Giant effect of negative differential conductance in graphene nanoribbon *p-n* hetero-junctions

V. Hung Nguyen,[1,2,a)] F. Mazzamuto,[1] J. Saint-Martin,[1] A. Bournel,[1] and P. Dollfus[1]
[1]*Institut d'Electronique Fondamentale, UMR8622, CNRS, University Paris Sud 11, 91405 Orsay, France*
[2]*Center for Computational Physics, Institute of Physics, VAST, P.O. Box 429 Bo Ho, Hanoi 10000, Vietnam*

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The *I-V* characteristics of graphene nanoribbon (GNR) *p-n* junctions have been investigated using atomistic quantum simulation. On the basis of results obtained for simple armchair GNR structures with large bandgap, it is suggested to improve significantly the device operation by inserting a small-bandgap section in the transition region between *n* and *p* zones. A giant peak-to-valley ratio (PVR) of negative differential conductance (higher than 10^3) can be achieved in such hetero-junctions. Additionally, the PVR is proved to be weakly sensitive to the transition length and not strongly degraded by the edge disorder, which is an important feature regarding applications. © *2011 American Institute of Physics*. [doi:10.1063/1.3616143]

Due to its excellent electronic properties such as high carrier mobility[1] and high critical current density,[2] graphene is expected to be a good candidate for RF electronic applications.[3,4] In semiconductor engineering, devices able to provide a negative differential conductance (NDC) behavior are known to offer great potential for high frequency applications as oscillator, frequency multiplier, and fast switching.[5] Therefore, the NDC effect has been explored and discussed in several graphene nanostructures (e.g., see Refs. 6–11). However, it was shown to be difficult to achieve a large peak-to-valley ratio (PVR) of NDC in such structures. This limitation is essentially due to the lack of bandgap of 2D-graphene sheets[6–8] or to the effect of edge defects in narrow graphene nanoribbons (GNRs).[10,11]

In a recent work,[12] we have investigated the transport characteristics of 2D-monolayer graphene *p-n* junctions and found that a strong NDC effect can be achieved, thanks to a finite energy bandgap opening, e.g., when the graphene sheet is epitaxially grown on SiC.[13] As in the conventional Esaki diode,[14] the peak current is governed by the interband tunneling through the junction at low bias (see Fig. 1(a)). The valley current occurs at high bias when the filled states in one side of the junction do not see any empty states available for tunneling on the other side (see Fig. 3 in Ref. 12). It was shown that an increase of bandgap reduces strongly the valley current and may result in a strong NDC effect. However, a large bandgap also raises the appearance of evanescent states in the transition region between *n* and *p* zones, which reduces the peak current. Additionally, due to the contribution of such evanescent states, the peak current and, hence, the PVR decrease strongly when increasing the transition length, which unfortunately is difficult to control.

Alternatively, similar *p-n* junctions can be also realized by using armchair graphene nanoribbons (AGNRs), wherein a finite bandgap opens according to the finite ribbon width.[15] It offers many possibilities of bandgap engineering though raising the issue of the precise control of ribbon edges and width. This motivates us to investigate in this letter, the transport characteristics of AGNR *p-n* junctions and suggests us to improve their operation by replacing the large-bandgap AGNR in the active region by another smaller-bandgap GNR section. It is likely to enhance the interband tunneling in the peak current regime while the small valley current controlled by the large bandgap in the doped regions is still maintained. We show that in such structures, the PVR is not only extremely high (a few thousands) but also weakly sensitive to the transition length and not strongly degraded by the edge disorder.

The structures under study, a simple AGNR junction and two hetero-structures (with *T*- and *AZ*- shapes), are schematized in Fig. 1. The *p*- doped and *n*- doped graphene regions can be generated by electrostatic doping[16] or by chemical doping.[17] The charge transport is investigated by using the non-equilibrium Green's function technique to

