



Electronic transport through a silicene-based zigzag and armchair junction

Dace Zha^a, Changpeng Chen^{a,b,*}, Jinping Wu^b

^a School of science, Wuhan University of Technology, Wuhan 430070 PR China

^b Material Science and Chemistry Engineering College, China University of Geosciences, Wuhan, 430074, PR China

ARTICLE INFO

Article history:

Received 15 May 2015

Received in revised form

15 June 2015

Accepted 18 June 2015

Communicated by Y.E. Lozovik

Available online 26 June 2015

Keywords:

A. Silicene nanoribbons

A. Zigzag and armchair junction

D. Negative differential resistance

D. Transport properties

ABSTRACT

Using density functional theory and non-equilibrium Green's function technique, we performed theoretical investigations on the transport properties of several ZAZ SiNRs junctions (a similar kind of silicene molecules junction combined by zigzag and armchair silicene nanoribbons). It is found that the differential conductances of the three systems decrease with an order of 5-ZAZ > 4-ZAZ > 3-ZAZ. Particularly, the Negative differential resistance (NDR) can be observed within certain bias voltage range only in 3-ZAZ SiNRs. In order to elucidate the mechanism the NDR behavior, the transmission spectra and molecular projected self-consistent Hamiltonian (MPSH) states are discussed in details.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

During the past decades, progress in micro-fabrication and self-assembly techniques [1] has made it possible to design molecular devices. A number of molecular devices have shown their peculiar current–voltage (*I*–*V*) properties, such as negative differential resistance (NDR) [2,3], rectification [4], and current switch [3,5], etc. On the other hand, recent advances in controllable synthesis and characterization of nanoscale materials, have opened up important possibilities for the investigation of ultra-thin 2D systems. The nanoribbons of graphene, MoS₂, BN etc. are found to possess variety of unusual properties which can be utilized in molecular devices [6–8]. The excellent research success of graphene has led to the investigation of other honeycomb monolayers composed of group IV elements, such as silicene, germanene, etc. Silicon, as an element resides in the same column of the periodic table with carbon, has recently attracted increasingly concern for its existence of a honeycomb monolayer [9]. As is well known, Silicon owns four valence electrons as carbon does, having many similar characters to carbon. However, Si also possesses some unique properties that carbon has not. Recent theoretical and experimental studies have shown that different from graphene, silicene is not planar but has a low-buckled honeycomb structure with buckled height of about 0.44 Å for stability [10–12]. The underlying reason is that silicene's sp³ hybridization is more stable than its sp² form [13,14]. Similar to graphene

nanoribbons (GNRs), silicene nanoribbons (SiNRs) also have two kinds of shapes: zigzag and armchair. Studies show that armchair SiNRs exhibit semiconductor behavior while zigzag SiNRs have stable anti ferromagnetic states [15–19]. The hydrogen-terminated GNR with either armchair- or zigzag-shaped edges has an energy gap which can be tuned by width or edge shape and shows interesting 3n rule, which was shown theoretically by Son et al. [20] and confirmed experimentally by Li et al. [21] and Ritter et al. [22]. As is well known, a transistor can potentially be made by using zigzag nanoribbon as source and drain and a semiconductor armchair nanoribbon as the channel on the same graphene layer [23,24]. So, it is naturally for one to consider a similar kind of silicene molecules junction combined by zigzag and armchair silicene nanoribbons, which is called ZAZ SiNRs junction (shown in Fig. 1).

In this present work, we study the electron transmission through the connections between zigzag SiNRs and armchair SiNRs using the nonequilibrium Green's function (NEGF) methodology. It is found that some interesting properties exist in certain kind of N-ZAZ SiNRs, such as negative differential resistance (NDR), which offer important insights into the potential application of SiNRs as both transistors and interconnects.

2. Model and method

The optimized geometric structure of ZAZ SiNRs is illustrated in Fig. 1. The N-ZAZ SiNRs are named after the number of the dimer lines across the ribbons width for the ZAZ SiNRs edges. The structures were optimized and the quantum transport calculations

* Corresponding author at: Wuhan university of Technology, School of Science, Luoshi Road, Wuhan 430070, China. Tel.: +862787391720

E-mail address: 16941612@qq.com (C. Chen).

