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Bias induced modulation of electrical and thermal conductivity and heat capacity of BN and BN/graphene bilayers

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ABSTRACT

By using the tight binding approximation and Green function method, the electronic structure, density of state, electrical conductivity, heat capacity of BN and BN/graphene bilayers are investigated. The AA-, AB_1- and AB_2-BN/graphene bilayers have small gap unlike to BN bilayers which are wide band gap semiconductors. Unlike to BN bilayer, the energy gap of graphene/BN bilayers increases with external field. The magnitude of the change in the band gap of BN bilayers is much higher than the graphene/BN bilayers. Near absolute zero, the σ(T) is zero for BN bilayers and it increases with temperature until reaches maximum value then decreases. The BN/graphene bilayers have larger electrical conductivity larger than BN bilayers. For both bilayers, the specific heat capacity has a Schottky anomaly.

1. Introduction

Graphene is a two-dimensional monoatomic layer system which has been most investigated experimentally and theoretically in the previous decade due to novel electronic properties [1,2]. Theoretically, it has been shown that graphene is a zero-gap semiconductor because its conduction and valence bands connect each other at the Dirac points [3–5]. Bilayer graphene can exist in the AA- and AB-stacked forms where in AA- stacked the layers are exactly aligned and in AB- stacked half of the atoms lie directly over the center of hexagon in the lower graphene sheet [6–8]. Similar to graphene, non-carbon graphene-like materials such as GaN, BN and BN/graphene have also been studied [9–11]. Two-dimensional hexagonal BN is similar to graphene with boron and nitrogen atoms Instead of carbon atoms. The main difference between graphene and BN sheet materials is in their electronic properties. Unlike graphene which is a semimetal with zero band gap, the BN is an insulator with a large energy gap [12].

Ribeiro et. al. investigated the ground state energies and interlayer distances of boron nitride bilayers using tight-binding approach [12]. They found the hopping parameters and the onsite energies by fitting an empirical tight binding model to the DFT results. In addition to the bilayers of graphene or BN materials, the graphene/hexagonal boron nitride bilayer system has been investigated in recent years [10,11,13–20].

Opening a tunable and sizable band gap in graphene, nanoribbons and nanotubes is a significant challenge [21–25]. The ability to control the band-gap can be obtained by different methods such as strain, doping, external fields and sandwiching graphene layer between other material sheets such as BN. Several theoretical calculations have been investigated the electronic properties and gap variations of BN and graphene bilayers, focusing on the influence on electric field and sandwiching the layers. Effect of doping of graphene either by boron, nitrogen, or co-doped by B and N is studied by density functional theory [26–28]. It is found that after co-doping of graphene by B and N, the energy gap appears at Fermi level and the system behaves as narrow gap semiconductor [26] and it does not show magnetic moment [28]. For BN bilayers, the ground state energies are computed using DFT and the hopping parameters and the onsite energies have been extracted by fitting a tight binding empirical model to the DFT results [12]. The electronic and transport properties of a biased multilayer hexagonal boron nitride have been calculated and it is shown that the band gaps of multilayer h-BN decrease with increasing electric field, irrespective of the layer number N and stacking manner [29].

Several theoretical calculations have investigated the electronic properties of the combination of the graphene and BN layers. Using density functional theory calculations, Quhe et. al. have shown that the band gap of single graphene layer sandwiched between two hexagonal boron nitride single layers can be opened with and without electric field [13]. Using first-principles calculations, it is shown that the band gap and electron effective mass (EEM) of graphene/boron nitride bilayers can be modulated by tuning the interlayer spacing and stacking arrangement [14]. The band structure of stable configuration of graphene/hexagonal boron nitride bilayer system has been studied and it was shown that an electric field significantly modifies the electronic structure of the system [10]. Theoretically the electronic structures of monolayer/bilayer of graphene/BN in the presence and

