Solid State Communications 202 (2015) 39–42

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Semiconductor–metal and metal–semiconductor transitions in twisting graphene nanoribbons

Ning Xu [a,*], Bolong Huang [b], Jianfu Li [b], Baolin Wang [a,*]

[a] Department of Physics, Yancheng Institute of Technology, Yancheng 224051, Jiangsu, China
[b] Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, Hong Kong, Hong Kong

ARTICLE INFO

Article history:
Received 1 September 2014
Received in revised form
7 October 2014
Accepted 14 October 2014
Communicated by E.L. Ivchenko
Available online 11 November 2014

Keywords:
Graphene nanoribbons
Transport properties

ABSTRACT

The electronic structure and transport properties of twisting graphene nanoribbons (TGNRs) are systematically investigated using the tight-binding model and the non-equilibrium Green's function method. We show that the energy gap and conductance around the Fermi energy can be reversibly modulated. Armchair TGNRs (ATGNRs) can be either metallic or semiconducting depending on the widths and the twist angles of the GNRs. Semiconductor–metal and metal–semiconductor transitions are observed in ATGNRs for $N=3i+1$ (where i is an integer and N is the number of atoms along the width of the nanoribbon) and $N=3i+2$, respectively. Narrow ATGNRs are semiconductors for $N=3i$, whereas zigzag TGNRs (ZTGNRs) are metallic regardless of the width and distortion of the GNRs.

1. Introduction

Graphene was first created in experiments in 2004 and become known for exhibiting unusual properties, such as electrons that behave as massless relativistic Dirac fermions [1], carriers with high-speed mobility [2,3], a room-temperature quantized Hall effect [2,3], a high mechanical strength [4], and unique electrical supercurrent properties [5]. Graphene can support Cooper pair transport, which results in the well-known Josephson effects [6]. All of these properties make graphene an important potential candidate for nanoelectronic applications.

Recently, quasi-one-dimensional graphene nanoribbons (GNRs) have attracted considerable attention because of their promising potential as elementary building blocks for nanoelectronic and spintronic applications. These GNRs have been prepared by mechanically cutting exfoliated graphene [7,8], unzipping single-walled nanotubes along the graphene axis [9,10], or patterning epitaxially grown graphene [11,12]. The electronic structures of GNRs with different edge shapes can be modulated by imposing hard-wall boundary conditions on the Schrödinger equation within the single π tight-binding model or on the Dirac equation for a two-dimensional massless particle [13–16]. The results indicate that GNRs with armchair-shaped edges can exhibit either metallic or semiconducting behavior depending on the GNR width and that GNRs with zigzag-shaped edges exhibit metallic behavior with unusual edge states on both sides of the ribbon regardless of the GNR width.

The physical properties of graphene, such as its broadband optical response, thermal conductance, and electronic structure, are generally known to depend strongly on the geometrical structure of graphene, which can be deformed because of the flexibility of graphene. Therefore, the geometry-dependent physical properties of various graphene structures have been recently explored [17–21].

In the present study, the geometry-dependent electronic properties of twisting graphene nanoribbons (TGNRs) are investigated using the tight-binding model and the non-equilibrium Green's function method [22,23]. GNRs with armchair-shaped edges and GNRs with zigzag-shaped edges on both sides can be conventionally classified in terms of the number N [15], as shown in Fig. 1. Semiconductor–metal and metal–semiconductor transitions are observed in armchair TGNRs for $N=3i+1$ (where i is an integer) and $N=3i+2$, respectively. The zigzag TGNRs are metallic, whereas the armchair TGNRs are semiconductors for $N=3i$. We used the aforementioned results to develop an armchair-TGNR-based metal–semiconductor modulator that performs analogous operations to those of a rheostat in electronic circuits.

2. Model and method

A planar GNR can be twisted along its central symmetrical axis (i.e., the x-axis) to produce two types of TGNRs. We denote an armchair TGNR of width N as an N-ATGNR and a zigzag TGNR of width N as an N-ZTGNR. The twist angle for a unit cell is denoted by $\theta=2\pi/p$, where

* Corresponding authors. Tel.: +86 51588298271; fax: +86 51588168221.
E-mail addresses: nxu@ycit.cn (N. Xu), blwang@pub.hy.jsinfo.net (B. Wang).

http://dx.doi.org/10.1016/j.ssc.2014.10.015
0038-1098/

a fixed cycle length of the TGNRs includes p unit cells of planar GNRs, and α denotes the twist angle of the TGNRs. Fig. 1 is the structural model of a 10-ATGNR with $\theta=2\pi/56$. In this calculation, the maximum distance between two near-neighbor atoms is restricted to 1.9 angstroms. Thus, the electronic properties of TGNRs can be effectively described using a single-π orbital. The electron mean-free path in graphene is much longer than the size of a TGNR; thus, electron–electron and electron–phonon interactions are neglected here. Throughout this paper, we assume that the dangling bonds on the edge sites are terminated by hydrogen atoms and that these bonds do not contribute to the electronic state around the Fermi level.

