however, is not necessarily mapped onto the height of the peak in the DOS.

From Fig. 4, one can observe that the largest DOS of hexagonal boron ribbon at the Fermi level dominates the largest current as compared with the two other boron ribbon junctions. The current of the hybrid hexagon-triangle boron ribbon device maintains a larger value than that of the flat triangle boron ribbon device, although the difference in transmission coefficient between these two junctions is not too large. Notably the hybrid hexagon-triangle boron flakes display a large low-bias current, which increases nonlinearly. Then it saturates at a value of about 5.2 μA. In contrast the I–V of the flat triangular boron flake is considerably lower at low bias and increases nonlinearly with bias. These phenomena mean that the barriers for electron transport of the devices with hexagonal structure and hybrid hexagon-triangle structure are reduced and the current-carrying capabilities are increased as compared with the flat triangular one.

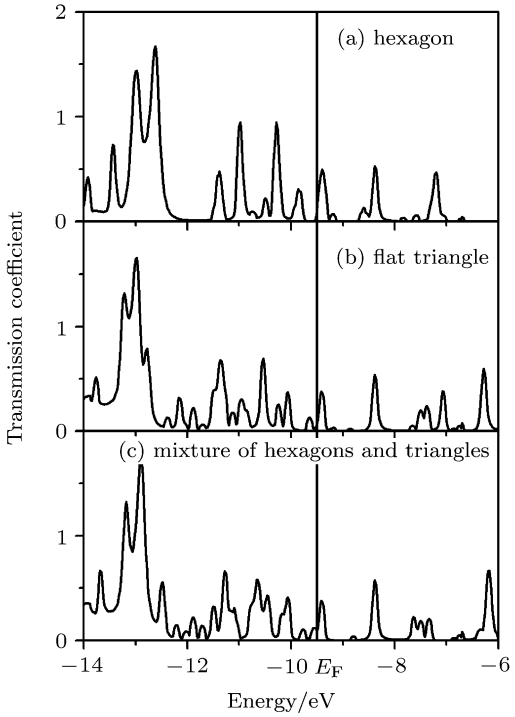


Fig. 3. Total transmission coefficients for the boron ribbon devices with structures of (a) hexagonal boron, (b) flat triangular boron, (c) hybrid hexagon-triangle boron.

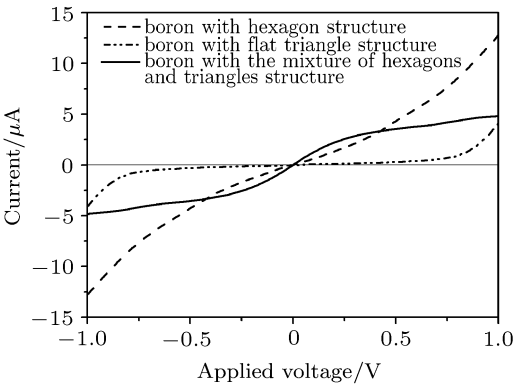


Fig. 4. Current–voltage characteristics for the three types of boron ribbon devices.

These different current characteristics could be related to the structures of these three boron junctions. The hexagonal boron is an sp^2 bonded system. Unlike graphene, in which four valence electrons per atom completely occupy the sp^2 and the p_z bonding states, a boron atom has only three valence electrons and not enough electrons to fully occupy some of the strong in-plane sp^2 bonding states, which results in a metallic plane. The hexagonal boron is highly prone to accepting electrons, and the hexagonal regions act as acceptors, which leads to the large current and the current tends to increase nonlinearly with the source–drain voltage in Fig. 4(a). For the flat triangular boron, each atom has six nearest neighbours and three valence electrons; a three-centre bonding scheme should be considered.[16] The flat triangular structure has a surplus of electrons in anti-bonding states. From a doping perspective, the three-centre flat triangular region should act as a donor, thereby leading the system to behave as a semiconductor with the voltage gap. In Fig. 4(b) one observes nonlinear current–voltage curves that exhibit a voltage gap at low applied bias. The current rises sharply as the source–drain voltage increases, showing that boron can transport charge carriers at higher bias. Thus, within a range of source–drain voltages, the system can be either insulating or conducting, depending on the field. For hybrid hexagon-triangle boron, the valence electrons per atom fully occupy all available in-plane sp^2 bonding states. The remaining electrons occupy the low energy p_z-derived states, leading to a metallic system. The current tends to increase as the source–drain voltage increases and then it saturates at a value of about 5.2 μA.

