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Rectifying behavior of graphene/h-boron-nitride heterostructure

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ABSTRACT

The rectifying behavior of a simple graphene/boron-nitride heterostructure between two semi-infinite electrodes is investigated by using the non-equilibrium Green's function method. Also a simple analytical model is used to explain the current–voltage characteristic of a typical heterostructure. The Hamiltonian of nanostructure is written in the tight-binding model and the interaction of heterostructure with left and right leads is studied in the wide-band approximation. The current–voltage curve of graphene/boron-nitride shows an asymmetric behavior and negative-differential-resistance in the positive bias voltage which is explained in the simple model. By increasing the ribbon width, current increases and the peak-to-valley current ratio decreases. All the G/h-BN shows a large rectification ratio in a certain voltage region. The rectification behavior in the hetero-junction is related to the barrier potential at the interface of two structures.

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1. Introduction

In recent years, transport through nanostructures such as nanowires or carbon nanotubes becomes an interesting topic in the experimental [1–13] and theoretical [14–21] nano-physics. The study of current–voltage characteristic of an asymmetric structure can reveal the new future of the under-lying physics of transport. Different kinds of heterostructure were fabricated in laboratory [1–6,13,22–24] which show the rectifying behavior [1–6,13,24] and NDR effect [3–5,22] but there are few theoretical works on this subject [25–30]. The graphene/h-boron-nitride (G/h-BN) heterostructure is a two dimensional nano structure which has interesting electronic and transport properties [22–24,31–36]. Also the G/h-BN multi-layers are synthesized in laboratory [37,38] and investigated theoretically [39,40]. Doped graphene nano-ribbons with boron and nitrogen show rectifying behavior in previous works based on the density-functional theory [25,26,35]. Also NDR was observed experimentally in the single-walled carbon nanotubes [28] and predicted in the doped caped-carbon nano tube by using the DFT [27]. The non-equilibrium Green's function formalism is a powerful method for investigation of transport through nano junctions [14–21,41]. Meir and Wingreen derived the equation of current through a lead-conductor–lead-junction [42]. In the absence of interaction between electrons the Meir–Wingreen relation is simplified to the well-known Landauer–Buttiker equation [14,15]. In recent years, the ab-initio calculations of electronic, optical and transport properties of solids attract a wide range of theoretical physicist and chemist. The ab-initio calculations are expensive so the parametric methods become more important in the nano device calculations. In this work the asymmetric behavior of current through a G/h-BN heterostructure was investigated using Green's function formalism. Also a simple model for a typical heterostructure was used to explain the important feature of a heterostructure. The Hamiltonian of junction is written in the tight binding model which is a cheap and applicable model for other structures. The difficulty of semi-infinite leads is solved by introducing the self-energy of left and right electrodes in the wide-band approximation.

2. Model

Fig. 1 shows the G/h-BN heterostructure between the left and right leads. The total Hamiltonian of the above system contains the Hamiltonian of different parts plus the coupling between G/h-BN and electrodes. The Hamiltonian of graphene and boron-nitride nanoribbon is written in the nearest neighbor tight-binding model:

$$H_0 = \sum_{i,\sigma} \varepsilon_i C^{\dagger}_{i,\sigma} C_{i,\sigma} - \sum_{\langle i,j\rangle,\sigma} t_{i,j} C^{\dagger}_{i,\sigma} C_{j,\sigma} \quad (1)$$

ε_i and $t_{i,j}$ are the on-site and hopping between the nearest neighbor, respectively. The index i run over the different sites of graphene and boron-nitride ribbons. The operator C_i^+ (C_i) creates/annihilates a π electron at the ith site of nano-ribbon. The voltage difference between the left and right electrodes produces an external electric field in the heterostructure. The presence of an effective external electric field in the central region changes the Hamiltonian [16,43]. In this situation, the total Hamiltonian of

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heterostructure is sum between the electronic part and the Hamiltonian of external electric field. The Hamiltonian of the electric field, which is assumed uniform along the molecule, is written as

$$H_E(V)=\sum_{i,\sigma}\left(\frac{V}{L}\right)\left[\frac{L}{2}-X(i)\right]C^{\dagger}_{i,\sigma}C_{j,\sigma} \quad (2)$$

where L is the ribbon length and $X(i)$ is the position of i-th atom in the G/h-BN structure. By adding the Hamiltonian of electric field, the total Hamiltonian and transmission become voltage dependent. The interaction of heterostructure with both electrodes is modeled using the self-energy of electrodes. The calculations of surface Green's function and self-energy of electrodes is explained in our previous work [21]. For the sake of simplicity electrodes are described in the wide-band approximation which the self-energy is assumed purely imaginary and energy independent [16,17]. The retarded Green's function of the isolated heterostructure in the absence of electric field is defined as,

$$G^r_0(\varepsilon)=\left[(\varepsilon+i\delta^+)I-H_0\right]^{-1} \quad (3)$$

where I is the identity operator and δ^+ is an infinitesimal positive real number. According to Dyson's equation Green's function of ribbon in the presence of interaction is calculated as,

$$G^r(\varepsilon)=G^r_0(\varepsilon)+G^r_0(\varepsilon)\Sigma^{tot}G^r(\varepsilon) \quad (4)$$