2. Model and method

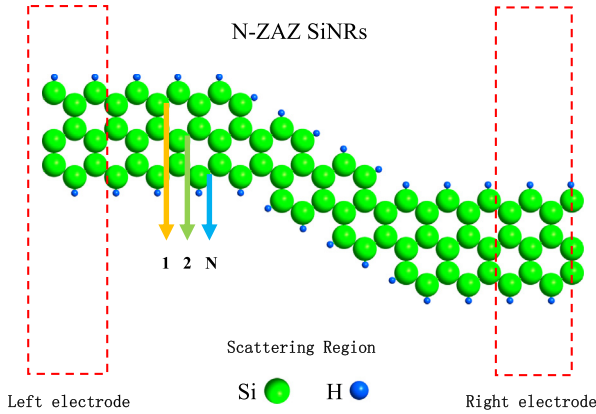


Fig. 1. The structure of the two-probe system of N-ZAZ SiNRs from top view. The N-ZAZ SiNRs are named after the number of the dimer lines across the ribbons width for the ZAZ SiNRs edges.

were carried out by the Atomistix ToolKit (ATK) package [25,26], which bases on the fully self-consistent non-equilibrium Green's functions and the density functional theory. Under external bias, the current through a molecular junction is calculated from the Landauer–Büttiker formula:

$$I(V) = 2e/h \int [f_L(E - \mu_L) - f_R(E - \mu_R)] T(E, V) dE$$

where $f_{L/R}$ is the Fermi–Dirac distribution for the left (L) and right (R) electrodes, $\mu_{L/R}$ is the electrochemical potential of the left (L) or right (R) electrodes and $T(E, V)$ is the transmission coefficient at energy E and bias voltage V .

$$T(E, V) = \text{Tr}[\Gamma_L(E, V) G^R(E, V) \Gamma_R(E, V) G^A(E, V)]$$

where $G^{R/A}$ are the retarded and advanced Green's functions, and coupling functions $\Gamma_{L/R}$ are the imaginary parts of the left and right self-energies, respectively. Self energy depends on the surface Green's functions of the electrode regions and comes from the nearest-neighbor interaction between the extended molecule region and the electrodes. For the system at equilibrium, the conductance G is evaluated by the transmission function $T(E)$ at the Fermi level (FL) E_F of the system: $G = G_0 T(E_F)$, where $G_0 = 2e^2/h$ is the quantum unit of conductance, and h is Planck's constant and e is the electron charge.

The geometric optimization and transport properties are calculated by ATK within local density approximation for exchange–correlation potential. The exchange correlation functional is set as local-density approximation (LDA) in the PerdewZunger (PZ) form. To save computational time of the transport calculations, a mesh cutoff is set to be 150 Ry and the Monkhorst–Pack ($1 \times 1 \times 100$) K-point grid is used. The basis set is adopted for elements of systems and the convergence criterion is 10^{-4} Hartree for the total energy. Test calculations with the larger basis set size, larger cutoff energy, and dense K-point (i.e. $3 \times 3 \times 100$) are also performed, which give similar results.

3. The transport properties of N-ZAZ SiNRs

The I – V characteristics of 3-ZAZ SiNRs, 4-ZAZ SiNRs and 5-ZAZ SiNRs in the range of [0 V, 0.6 V] are calculated in Fig. 2. It can be found that the 5-ZAZ SiNRs show the metal behavior and the I – V curve displays a linear behavior at a bias voltage. The current through the three systems decrease with an order of 5-ZAZ > 4-ZAZ > 3-ZAZ. In particular, the current through 5-ZAZ is much higher than that through 3-ZAZ under the same applied bias. This

