Robust low-bias negative differential resistance in graphene superlattices

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Abstract
In this work, we present a detailed theoretical study on the low bias current–voltage (I–V) characteristic of biased planar graphene superlattice (PGSL), provided by a heterostructured substrate and a series of grounded metallic planes placed over a graphene sheet, which induce a periodically modulated Dirac gap and Fermi velocity barrier, respectively. We investigate the effect of PGSL parameters on the I–V characteristic and the appearance of multipeak negative differential resistance (NDR) in the proposed device within the Landauer–Buttiker formalism and adopted transfer matrix method. Moreover, we propose a novel venue to control the NDR in PGSL with Fermi velocity barrier. Different regimes of NDR have been recognized, based on the PGSL parameters and external bias. From this viewpoint, we obtain multipeak NDR through miniband aligning in PGSL. The maximum pick to valley ratio (PVR) up to 167 obtained for $\nu_c$, the Fermi velocity correlation (ratio of Fermi velocity in barrier and well region), is 1.9 at bias voltages between 70–130 mV. Our findings have good agreement with experiments and can be considered in designing multi-valued memory, functional circuit, low power and high-speed nanoelectronic device applications.

Keywords: negative differential resistance (NDR), planer graphene superlattices (PGSLs), Fermi velocity barrier, Dirac gap

1. Introduction
Graphene, an atomically thin 2D material, has attracted a great deal of interest, due to its superior electrical and optical properties [1–3], which has become one of the most promising materials for nanoelectronic and nanophotonic devices [4–6]. The charge carriers in monolayer graphene behave like massless Dirac fermions with linear energy dispersion, and can be governed by an effective Dirac equation, which leads to many novel electronic and transport properties [7–10]. However, due to the lack of energy gap in the pristine graphene electronic band structure, the Klein tunneling prevents the Dirac electrons in graphene from being confined by an electrostatic potential, which impedes its use in electronic devices. In order to overcome this limitation, several schemes have been proposed which lead to the suppression of Klein tunneling and confinement of the Dirac electrons in graphene. For instance, an energy gap can be induced by doping [7–9], substrate [10–12], strain [13–15], quantum confinement effects [16–19], spatial modulation of Dirac gap and external periodic potentials [20–23]. The Fermi velocity is another key concept to study the electronic properties of graphene. According to the Lorentz invariant theory, by controlling the electron–electron interaction, one can regulate the Fermi velocity in graphene. This implements various procedures, such as dielectric screening [24, 25], carrier concentration [26–28], periodic potentials [29], curvature of the graphene sheet [30] and substrate modulation [31]. Recently, graphene superlattice, graphene under periodic potentials, has been extensively studied both experimentally and theoretically [20–23, 32–38]. These works have considered the periodic potentials of different natures (electric and magnetic) and profiles. This considerable interest is motivated by discovering the novel transport properties of charge carriers through planar graphene superlattice (PGSL) structures (e.g. extra Dirac points, highly anisotropic Dirac points), which has not been observed in the pristine
graphene, and also by promising potential applications in a diverse area of nanoelectronic devices.

Beyond the usual linear or saturation performances expected to occur in graphene based devices, the appearance of prominent non-linear effects, such as the negative differential resistance (NDR) in the current–voltage characteristics, has attracted strong research interest both theoretically and experimentally [39–48], since it could potentially impact the number of key applications, such as high frequency oscillators, reflection amplifiers, memories, multi-level logic devices and fast switches [49].

NDR at high bias voltages (1–2 V) in narrow nanoribbons have been studied in lots of works [40, 42]. NDR at low bias regime can also be achieved in monolayer and bilayer graphene, and graphene nanoribbon superlattices systems [41, 46, 47].