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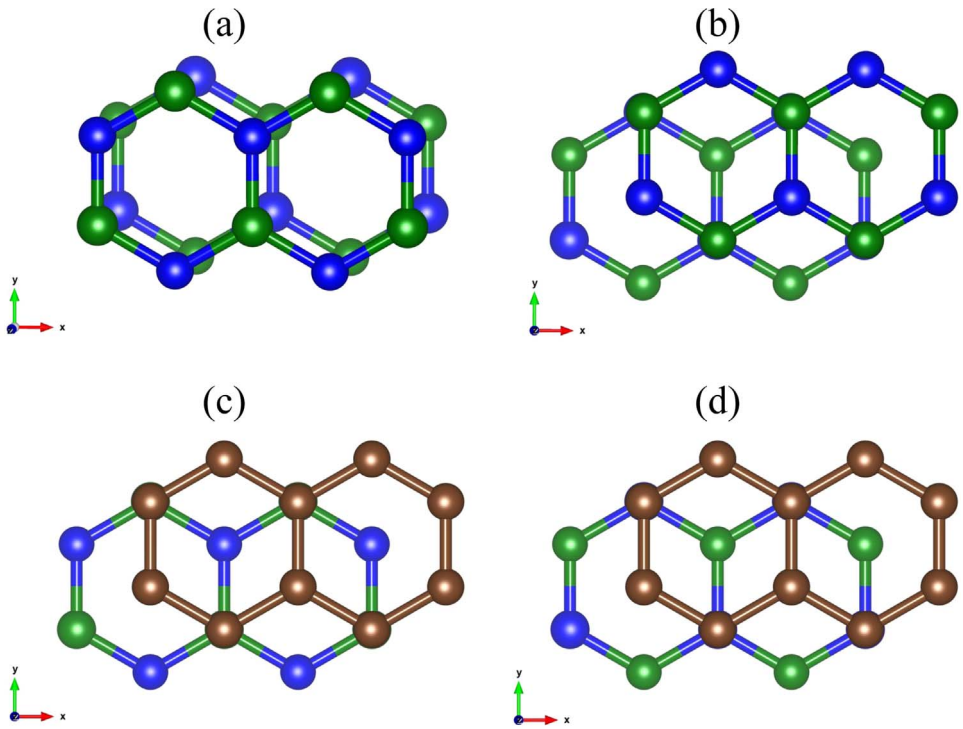

Fig. 1. Schematic picture of a (a) AA-, (b) AB- stacked BN bilayers and (c) AB_1- and (d) AB_2- BN/graphene bilayers. Brown, green and blue show Carbon, Boron and Nitrogen atoms. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

absence of magnetic field were investigated and it has been shown that magnetic field leads to band modifications such as the gap opening [30]. The electrical conductivity, electronic heat capacity and thermal conductivity of single- and few-layers graphene were investigated within the tight-binding model and it is found that the electrical conductivity of the gapped graphene reduces in terms of temperature compared to the pristine case [31–34].

In this study, we calculated the heat capacity, electrical and thermal conductivity for simple (AA-stacked) and Bernal (AB-stacked) bilayer BN and BN/graphene through tight-binding Hamiltonian model by using of the Kubo-Greenwood formula. Also the effects of electric field is included in our calculations. For this purpose, we first investigate the band structure and density of state (DOS) for BN and BN/graphene bilayers. The remainder of this paper is organized as follows. In the next section, we explain the theoretical aspects of our work. In Section 3, for obtaining the heat capacity, electrical and thermal conductivity the Kubo-Greenwood formula are calculated.

2. Theoretical method

We employed the tight binding model to investigate the electronic properties of AA- and AB-stacked BN and BN/graphene bilayers in presence of electric field. The bilayer unit cell contains four in-equivalent atoms A_i and B_i [i=1,2] where A_i and B_i refer to atoms on two sub-lattices in the same layer *i*. In AA- stacking, the A(B) atoms in one layer are located directly above the A(B) atoms in the neighboring layer and for AB- stacking, the A atoms of one plane sit over the center of hexagons in the other plane and only half of the atoms are located directly above each other.

