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Controlling the transport gap of wedge-shaped graphene nanoconstriction by strain

Baihua Gong [a,b,*], Xin-Hui Zhang [c], Shengli Zhang [a,b]

[a] Department of Applied Physics, Xi'an Jiaotong University, Xi'an 710049, China
[b] MOE Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, Xi'an Jiaotong University, Xi'an 710049, China
[c] School of Science, Xi'an University of Architecture and Technology, Xi'an 710055, China

HIGHLIGHTS

- Numerical computation shows that wedge-shaped graphene nanoconstrictions (WGNCs) have a transport gap decreasingly dependent on the transverse strain.
- An analytical formula of the transport gap as a function of transverse strain is obtained confirming the numerical results.
- The transport gap is inversely proportional to the width of the WGNC, while having nothing to do with other geometry parameters.

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ABSTRACT

The Landauer transport theory is used to study the electron transmission of wedge-shaped graphene nanoconstrictions (WGNCs) under transverse strain. It is found that WGNCs have a transport gap decreasingly dependent on the strain. Further analysis shows that the strain dependence of the transport gap origins from the sensitiveness of confined states to strain. And on this basis, an analytical formula of the transport gap as a function of transverse strain is obtained confirming the numerical results. Our results suggest that WGNCs can be useful for the future graphene-based nanoelectromechanics.

1. Introduction

Apart from its excellent electronic properties, graphene has attracted much interest recently due to its exceptional mechanical performance [1–3]. Graphene has been confirmed as the strongest material being able to sustain as high as 30% strain [4], and recent experiments show that reversible and controlled strain can be produced in graphene with measurable impact on its electronic structure and transport properties [5–9]. These experimental works reveal the potential of strain in controlling graphene's electronic properties, offering a tempting prospect for the application of graphene in nanoelectromechanics.

Motivated by experimental progress, much theoretical research has been done to understand the underlying physics of strain effects on graphene's electronic properties, which is crucial to fabricate graphene-based nanoelectromechanical devices of customized functionality. Among other factors, edge shape plays an important role in the mechanism that strain modulates the electronic properties of graphene-based devices. For example, uniaxial strain modifies the band gap of armchair graphene nanoribbons (AGNRs) in a periodic way, while has little influence on the low-energy band structure of zigzag graphene nanoribbons (ZGNRs) [10]. This distinctness origins from the fact that the low-energy bands of ZGNRs are contributed by the edge states associated with the zigzag borders, which are robust against uniaxial strain. In this sense, it seems that ZGNRs, compared with AGNRs, are unsuitable to be used in graphene nanoelectromechanical devices [10–12].

In this paper, we propose that the insusceptibility of ZGNRs' electronic properties to strain can be overcome by etching the ZGNRs into wedge-shaped graphene nanoconstrictions (WGNCs), e.g., see Fig. 1. WGNCs have a transport gap where the conductance is totally suppressed [13], and moreover, we will show that this gap is monotonically dependent on transverse strain, i.e., compression enlarges the gap while tension reduces it. Further analysis reveals that the energy interval of transport gap of WGNCs is exactly identical

* Corresponding author.
E-mail address: baihuagong@mail.xjtu.edu.cn (B. Gong).

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to the energy interval of edge states of ZGNRs with the same width, indicating that in WGNCs edge states are totally reflected while confined states are partially transmitted. Thus the strain-dependence of transport gap of WGNCs can be deduced from the corresponding strain-dependence of energy bands of ZGNRs. The monotonic dependence of transport gap of WGNCs on strain has potential application in nanoelectromechanical devices, especially when a graphene-based transistor with a tunable on-off conductance ratio is needed.

The rest of the paper is organized in the following way. In Section 2, we introduce a tight-binding model for strained WGNCs and the computational method. We then present the main results and give a simple analysis of the dependence of WGNCs' transport gaps on transverse strain in Section 3. In the end, a brief summary is provided in Section 4.

2. Model and method

The geometry studied in this paper is schematically shown in Fig. 1, it consists of the left and right semi-infinite ZGNR leads, and the middle constriction region. Three vectors connecting A sites to B sites are

$$\vec{r}_1 = a(-\tfrac{\sqrt{3}}{2}, \tfrac{1}{2}), \quad \vec{r}_2 = a(\tfrac{\sqrt{3}}{2}, \tfrac{1}{2}), \quad \vec{r}_3 = a(0, -1), \tag{1}$$

where a is carbon–carbon bond length. A nearest-neighbor tight-binding model is employed here to describe the device