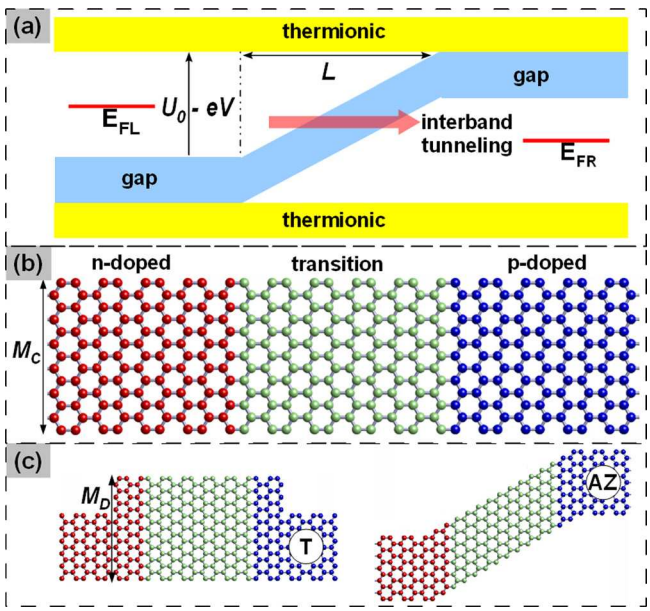

FIG. 1. (Color online) (a) Band profile along the transport direction of graphene *p–n* junctions and (b) schematic of a simple AGNR one. The junctions are characterized by two important parameters, the potential barrier U_0 and the transition length *L*. (c) Other hetero-structures under study, namely, *T*-and *AZ*-junctions. $M_{C,D}$ is the number of carbon chains between two ribbon edges in the two junction sides and in the center, respectively.

a)Electronic mail: viet-hung.nguyen@u-psud.fr.

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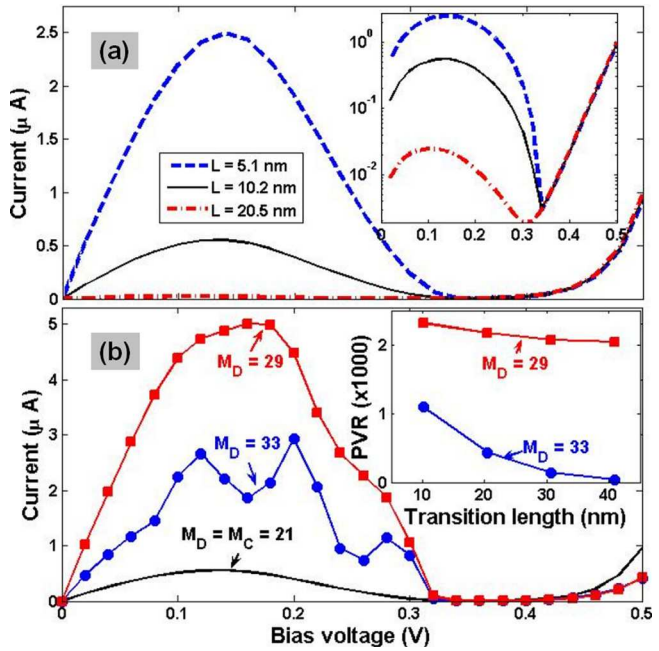

FIG. 2. (Color online) *I-V* characteristics (a) of the simple junction with different L and (b) of the T-junctions with different indexes M_D. The insets show the current plotted on the logarithm scale in (a) and the L-dependence of PVR in (b). Other parameters: $U_0 = 0.7$ eV, $M_C = 21$, and $L = 10.2$ nm in (b), and the device length $D \approx 42.6$nm.

solve the tight-binding Hamiltonian as in Ref. 18. Moreover, to take into account the bond relaxation at the AGNR edges,[19] we use a different tight binding parameters $t_e = C_e t_0$ ($C_e = 1.12$) for the edge bonds, where $t_0 = 2.7$ eV is for the other bonds. Throughout the work, the ballistic current is computed at room temperature.

First, we display in Fig. 2, the *I-V* characteristics of the AGNR-junctions (with simple and T-shapes). Fig. 2(a) shows that, thanks to the large bandgap ($\sim$0.37 eV for $M_C = 21$), a strong NDC behavior can be observed in the simple junction, e.g., a PVR of $\sim$857 is obtained for $L = 5.1$ nm. However, the peak current and then the PVR are reduced strongly when increasing L, e.g., the PVR falls to $\sim$188 and 13 for $L = 10.2$ nm and 20.5 nm, respectively. This behavior is very similar to that observed and explained for 2D-monolayer graphene *p-n* junctions in Ref. 12. To reduce the sensitivity of the peak current to L, we propose to replace the large-bandgap ribbon in the active region by another smaller-bandgap one. Without changing significantly the valley current, this configuration can reduce the role of evanescent states in the transition region and, therefore, enhance the peak current and the PVR. Indeed, this idea is clearly demonstrated by the maps of local density of states (LDOS) and the transmission probability in Fig. 3 and by the *I–V* characteristics in Fig. 2(b). In particular, Fig. 3 shows that while the evanescent states around the neutral point in the transition region are observed clearly in the simple junction (Fig. 3(a)), they are not visible in the T-one (Fig. 3(b)), wherein the central GNRs bandgap E_{gD} is small. This leads to the enhancement of the interband tunneling in the latter junction as shown in Fig. 3(c). As a consequence, Fig. 2(b) shows that while the valley current (due to the fixed transmission gaps seen in Fig. 3(c)) is always small, the peak current and, hence, the PVR increase significantly when reducing E_{gD}. For instance, the PVR is $\sim$1095 and 2318 for $M_D = 33$ ($E_{gD} \approx 0.233$ eV) and 29 (0.062 eV), respectively. Such a giant PVR can not be achieved in the simple junction with the same transition length ($L = 10.2$ nm). Moreover, it is worth noting that as shown in the inset of Fig. 2(b), the smaller E_{gD}, the weaker the sensitivity of the PVR to the length L.