The tight-binding Hamiltonian of the system can be written as

$$H=\sum_i \varepsilon_i c_i^+ c_i+\sum_{i,j}\gamma_0 f(r_{ij})c_i^+ c_j, \tag{1}$$

where ε_i denotes the on-site potential. The hopping parameter $\gamma_0=-2.7$ eV and is modified by the factor $f(r_{ij})=e^{-3.37(r_{ij}/a_0-1)}$ [24] (r_{ij} is the distance between the i and j atoms and $a_0=1.42$ Å). The creation and annihilation operators at sites i and j are denoted by $\{c_i^+, c_j\}$, respectively. The transmission coefficient between the left and right leads can be calculated using [22,23]

$$T=Tr(\Gamma_L G^r \Gamma_R G^a), \tag{2}$$

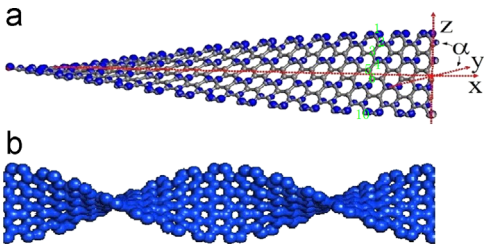

Fig. 1. (a) Structural model of a 10-ATGNR with $\theta=2\pi/56$: the ribbon is assumed to be infinite in the x-direction; carbon atoms are depicted as gray balls, and blue balls denote the spatially resolved LDOS of the ATGNR at the Fermi energy ($\alpha=\pi/2$); (b) spatially resolved LDOS for the 10-ATGNR for $\theta=2\pi/14$ at the Fermi energy ($\alpha=2\pi$). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

where $\Gamma_{L(R)}=i[\Gamma^{\dagger}_{L(R)}-\Gamma_{L(R)}]$ denotes the coupling of the device to the left and right leads. $G^{r,a}$ are the retarded and advanced Green's function matrices of the device, respectively. From Landauer theory, the conductance G through the central sample is given by $G=(2e^2/h)T$. The density of states (DOS) of the corrugated GNRs is calculated using the formula $\mathrm{DOS}=-(1/\pi)\mathrm{Im}[TrG^r(E)]$.

The generalized Landauer approach can be used to derive the tunneling current as

$$I=\frac{2e}{\hbar}\int dET(E)[f_1(E-u_L)-f_2(E-u_R)], \tag{3}$$

where the factor of 2 accounts for degeneracy, and $f_1(E-u_L)$ and $f_2(E-u_R)$ are the Fermi energy functions of the incident waves from the two leads to the TGNRs. Note that the objective of this study is only to calculate the phase-coherent transmission coefficient. Therefore, the effect of electron–phonon interaction can be neglected, and the temperature dependence only arises from the Fermi factors of the electrons.

3. Results and discussions

First, we compute the band gaps of the armchair GNRs as a function of the ribbon width N, as shown in Fig. 2(a). The variation in the band gaps exhibits two distinct types of behavior, which is similar to that reported in Ref. [16]. An armchair GNR is shown to be semiconducting for $N=3i$ and $N=3i+1$; otherwise, the armchair GNR is metallic. The band gaps of the semiconducting GNRs decay exponentially with increasing width. Incorporating the twist effect results in three well-separated categories (or families of structures) of band gaps as a function of θ, as shown in Fig. 2(b)–(d). The energy gap of an N-ATGNR for $N=3i$ first increases and then decreases with increasing θ. A narrow N-ATGNR behaves as a semiconductor for $N=3i$. The trends of the band gaps shown in Fig. 2(b) are used to predict a semiconductor–metal transition for wide ATGNRs with increasing θ. Fig. 2(c) and (d) show that the semiconductor–metal–semiconductor and metal–semiconductor

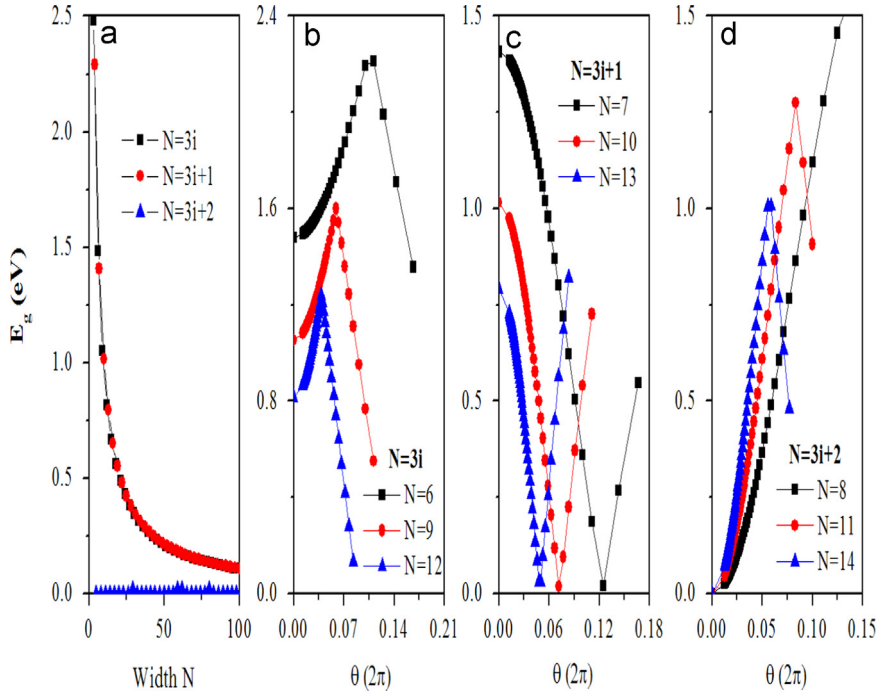

Fig. 2. Variation in band gaps of ATGNRs for various N versus twist angle θ, as obtained from tight-binding calculations for $t=3$ eV: (a) $N=3i$, (b) $N=3i+1$, and (c) $N=3i+2$.