In the present study, for the first time, we investigate the NDR features of graphene based planar superlattices composed of periodically modulated Fermi velocity, Dirac gap and electrostatic potential at low bias voltages $V_{SD} < 200$ mV. The above mentioned effects are induced by means of velocity barrier, nanostructured substrate and 1D potentials of square barriers, respectively. Transmission properties of Dirac fermion beams tunneling through PGSL are investigated by an adopted transfer matrix method (TMM) in detail. We have found that the transmission properties of PGSL can be tuned readily by changing the main parameters of the PGSL, i.e. the well and barrier widths, energy and angle of the incident electrons, the number of periods of PGSLs, Dirac gap and Fermi velocity barrier. Current–voltage characteristics are obtained within the Landauer–Buttiker formalism. We have found that the NDR appears with appropriate structural parameters, which means that NDR could be controlled and tuned by PGSL parameters. More interestingly, we investigated the effect of the Fermi velocity barrier on the $I–V$ characteristics of a PGSL resonant tunneling diode (PGSLRTD). We found that the pick to valley ratio (PVR) in PGSLRTD is enhanced exponentially by increasing the Fermi velocity correlation.

2. Model and method

A schematic view of our proposed device is shown in figure 1. A monolayer of graphene is placed on a planar heterostructured substrate composed of two different materials shown by I, II. This composed substrate opens different energy gaps in different regions of the graphene sheet, denoted by $\Delta_W$ and $\Delta_B$. W, B refer to the well and barrier, respectively. Moreover, according to the Lorentz invariant theory, Fermi velocity differs in the well and barrier regions of graphene placed on different materials of substrate [49]; thus, the composed substrates can also modify the Fermi velocity in graphene. The Fermi velocity in each region will be denoted by $\nu_W$ and $\nu_B$. We define $v_F = \nu_B/\nu_W$ as the Fermi velocity correlation between the barrier and well regions. A series of grounded metallic planes are placed over the graphene sheet, which induce a periodic velocity barrier. Metallic planes do

electron–electron interaction weaker; therefore reducing the Fermi velocity in the relevant region [25]. Metal electrodes in the left and right create an electrostatic potential across the graphene sheet, acting as source–drain voltage, $V_b = V_R - V_L$.

The Kronig–Penney (KP) model is applied for investigation of the PGSL electrostatic potential profile. In the vicinity of the Dirac points, the PGSL electronic structure can be described by the Dirac-like equation. The effective 2D Dirac Hamiltonian for a PGSL with a position dependent energy gap and Fermi velocity, $v_F$, is written as:

$$H = -i\hbar (\sqrt{v_F(x)} \sigma \partial_x \sqrt{v_F(x)} + v_F(x) \sigma \partial_x) + V(x) \mathbf{1} + \Delta(x) \sigma_z$$

(1)

where $\sigma_i$ are the Pauli matrices and $\mathbf{1}$ is the $2 \times 2$ unitary matrix, $\Delta(x)$ is the position dependent graphene energy gap, $V(x)$ is an external position dependent electrostatic potential that is composed of two parts: first, the KP potential $(V_{KP})$ that takes as zero in the well region and 400 meV in barrier region. The second part indicates the applied external potential bias that is taken as $eEx$ ($e$ is the electron charge, $E$ is the electric field and $x$ is the growth direction of PGSL)

$$V(x) = \begin{cases} V_W(x) & V_{KP} - eEx \text{ for barrier} \\
V_W(x) - V_{KP} - eEx \text{ for well}, \end{cases}$$

(2)

where indices W, B refer to the well and barrier regions, respectively. According to Bloch’s theorem, it is straightforward to obtain the electronic dispersion for the periodic structure of PGSL by the following equation:

$$\cos(k_d) = \cos(k_{dw}) \cos(k_{wdw}) + \frac{k_d^2 - (E - V_W(x))^2 - \Delta_W^2/h^2}{k_w^2 - (E - V_B(x))^2 - \Delta_B^2/h^2} \times \sin(k_{dw}) \sin(k_{wdw})$$

(3)

where $k_w = ((E - V_W(x))^2 - \Delta_W^2)/h^2$, $k_B = ((E - V_B(x))^2 - \Delta_B^2)/h^2$, $k_d = (E \sin \theta / h \nu_F)^{1/2}$, $\theta$ is the incident angle of the electron beam that is defined as the angle between the growth direction of planar PGSL and the direction of incidence, $d_w$ and $d_B$ are the well and barrier widths, respectively. We choose $V_{KP} = 0$, $V_{KP}^B = 400$ meV, $\Delta_B = 0$, $\Delta_w = 0$.