Actually, the edge disorder is known to lead to quasi-localized states around the edge defects,[20] which may drastically affect the transmission processes[21] and then limit the performance of GNR devices.[10,11,22] In particular, it can result in an increased valley current which limits the value of PVR (Refs. 10 and 11) and on/off current ratio.[22] To evaluate its effects in the junctions considered here, we show in Fig. 4, the *I–V* characteristics for different disorder configurations. The edge defects are simply generated by randomly removing the carbon atoms with a percentage of 15% along both sample edges. The study shows that differently from other structures, the valley current in these junctions is not enhanced but actually reduced by the disorder. This can be explained by the different physical origins of the valley current, i.e., the confinement effects in Ref. 10, the parity selective rule in Ref. 11, and the transmission gaps (due to the bandgap in the two junction sides as seen in Fig. 3) in this work. While the edge disorder can break the two former factors, it generally reduces the transmission probability[21] and hence enlarges the transmission gaps in the present case. Therefore, as demonstrated clearly in Fig. 4, though the peak current is slightly affected, the device operation is not

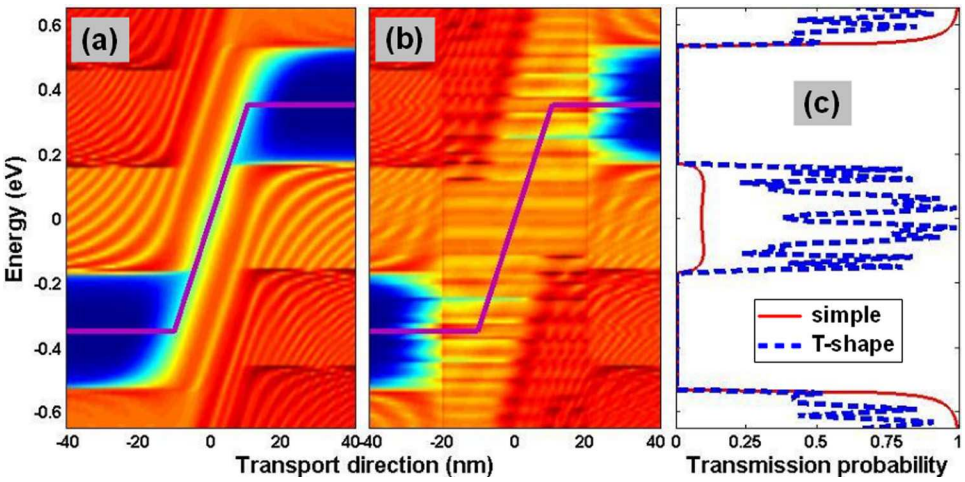

FIG. 3. (Color online) Local density of states of (a) simple ($M_C = M_D = 21$) and (b) T-junctions ($M_C = 21$ and $M_D = 29$). (c) shows the corresponding transmission probability as a function of energy. The structures are unbiased.

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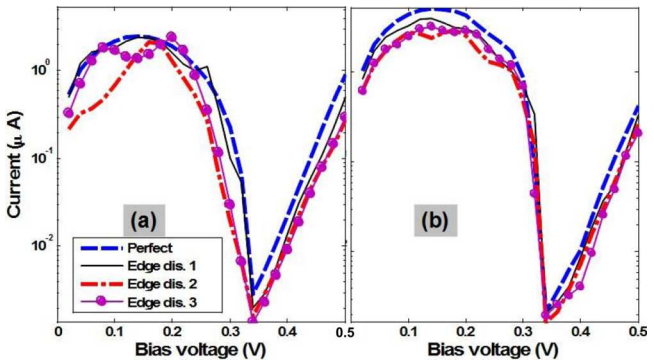

FIG. 4. (Color online) *I-V* characteristics of (a) the simple junction and (b) the *T*-one with different edge disorder configurations. Other parameters: $U_0 = 0.7$ eV, $M_C = 21$, $M_D = 29$, $L = 5.1$ nm, and $D \approx 42.6$nm.

degraded significantly by such disorder effects, i.e., a PVR as large as $\sim 10^3$ can still be achieved. It is worth noting that this is an important outcome regarding applications, because though expected to be realized soon,[23–25] the precise control of the ribbon edges is still a technological challenge.