$$H = -\sum_{\langle i,j \rangle} t_{ij} a_i^+ a_j, \tag{2}$$

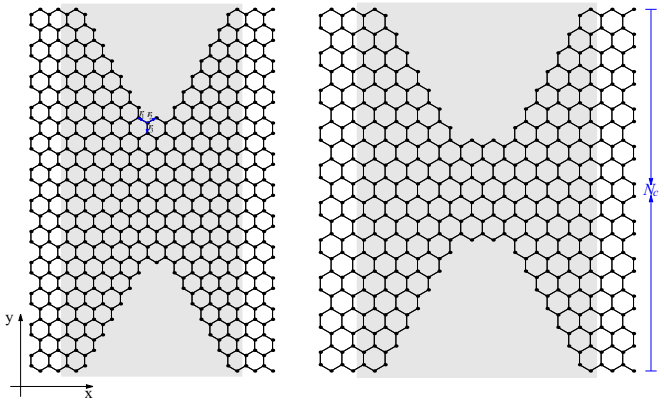

Fig. 1. Schematic diagram of two examples of WGNCs, where $\vec{r}_i$, $i=1, 2, 3$ are the nearest-neighbor vectors connecting A atoms to B atoms. The central scattering regions are indicated by the gray shadow. The width of the left structure is $N_c = 35a$ and that of the right one is $N_c = 29a$, where a is carbon–carbon bond length.

where t_{ij} is transfer integral between neighboring atoms i and j. The zero-temperature ground state of electrons at zigzag edges is spin-polarized [14], however, this spin-polarized state is unstable with respect to the spin-unpolarized states at finite temperature [15]. Hence we focus on the spin-unpolarized states in the following.

The uniaxial strain in graphene plane has a tensor form [16]

$$\boldsymbol{\epsilon} = \epsilon \begin{pmatrix} \cos^2\theta - \nu \sin^2\theta & (1+\nu)\cos\theta \sin\theta \\ (1+\nu)\cos\theta \sin\theta & \sin^2\theta - \nu \cos^2\theta \end{pmatrix}, \tag{3}$$

where θ is the direction of the strain with x-axial, and $\nu = 0.165$ is Poisson's ratio [17]. For transverse strain, θ equals $\pi/2$ and the strain tensor can be written as

$$\boldsymbol{\epsilon} = \epsilon \begin{pmatrix} -\nu & 0 \\ 0 & 1 \end{pmatrix}. \tag{4}$$

A general vector v_0 in the undeformed graphene plane has its deformed counterpart $v = (1+\boldsymbol{\epsilon}) \cdot v_0$, thus the three bond lengths under transverse strain (4) change into

$$\begin{cases} r_3 & \to (1+\epsilon) r_3 \\ r_{1,2} & \to \sqrt{\left[\cos\frac{\pi}{3}(1+\epsilon)\right]^2 + \left[\sin\frac{\pi}{3}(1-\nu\epsilon)\right]^2}\, r_{1,2} \end{cases}. \tag{5}$$

The change of the bond lengths results in variation of the hoping energies, which can be modeled by the inverse-square relation $t_i = t/(r_i/a)^2$ [18], where t is the hopping energy of the unstrained bond.

For calculating electron transport in nanometer-sized devices, the natural framework is the Landauer formula which relates the conductance $G(E)$ to the transmission $T(E)$ [19]

$$G(E) = \frac{2e^2}{h} T(E), \tag{6}$$

where $T(E) = \sum T_i(E)$ is the total transmission at energy E and is equal to the sum of the transmission probabilities across every conducting eigenchannel. When scattering is absent, i.e., $T_i(E) = 1$ for each i, the total conductance becomes $N(2e^2/h)$, where N is the total number of eigenchannels that are conducting the electrons of energy E. We calculate $T(E)$ in terms of the recursive Green's function method which provides high efficiency and accuracy for numerical calculations.

3. Results and analysis

In Fig. 2, we present the transmission curves of WGNCs, compared with those of ZGNRs with the same width. From this figure, it is clear that electron transmission is globally suppressed

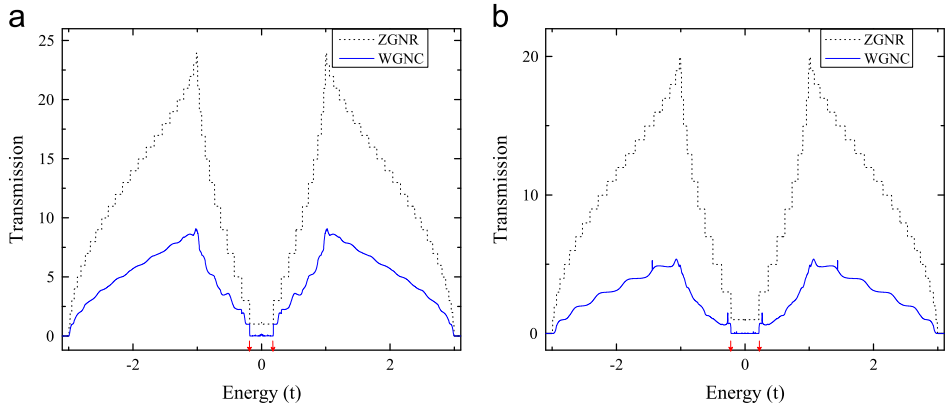

Fig. 2. Transmission curves of WGNCs and ZGNRs with the same width: (a) $N_c = 35a$ and (b) $N_c = 29a$. Arrows in the figure indicate the energy intervals of the transport gaps of WGNCs as well as those of edges states of ZGNRs.