In order to adopt the well known TMM to the graphene superlattice under bias in this work, we consider the m layers containing barrier and well with the potential mentioned in equation (2) that can be rewritten as:

$$V_m = V_{KP}^m - eV_{RL} \cdot x_m/L.$$  

(4)

Index $m$ refers to the number of layers ($m = 1, 2, 3, \ldots N$). $V_{RL}$ is the difference of the potential applied between two left and right end electrodes.

The solution to the Dirac equation, $H\psi(x, y) = E\psi(x, y)$ is a two component spinor that illustrates the two graphene sublattices:

$$\psi_m(x, y) = \psi_m(x)e^{ik_x y}.$$  

(5)
and defining $\nu(x_m) \psi_m(x) = \phi_m(x)$, the solution to the Dirac equation in the $x$ direction can be written as a linear combination of forward/backward plane-waves [52]:

$$\phi^1_m(x, y) = \sqrt{\nu(x_m)} (A_m e^{i k x} + B_m e^{-i k x}) e^{i k y},$$

$$\phi^2_m(x, y) = \sqrt{\nu(x_m)} (A_m e^{i k x} + B_m e^{-i k x}) e^{i k y},$$

where $A_m$ and $B_m$ are the transmission amplitudes, and $k = (E \sin \theta / \hbar \nu)^{1/2}$. $\theta$ is the incident angle of the electron beam that is defined as the angle between the growth direction of planar PGSL and the direction of incidence $\alpha_m = \tan^{-1}(k/E_k)$. The external potential in our work is linear with $x$. To construct the transfer matrix for this structure we divided the linear potential to very small potential steps where the transfer matrix of each small step in the $m$th region can be written simply through continuity conditions between spinors as [53]:

$$M^1_j = \begin{pmatrix} e^{i k x J} & e^{-i k x J} \\ e^{-i k x J} & e^{i k x J} \end{pmatrix},$$

$$M^2_m(x) = \prod_j M^j_m(x)$$

where index $j$ refers to the $j$th division in the $m$th region of PGSL. The transfer matrix of the whole system, connecting the left electrode to right electrode, is obtained as:

$$t = \prod_m M^m_{m+1}(x_{m+1}) M^m_{m+1}(x_{m+1}).$$

From the current density in the $m$th region, $J_m(x) = \nu(x) \psi^\dagger_m(x) \sigma_i \psi_m(x)$, the current flow must be conservative at the left and right sides of PGSL, which implies $J_L(x) = J_R(x)$. From which, we identify the transmission coefficient, $T_{LR}$ [43, 50]:

$$T_{LR}(E, k, V_b) = \frac{J_R}{J_L} = \frac{\cos \theta_R}{\cos \theta_L} \left| \frac{E}{k} \right|^2.$$}

In our model, the potential drop from source to drain follows a linear function. The zero-temperature ballistic net current as a function of bias is computed by the Landauer–Büttiker formalism [51, 54, 55]:

$$I = \int_{-\pi/2}^{\pi/2} dE |E| \times \int_{-\pi/2}^{\pi/2} T(E, \alpha, v_b) \cos \alpha d\alpha$$
where $I_0 = 2geW/v_t h^2$, $g = 4$ is the degeneracy of the electron states in graphene, $W$ is the sample width that we chose as $d_B$ and $V_b$ is applied voltage between the left and right electrode ($V_{\text{bias}}$ in figure 1), a linear voltage along the $x$-direction defined as $eV_b = \mu_L - \mu_R$ and $\mu_L, \mu_R$ is the bias-dependent local Fermi energy in the left (right) electrode.

3. Results and discussions

Due to the significant roles of the device dimension and geometry in the $I$–$V$ characteristics, we first analyze the effect of the well and barrier width, $d_W, d_B$, and the number of periodicity, $N$, on NDR. In figure 2, we present the $I$–$V$ diagram of the device for different values of $d_W$ and certain values of $d_B$. 

Figure 2. $I$–$V$ characteristic for three values of well width, $d_W$, for $d_B = 5$ nm, $N = 10$ and $\Delta_B = 150$ meV.

Figure 3. (a) Map of transmission spectrum for different values of $N$. Incident angle, $\theta$, is $\pi/6$. (b) $I$–$V$ characteristics for different values of $N$. $d_W = 40$ nm, $\Delta_B = 150$ meV and $d_B = 5$ nm.
Figure 4. The effect of gap opening in barrier region, $\Delta_B$, on the $I-V$ characteristic. $N = 10, d_W = 40$ nm, $d_B = 5$ nm.