We now discuss another possibility of improving the junction operation, which consists in using the *AZ*-structure schematized in Fig. 1(c). Previous studies have shown that the transport through a zigzag graphene nanoribbon (ZGNR) is governed by two important rules: the matching of transmission modes along the transport direction[11] and the parity selective rule.[9,26] While the former one can lead to the current enhancement, the latter rule manifests only when the number M_Z of zigzag lines is even and results in the reduction of the transmission probability. In Fig. 5, we display the *L*-dependence of the PVR in two typical cases: the number of zigzag lines $M_Z = 11$ and 16 (with $M_C \equiv 2M_Z - 1$). It is shown that due to the gapless character of perfect ZGNRs, the peak current and the PVR increase when replacing the AGNR in the active region by a ZGNR. For instance, the PVR is $\sim$1500 for $M_Z = 11$ ($M_C = 21$) and $L = 5.1$ nm in Fig. 5, while it is only $\sim$857 in Fig. 2(a) for the simple AGNR structure. However, when increasing the length *L*, we distinguish two different cases depending on M_Z parity: the PVR increases for odd M_Z (circle-solid line), but decreases for even M_Z (square-solid line). The former (surprising) feature can be explained well by the role of the matching of transmission modes discussed in Ref. 11, i.e., the larger the transition length, the smaller the slope of $U(x)$ in the transition region, the higher the number of allowed transmission channels within a given energy range and, thus, the higher the peak current. Of course this increase of PVR as a function of *L* should be valid only in the ballistic approximation and is limited to *L*-values close to the mean-free-path, i.e., typically a few hundreds of nm.[2] In the case of even M_Z, the parity selective rule applies and results in gaps in the transmission between two regions of different doping.[9,26] Hence, the wider the transition region where the transmission processes are affected, the lower the total current. Additionally, in the presence of edge disorder, Fig. 5 shows that as in the *T*-junction, though reduced a PVR as large as $\sim 10^3$ is still achieved for $M_Z = 11$, while for even M_Z ($= 16$), the parity selective rule is broken, which hence enhances significantly the peak current and the PVR.

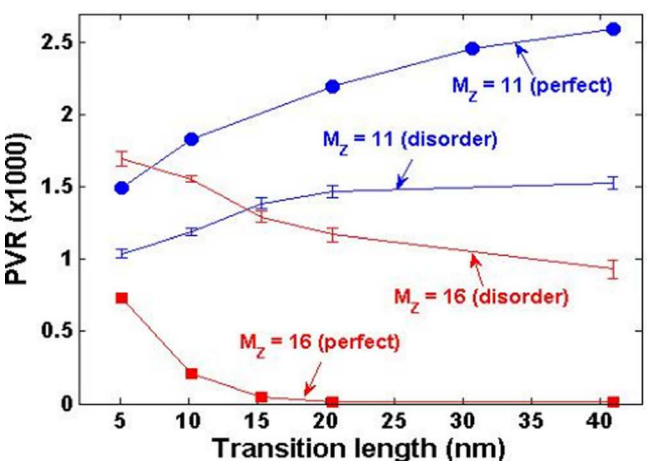

FIG. 5. (Color online) *L*-dependence of the PVR in the *AZ*-junction for different numbers M_Z of zigzag lines without and with (averaged over ten configurations of) the edge disorder. Others parameters: $U_0 = 0.7$ eV and $D \approx 42.6$nm.

In summary, we have shown that by designing GNR *p-n* hetero-junctions with a small-bandgap section in the transition region, it is possible to achieve a giant PVR of NDC, of typically a few thousands at room temperature. This small-bandgap section may be either an AGNR larger than the doped regions (*T*-structure) or a ZGNR (*AZ*-structure) where the parity selective rule does not exist or is broken by edge disorder effects. Most importantly, besides this high PVR value, it was proved that in such hetero-structures where the valley current is essentially controlled by the bandgap in the doped regions, the PVR is weakly sensitive to the transition length and not strongly degraded by the edge disorder, which makes this design strategy viable for future applications.

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