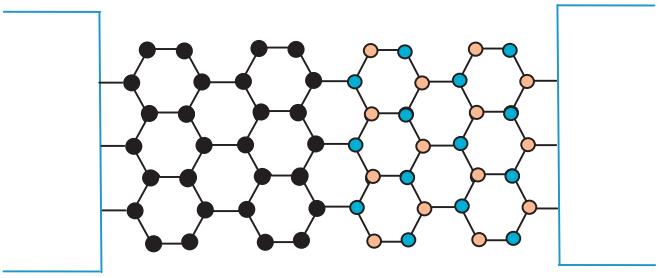

Fig. 1. The G/h-BN heterostructure between two semi-infinite electrodes.

where $\Sigma^{tot}=\Sigma_L+\Sigma_R$ is the total self-energy which includes the effect of left and right leads. At last, the retarded Green's function of the electrode/heterostructure/electrode in the presence of an external electric field is written as,

$$G^r(\varepsilon)=\left[(\varepsilon+i\delta^+)\mathrm{I}-H^{tot}\right]^{-1}=\left[(\varepsilon+i\delta^+)\mathrm{I}-H_0-H_E-\Sigma_L-\Sigma_R\right]^{-1} \quad (5)$$

The self-energy of left and right electrodes $\Sigma_{L/R}$ is a matrix which has only non-zero elements in the edge of the ribbon. By using the retarded Green's function, the current flow between two electrodes, through the heterostructure, is calculated. In the absence of many-body interactions, current is written as the Landauer–Buttiker formula [16,17,21,41,43],

$$I(V)=\frac{e}{h}\int_{-\infty}^{+\infty}d\varepsilon T(\varepsilon)\left[f_L(\varepsilon)-f_R(\varepsilon)\right] \quad (6)$$

where $f_{L/R}(\varepsilon)$ is the Fermi distribution function in the left/right electrode with chemical potential $\mu_{L/R}=\varepsilon_f\pm(eV_b/2)$ and Fermi energy ε_f which is set in the middle of the electronic band gap. The $T(\varepsilon)$ is the transmission coefficient as a function of energy for electrons and can be written as follows:

$$T(\varepsilon)=Tr\ \left[\Gamma_L G^r(\varepsilon)\Gamma_R G^a(\varepsilon)\right] \quad (7)$$

In the above equation $G^a(\varepsilon)$ is the advance Green's function which is simply the complex conjugate of the retarded Green's function.

3. Results

The tight-binding parameters that include the on-site energy and hopping between carbon, boron and nitrogen are extracted from our previous work [21]. The imaginary part of self-energy is considered energy dependent and set to 0.5 eV. We use a nanoribbon with 7 and 9 atoms wide and compare the I–V curve with a narrower ribbon. Fig. 2 shows the transmission as a function of energy for different bias voltages in the case of $W=7$. The transmission peaks correspond to the eigenvalues of the heterostructure. By increasing the bias voltage the energy window

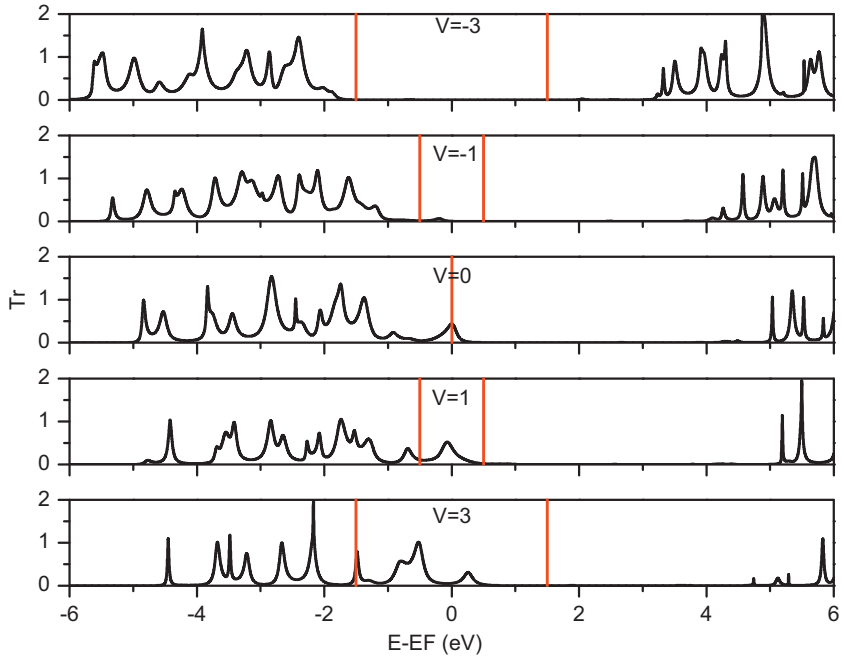

Fig. 2. Transmission through the G/h-BN as a function of energy in the negative and positive bias voltages. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

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