Figure 5. (a) Counter plot of transmission spectrum for different values of correlation velocity, $v_C$ for incident angle of $\theta = \pi/6$.
(b) $I-V$ characteristics for different correlation velocities $\Delta_B = 150$ meV, $N = 10$, $d_W = 40$ nm and $d_B = 5$ nm.
We consider the well width to be bigger than barrier width, and \( N = 10 \).

As can be seen from figure 2, for wider wells, the corresponding current peaks values are smaller than that of thinner wells. Also, peaks are shifted to lower biases. This behavior can be attributed by the red shifting of resonant energies with increasing well width. In the case of wider wells, lower biases are needed to align the resonant states. We found that transmission oscillations increase with increasing well widths (not shown here), which is because of the increasing resonant states. On the other hand, increasing oscillations reduce the area under the transmission curve that subsequently reduces the current value for wider wells (equation (4)). We found that, for a barrier width remarkably bigger than and comparable with well width, applying a bias aligns the resonant modes, so that the resonant sequential resonant tunneling occurs and current increases to reach a peak. By increasing the bias more, the resonant states are misaligned and strong tunneling suppression appears, leading to the current decreasing and a pronounced spike in the \( I-V \) curve.

Now, we turn our attention to the impact of \( N \) on NDR and discuss its different distinct regimes in our system. Figure 3 depicts the transmission spectrum (\( t \)) of PGSL as a function of \( N \). From the figure, it is observed that, by increasing \( N \) and subsequently increasing interfaces, Fabry–Perot like interferences are increased and lots of resonant modes are created. Furthermore, resonant modes show up below and above the stop band for all values of \( N \). In the case of the thin barriers in figure 3(b), for a small value of \( N \) as 2, the current increases monotonically upon resonant mode alignment and sequential resonant tunneling occurs. Higher external biases misalign the resonant modes and tunneling is completely suppressed, resulting in a decreasing current value and NDR appearing as a peak (curve of \( N = 10 \)). This trend indicates a classical regime.

For large number of \( N \) (10 and more), resonant modes form superlattice minibands. At low biases, the current is dominated by transmission across these minibands, called the miniband regime. With an increasing bias, resonant modes (responsible for formation of minibands) are misaligned, breaking up the minibands into off resonant Wannier Stark ladders with suppressed transmission, leading to the current decreasing. By increasing the bias, rungs of ladders from distinct minibands cross, showing new resonant peaks in the transmission and system, encountering Wannier–Stark regimes. Such an alternation process from miniband to Wannier–Stark regime is the reason for multi-peak NDR. In the other words, this trend of NDR for larger numbers of barriers originates from the destructive-constructive interferences of Dirac fermions, creating several peaks in the transmission spectrum and \( I-V \) diagram. Hereafter, we consider the case of the miniband and Wannier–Stark regime by taking the number of barriers as \( N = 10 \).

It is worth mentioning that Fabry–Pérot like resonances appear for the non-perpendicular incident (i.e. \( k_y \neq 0 \)), while for \( k_y = 0 \), Klein tunneling suppresses resonant tunneling.
and NDR. Figure 4 illustrates the Dirac barrier gap ($\Delta B$) effect on $I-V$ characteristic in low bias regime. Based on our calculations, with an increasing Dirac barrier gap, wider stop bands in the transmission spectrum cause the decreasing of the current. On the other hand, increasing the Dirac barrier gap inhibits the Dirac carrier transport, meaning that PVR increases. Also, a multi peak trend appears for bigger Dirac barrier gaps, caused by resonant tunneling enhancement. This finding has good agreement with that of Song et al and Sollner et al [56, 57]. Appropriate structural parameters to reach the maximum NDR are obtained as $v_C = 1.9$, $V_b = 70–130$ mV, $N = 10$, $d_w = 40$ nm and $d_b = 5$ nm. The considerable value of PVR as 167 obtained for a Dirac barrier gap of 150 meV, which is a very good value for the optimal performance of RTD based on PGSL, can be realized experimentally. In order to compare with other works done on graphene based NDR, we consider when Song et al [56] reported a maximum value of PVR as almost 2. They used double barrier RTD based on graphene strips to obtain PVR. The advantage of our model is in obtaining a very big PVR in an ultra-low bias regime by the means of PGSL. In our work, a variety of parameters have been taken into account to control NDR and obtain a high value of PVR, when NDR appears for suitable values. For example, a very high value of barrier width prohibits the tunneling of electrons and the current increases with the increasing bias voltage linearly, leading to the prohibition of NDR’s appearance. The optimization of parameters should be done to find a high value of PVR.

