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Graphene Nanoribbon Field Effect Transistor Designing from Numerical Simulations

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Abstract

We have theoretically examined carrier localization in edge-disordered armchair graphene nanoribbons (ED-AGNRs) whose lengths correspond to the typical gate length for current field-effect transistors (FETs). The GNR width dependence and the edge roughness concentration dependence on the localization length of ED-GNRs is clarified, which provides essential guideline for the design of GNR-based FETs.

1. Introduction

Graphene is expected to be a channel material of field effect transistors (FETs) because of its high carrier mobility [1, 2]. However, zero bandgap is a serious problem of graphene for its FET application. One possible way to overcome the gap-opening problem is to process graphene into a nanometer width ribbon, referred as graphene nanoribbons (GNRs) [3, 4]. They have been successfully applied to FETs with high carrier mobility [5, 6]. A recent experiment reported that the resistance of GNRs increases exponentially with their length even at the room temperature [7]. This non-Ohmic behavior is due to the edge-vacancy of GNRs. The effects of edge-vacancy become more remarkable when the ribbon width becomes narrower in the future. However, the electronic transport properties of such narrow GNRs have not been clarified yet.

Most recently, we have theoretically explored the conductance fluctuation of semiconducting ED-GNRs and provided conclusive proof of such Anderson localization, in that the conductance histogram has a non-Gaussian log-normal shape when $L_c \gg \xi$ [8].

In this study, we have thoroughly investigated roughness concentration dependence and width dependence of localization length ξ.

2. Simulation method

Here, we have investigated electronic transport in edge-disordered armchair graphene nanoribbons (ED-AGNRs) and figure 1 shows a schematic illustration of the simulation model. We included the hydrogen atoms for passivation at the AGNR edge but they are not represented in Fig. 1 for simplicity. In the model, the edge disorder is expressed by the addition and removal of pairs of carbon atoms at the edges, and we chose these edge defects location randomly in a central region of length L_c.

The simulation method is based on Landauer's quantum transport theory combined with a tight-binding approximation and the non-equilibrium Green's function method [9]; all simulations were performed using ATK-SE (Ver.12.8.2) [10]. Slater-Koster parameters were selected for the carbon-carbon and carbon-hydrogen interactions [11]. ED-AGNRs ware calculated for 5,000 configurations of different edge defects locations. The 5,000 configurations were, then, selected randomly using the Mersenne-Twister algorithm [12].

3. Simulation result

In figures 2(a)-2(c), we represent the energy dependence of $\xi(\epsilon)$ for ED-AGNRs with W = 1.48, 2.21, and 2.95 nm and with various P, where P = 0.04 (filled circles), 0.06 (squares), 0.1 (diamonds), 0.2 (triangles), and 0.3 (open circles), 0.4 (open squares), 0.5 (open diamonds). The fermi level of the ϵ is chosen to be 0 eV (the middle of the energy band gap E_g) and the band gap decreases in almost inverse proportion to the ribbon width W, as is well known. At first, focusing P dependence of $\xi(\epsilon)$ with fixed W = 1.48 nm (Fig. 2(a)), $\xi(\epsilon)$ decreases monotonically with P for any energy. We also found similar behavior for other GNR widths W = 2.21 nm (Fig. 2(b)) and W = 2.95 nm (Fig. 2(c)). It caused by increasing the electron scattering rate with edge defects. Therefore these results are also reasonable. Next, we discuss the dependence of $\xi(\epsilon)$ on W. For example, with P = 0.04, as indicated by the filled circles in Figs. 2(a)-2(c), $\xi(\epsilon)$ increases with W for any energy. Similar behavior is observed for all P values. Typically, edge-scattering effects decrease as W increases. Therefore, these results are also reasonable

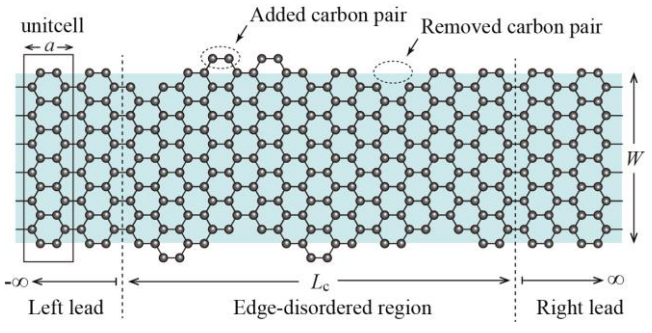

Fig. 1 Schematic illustration of an ED-GNR.