4. Conclusions

The conductances of different geometric conformations of boron ribbon devices are calculated by using the non-equilibrium Green function technique. The tight-binding Hamiltonian is used in calculation. Although three valence electrons of boron could in principle form an sp^2 hybrid orbital, different structures exhibit either acceptor or donor or full filler natures because each atom has a different number of neighbours. As a consequence, the I–V characteristics of the three geometry conformations are rather different from each other. The hexagonal boron device has the largest current increasing nonlinearly with the source–drain voltage. The hybrid hexagon-triangle boron device has the second largest current, which displays a large low-bias nonlinear current and saturates at a value of about 5.2 μA. The nonlinear current of the flat triangular boron flake is lowest and exhibits a voltage gap at low applied bias. Thus, within a range of source–drain voltages, the flat triangular boron flake can be either conducting or insulating, depending on the field. These phenomena mean that the current-carrying capabilities of the hexagonal and hybrid hexagon-triangle devices are stronger as compared with the flat triangular one. These results may serve as a reference in fabricating nanoscale electronic devices experimentally.

References

[1] Kroto H W, Heath J R, O'Brien S C, Curl R F and Smalley R E 1985 *Nature* **318** 162
[2] Ijima S 1991 *Nature* **354** 56
[3] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 *Science* **306** 666
[4] Novoselov K S, Geim A K, Morozov S V, Jiang D, Katsnelson M I, Grigorieva I V, Dubonos S V and Firsov A A 2005 *Nature* **438** 197
[5] Berger C, Song Z, Li X, Wu X, Brown N, Naud C, Mayou D, Li T, Hass J, Narchenkov M A, Conrad E H, First P N and de Heer W A 2006 *Science* **312** 1191
[6] Li Z Y, Qian H Y, Wu J, Gu B L and Duan W H 2008 *Phys. Rev. Lett* **100** 206802
[7] Lipscomb W L 1963 *Boron Hydrides* (New York: Benjamin W A)
[8] Meutterties E L 1975 *Boron Hydride Chemistry* (New York: Academic)
[9] Cotton F A, Wilkinson G, Murillo C A and Bochmann M 1999 *Advanced Inorganic Chemistry* (New York: Wiley)
[10] Jemmis E D, Balakrishnarajan M M and Pancharatna P D 2002 *Chem. Rev.* **102** 93
[11] Wang X J, Tian J F, Bao L H, Yang T Z, Hui C, Liu F, Shen C M, Xu N S and Gao H J 2008 *Chin. Phys.* B **17** 3827
[12] Boustani I, Quandt A, Hernandez E and Rubio A 1999 *J. Chem. Phys.* **110** 3176
[13] Evans M H, Joannopoulos J D and Pantelides S T 2005 *Phys. Rev.* B **72** 045434
[14] Lau K C and Pandey R 2007 *J. Phys. Chem.* C **111** 2906
[15] Kunstmann J and Quandt A 2006 *Phys. Rev.* B **74** 035413
[16] Cabria I, Lopez M J and Alonso J A 2006 *Nanotechnology* **17** 778
[17] Tang H and Ismail-Beigi S 2007 *Phys. Rev. Lett.* **99** 115501
[18] Nitzan A and Ratner M A 2003 *Science* **300** 1384
[19] Venkataraman L, Klare J E, Nuckolls C, Hybertsen M S and Steigerwald M L 2006 *Nature* **442** 904

[20] Li Z L, Wang C K, Luo Y and Xue Q K 2005 *Chin. Phys.* 14 1036

[21] Li G Q and Cai J 2009 *Acta Phys. Sin.* **58** 6453 (in Chinese)

[22] Ulrich J, Esrail D, Pontius W, Venkataraman L, Millar D and Doerrer L H 2006 *J. Phys. Chem.* B **110** 2462

[23] Ramachandran G K, Hopson T J, Rawlett A M, Nagahara L A, Primak A and Lindsay S M 2003 *Science* **300** 1413

[24] Soler J M, Artacho E, Gale J D, García A, Junquera J, Ordejón P and Sánchez-Portal D 2002 *J. Phys: Condens. Matt.* **14** 2745

[25] Emberly E G and Kirczenow G 1998 *Phys. Rev.* B **58** 10911

[26] Andriotis A N and Menon M 2001 *J. Chem. Phys.* **115** 2737

[27] Datta S 1995 *Electronic Transport in Mesoscopic Systems* (Cambridge: Cambridge University Press) p117

[28] Zahid F, Paulsson M and Datta S 2003 *Electrical Conduction through Molecules*, chapter in 2003 *Advanced Semiconductors and Organic Nanotechniques* (New York: Academic Press)
Paulsson M, Zahid F and Datta S 2005 *Huckel-IV on the nanoHub*, https://www.nanohub.org/resources/422/

[29] Lide D R 2000 *CRC Handbook of Chemistry and Physics* (Boca Raton FL: CRC)