One of the key parameters in the $I-V$ characteristic is the ratio of Fermi velocity in barrier/well regions ($\nu_{C}$). It is very important to study the effect of this parameter to control NDR. In figure 5(a) we report the transmission coefficient spectrum for different values of $\nu_{C}$. It can be seen that transmission is enhanced for a special value of $\nu_{C}$ and energies. A closer view of figure 5(a) determines that the oscillatory behavior in the transmission spectrum becomes more pronounced at specific values of $\nu_{C}$. In contrast, at higher values of $\nu_{C}$, the oscillation diminishes and the energy gap is increased. Figure 5(b) depicts that big values of current are obtained for smaller $\nu_{C}$. This finding can be explained by the transmission spectrum in figure 5(a), where a larger area under the transmission curve can be observed that leads to a bigger current (equation (4)).

Two main peaks are observed in low bias regime around 70 mV and 130 mV, which implies the appearance of NDR. Such phenomena originate from this fact that bigger $\nu_{C}$ creates a higher Fermi velocity barrier, so that it is difficult for Dirac electrons to be able to tunnel from them, leading to the reduction of current. NDR results from resonant tunneling occurring in the miniband and Wannier–Stark regime, as discussed before. To get a closer insight, we focus on the trends of PVRs related to two main peaks versus $\nu_{C}$, $d_w$, $N$, $\Delta \nu$ in figure 6. It is clear that the PVR’s values are increased with increasing these parameters, except for $N$. Figure 6(c) illustrates that an increasing number of periods, $N$, increases PVR1 but decreases PVR2. The optimum values of structural parameters to enhance the PVR at low biases can be obtained from figure 6. Our results show that, among the structural parameters, $\nu_{C}$ has remarkable effects on the value of PVR1 and PVR2, hence it is very important in the characterization of the electronic device through the cut-off frequency, which is a fundamental parameter in high frequency PGSLRTD based oscillators and switches. Our obtained high value of PVR at low biases is desired for implementation in novel low power digital logic circuits and multi-valued memory.

Finally, in order to verify our results, we compared our findings with those of Antonova et al [58]. They investigated NDR in the films fabricated from partially fluorinated graphene suspension. The formation of graphene islands (quantum dots) are observed in these films. Various types of NDR and a step-like increase in the current are found for films created from the fluorinated graphene suspension. NDR resulting from the formation of the potential barrier system in the film and graphene quantum dots was reported in their study. We model this system by quantum well/barrier systems according to our theoretical framework. The $I-V$ characteristic found by our calculation has very good agreement with the $I-V$ characteristic measured by them in low biases.

4. Conclusion

In summary, we theoretically studied the $I-V$ characteristics of PGSL modeled by patterning graphene on a nanostructured substrate and top grounded metal planes. To reach this goal, we adopted a TMM to obtain the transmission spectrum under external bias. The effects of the parameters, such as the number of periods, $N$, well and barrier width, $d_w$, $d_b$ and ratio of Fermi velocity in each region, $\nu_{C}$. Dirac barrier and electrostatic barrier, have been analyzed in detail to enhance the peak to valley ratio, PVR, in the $I-V$ curve at very low external biases within the Landauer–Buttiker formalism. Different regimes of NDR were discussed according to the parameters used in our model device. The appropriate structural parameters to reach a maximum NDR were obtained as $\nu_{C} = 1.9$, $V_b = 70–130$ mV, $N = 10$, $d_w = 40$ nm and $d_b = 5$ nm. A robust value of PVR as 167 was obtained for a Dirac barrier gap of 150 meV at ultra-low biases. Our proposed device paves a novel way in PGSL based NDR devices, such as RTDs, multilevel memory, low power and high-speed electronic devices working at a low bias.

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