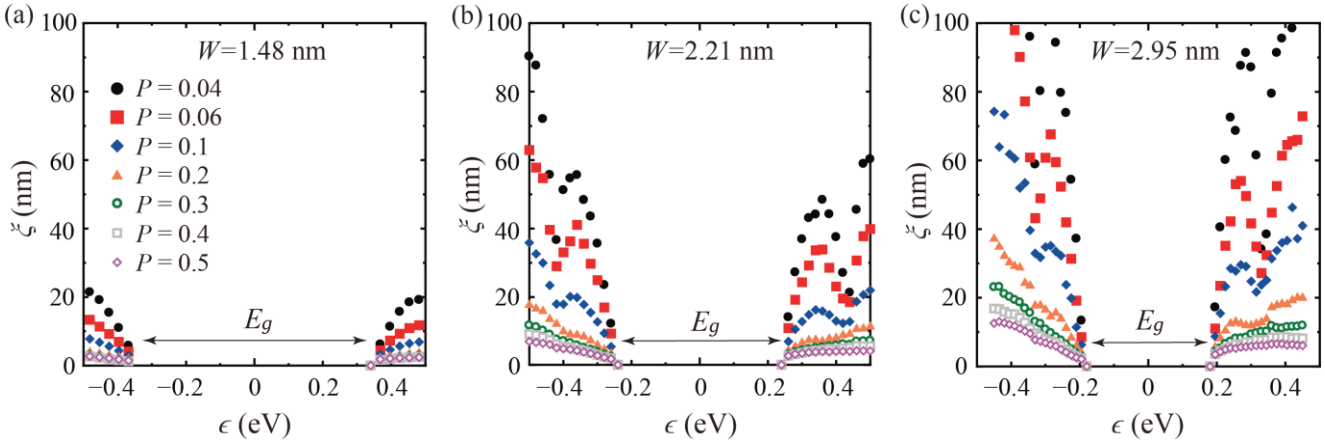

Fig. 2 Localization length $\xi(\epsilon)$ for ED-GNRs with three different widths of (a)W = 1.48, (b) 2.21, and (c) 2.95 nm and with various edge-disorder concentrations of P = 0.04 (filled circles), 0.06 (squares), 0.1 (diamonds), 0.2 (triangles), and 0.3 (open circles), 0.4 (open squares), 0.5 (open diamonds).

From the value of the $\xi(\epsilon)$ on various P and W, we can obtain essential information for the design of GNR-based FETs. We consider GNR-based FET which is L_c = 20 nm. The L_c length corresponds to the gate length of a current Si-MOSFET. If 1.48 nm-width ED-GNRs (or more narrow ED-GNRs) are used for the FETs, then the on-state cannot be realized, even if P is decreased to a small value of 0.04. It is because $\xi(\epsilon)$ is lower than or comparable to L_c set at 20 nm, as shown in Fig. 2(a). When $L_c \gg \xi$, electric flow dese not occur due to carrier localization [8]. While, in wider ED-GNR (Fig. 2(c), 2.95 nm-width), when the edge-defect concentration is less than approximately 10% ($P < 0.1$), because $\xi(\epsilon)$ becomes longer than L_c = 20 nm. ED-GNRs have potential for use as FET channels in that condition. In addition, the 2.95nm-width GNRs have a moderate energy gap of E_g = 0.4 eV. Therefore 2.95 nm-width GNR-based FETs with $P < 0.1$ could possibly even be operated at room temperature.

3. Conclusions

In summary, the localization length ξ, which can provide an essential information for designing graphene nanoribbons based field effect transistor, was investigated for various types of semiconducting edge-disordered armchair graphene nanoribbons (ED-AGNRs) using the non-equilibrium Green's function method combined with a tight-binding approximation. We have found that GNR-based FETs could operate even with edge disorder when and the width is 2.95 nm and the edge-defect concentration is less than approximately 10%, because ξ becomes longer than the GNR length of 20 nm. The same GNR-based FETs could operate even at room temperature because they have moderate energy gap for switching operation.

Acknowledgements

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References

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, Nature **438**, 197 (2005).

[2] A. K. Geim and K. S. Novoselov, Nat. Mat. **6**,183 (2007).

[3] M. Fujita, K. Wakabayashi, K. Nakada, and K. Kusakabe, J. Phys. Soc. Jpn. **65**, 1920 (1996).

[4] K. Nakada, F. Fujita, G. Dresselhaus, and M. S. Dresselhaus, Phys. Rev. B **54**, 17954 (1996).

[5] L. Jiao, X. Wang, G. Diankov, H. Wang, and H. Dai, Nano-tech. **5**, 321 (2010).

[6] P. B. Bennett, Z. Pedramrazi, A. Madani, Y.-C, Chen, D. G. de Oteyza, C. Chen, F. R. Fischer, M. F. Crommie, and J. Bokor, Appl. Phys. Lett. **103**, 253114 (2013).

[7] G. Xu, C. M. Torres, J. Tang, J. Bai, E. B. Song, Y. Huang, X. Duan, Y. Zhang, and K. L. Wang, Nano Lett., **11**, 1082 (2011).

[8] K. Takashima and T. Yamamoto, Appl. Phys. Lett. **104**, 093105 (2014).

[9]S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, England, 1995).

[10] K. Stokbro, D. E. Petersen, S. Smidstrup, A. Blom, M. Ipsen and K. Kaasbjerg, Phys. Rev. B **82**, 075420 (2010).

[11]P. Koskinen and V. M□akinen, Comput. Mater. Sci. **47**, 237 (2009).

[12]M. Matsumoto and T. Nishimura, ACM Transactions on Modeling and Computer Simulation **8**, 3 (1998).

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