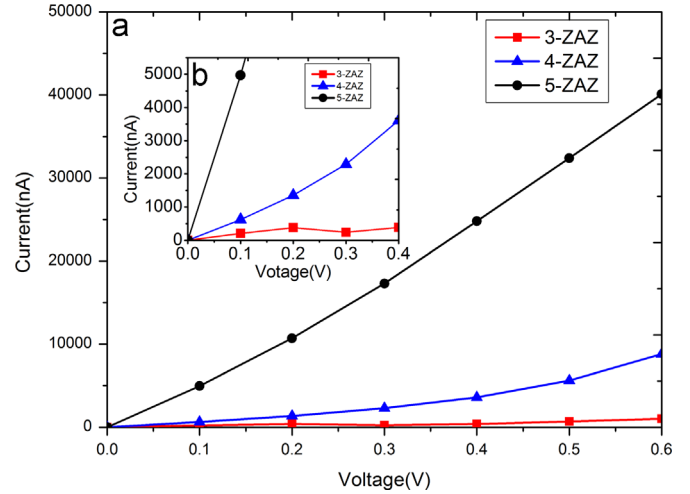


Fig. 2. The currents as functions of the applied bias for N-ZAZ SiNRs. The inset shows the local expansion for lower bias range.

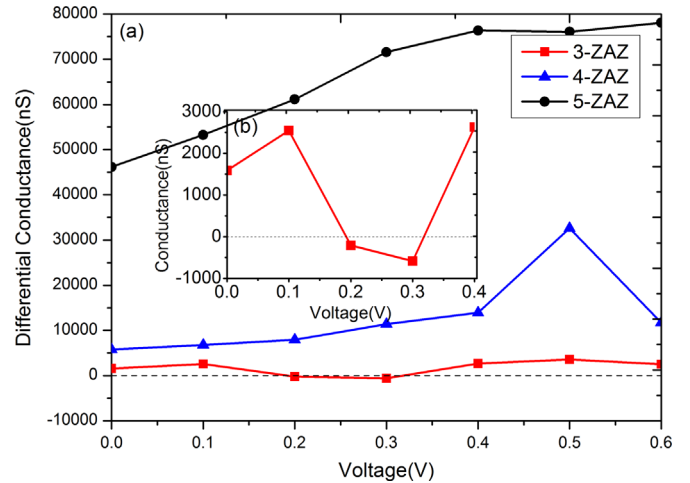


Fig. 3. Differential conductance–Voltage curves of N-ZAZ SiNRs. The inset shows the local expansion for lower bias range in 3-ZAZ SiNRs.

means that 3-ZAZ can weaken the electron transport at the same bias voltage. In addition, when the bias takes a value between 0.1 V and 0.3 V, the current of 3-ZAZ SiNRs shows NDR behavior in the bias range. When $V > 0.4$ V, the currents rapidly increase with bias voltage. However, the currents of 4-ZAZ SiNRs and 5-ZAZ SiNRs always increase with bias voltage. The NDR behaviors for 4-ZAZ SiNRs and 5-ZAZ SiNRs are not found. In Fig. 3(a), we plot the corresponding conductance (dI/dV) curves for 3-ZAZ SiNRs, 4-ZAZ SiNRs and 5-ZAZ SiNRs. Under zero bias, the conductance of 3-ZAZ SiNRs, 4-ZAZ SiNRs and 5-ZAZ SiNRs is 1.59×10^3 nS, 5.57×10^3 nS, and 4.62×10^4 nS, respectively. The differential conductance of 4-ZAZ SiNRs and 5-ZAZ SiNRs first increases with the applied bias increasing, which means that the corresponding transmission channels are opened and make contributions to the electronic transport. However, as for 3-ZAZ structure, the differential conductance is depressed in comparison with that of 4-ZAZ and 5-ZAZ structure, which indicates that 3-ZAZ depress the transport properties. Especially, the negative value of conductance can be found in bias range of [0.2 V, 0.3 V] for 3-ZAZ SiNRs, which matches well with I – V curves for the explored bias region.

The characteristic of I – V depends on the transmission spectrum of zero bias when the external bias is very low. The transmission spectra $T(E, V)$ of N-ZAZ SiNRs is calculated under zero bias voltage in Fig. 4. We can clearly see that there are strong transmissions for

Download English Version:

<https://daneshyari.com/en/article/1591481>

Download Persian Version:

<https://daneshyari.com/article/1591481>

[Daneshyari.com](https://daneshyari.com)