In order to calculate the band structure and DOS of these structures, we derive their respective Hamiltonians. In the second quantization notation, the Hamiltonian becomes:

$$H=-t\sum_{\alpha,\beta=A,B}\sum_{n,\sigma}c_{n,\sigma}^{\alpha\dagger}c_{n+\delta,\sigma}^{\beta}+\sum_{\alpha=A,B}\sum_{n,\sigma}\varepsilon_0^{\alpha}(\boldsymbol{F})\quad c_{n,\sigma}^{\alpha\dagger}c_{n,\sigma}^{\alpha}$$

where α and β indicate the A and B sites inside the Bravais lattice unit cell. $c_{n,\sigma}^{\alpha\dagger}(c_{n,\sigma}^{\alpha})$ represents the creation (annihilates) of an electron with spin σ on site n at sub-lattice α. $\varepsilon_0^{\alpha}(\boldsymbol{F})$ is the on-site energy for α type atom in the presence of electric field. In the absence of electric field, the difference between the on-site energies of two in-equivalent A and B sub-lattices is zero. For AA and AB stacked bilayers, the Hamiltonian has three parts:

$$H=H_0+H_{inter-layer}+H_{bias}$$

where the H_0, $H_{inter\text{-}layer}$ and H_{bias} are:

$$H_0=-t\sum_{m=1}^{2}\sum_{\alpha,\beta=A,B}\sum_{n}c_{n,\sigma}^{\alpha_m\dagger}c_{n+\delta_m}^{\beta_m}$$

$$H_{inter-layer}=\gamma\sum_{m,m'=1}^{2}\sum_{\alpha,\beta=A,B}\sum_{n}c_{n,\sigma}^{\alpha_m\dagger}c_{n}^{\beta_{m'}}$$

$$H_{bias}=\sum_{m=1}^{2}\sum_{\alpha=A,B}\sum_{n}[\varepsilon_0^{\alpha_m}+\varepsilon_1^{\alpha_m}(\boldsymbol{F})]c_{n}^{\alpha_m\dagger}c_{n}^{\beta_m}$$

The *t* and *δ* are the hopping to the nearest neighbors and positions of the nearest neighbors of each sub-lattice, respectively. The indexes m, m′=1,2 refer to the first and second layer, respectively. The $\varepsilon_0^{\alpha_m}[\varepsilon_1^{\alpha_m}(\boldsymbol{F})]$ is the on-site energy for α atom at the layer m in the absence (presence) of the electric field. For the positive and negative bias we assume that $\varepsilon_1^{\alpha_m}(\boldsymbol{F})=\pm\frac{U}{2}$, respectively. For AA- and AB- stacked bilayers the total Hamiltonian, in the matrix form are given by:

$$H_{AA}=\begin{pmatrix}\varepsilon_1+(-1)^i\Delta/2 & \phi(k) & 0 & \gamma\\ \phi^*(k) & \varepsilon_2+(-1)^i\Delta/2 & \gamma & 0\\ 0 & \gamma & \varepsilon_3+(-1)^{i+1}\Delta/2 & \phi^*(k)\\ \gamma & 0 & \phi(k) & \varepsilon_4+(-1)^{i+1}\Delta/2\end{pmatrix}$$

$$H_{AB}=\begin{pmatrix}\varepsilon_1+(-1)^i\Delta/2 & \phi(k) & 0 & 0\\ \phi^*(k) & \varepsilon_2+(-1)^i\Delta/2 & \gamma & 0\\ 0 & \gamma & \varepsilon_3+(-1)^{i+1}\Delta/2 & \phi(k)\\ 0 & 0 & \phi^*(k) & \varepsilon_4+(-1)^{i+1}\Delta/2\end{pmatrix}$$