Physics Letters A 380 (2016) 282–287

Contents lists available at ScienceDirect

Physics Letters A

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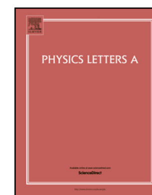

Tunable electronic and transport properties for ultranarrow armchair-edge silicene nanoribbons under spin–orbit coupling and perpendicular electric field

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ARTICLE INFO

Article history:
Received 8 August 2015
Received in revised form 25 September 2015
Accepted 28 September 2015
Available online 13 October 2015
Communicated by R. Wu

Keywords:
Electronic structure
Transport property
Spin–orbit coupling
Perpendicular electric field
ASiNR
NEGF

ABSTRACT

The electronic and transport properties for armchair-edge silicene nanoribbons (ASiNR) with effective spin–orbit coupling and potential energy were investigated by using the non-equilibrium Green's function method. The energy gaps and the conductance for ASiNRs can be effectively modulated by effective spin–orbit coupling λ_{SO} and the potential energy V_0. With increasing λ_{SO}, the energy gap for 6-ASiNR and 7-ASiNR decreases, while it remains zero for metallic 8-ASiNR. Interestingly, an energy gap appears for 8-ASiNR in presence of V_0, which results in the appearance of a conductance gap for 8-ASiNR system. Additionally, the dependence of conductance on Anderson disorder strength has been studied.
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1. Introduction

Silicene, a monolayer of silicon atoms forming a two-dimensional honeycomb lattice, has been synthesized [1–5] and attracts much attention [6–10]. Almost every striking property of graphene could be transferred to this innovative material. However, silicene has a buckled structure and its relatively strong spin–orbit coupling (SOC) opens a gap between the conduction and valence bands. Facilitated by this buckling, the band-gap edges of silicene are split by an external perpendicular electric field [7]. Furthermore, silicene has the advantage with its easy incorporation into modern silicon-based electronic technology. This advantage with the dissipationless spin currents may make the silicene particularly attracting for technological applications in spintronics [11,12].

On the other hand, silicene nanoribbons (SiNRs) have been synthesized on Ag(110) and (100) surfaces [13–15]. Theoretical studies have been performed on the electronic properties of SiNRs. For example, Yi Ding and Jun Ni have investigated that the gap of armchair-edge SiNR (ASiNR) oscillates with a period of 3 dimers as nanoribbon width is increasing, and the zigzag-edge SiNR (ZSiNR) becomes half metal under a transverse electric field [16]. Based on the first-principles calculation, Dong et al. have found that Stone–Wales defects can make semiconducting ZSiNRs become metallic or half-metallic [17]. An et al. have studied the interplay between the edge and bulk states induced by the Rashba SOC for a ZSiNR [18]. Furthermore, the transport properties for ZSiNRs have been studied vastly. Kang et al. have found that ZSiNRs show symmetry-dependent transport property similar to those of zigzag graphene nanoribbons (ZGNRs) [19]. Giant magnetoresistance in a ZSiNR connecting to two silicene sheets has been predicted by Xu et al. [20]. Tsai and collaborators have predicted that a gated silicene quantum point contact can be used as a tunable spin polarizer with 98 percent spin polarization [12]. Using non-equilibrium Green's function, Farokhnezhad et al. have found that complete spin polarization can take place in the presence of perpendicular electric field for anti-parallel configuration and the nanoribbon can work as a perfect spin filter [21]. However, the previous works on electronic and transport properties through a silicene-based system are mainly focused on ZSiNR systems [17–21]. Investigation

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http://dx.doi.org/10.1016/j.physleta.2015.09.054
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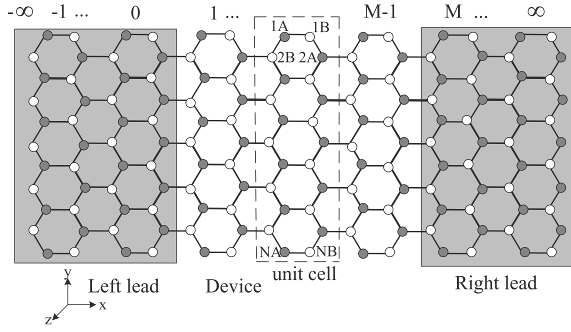

Fig. 1. An ideal ASiNR with width $N = 11$ is connected to planar silicene nanoribbons as left and right leads (gray areas). A unit cell of an ASiNR represented by dashed lines contains $2n$ numbers of lattice sites labeled as 1A, 1B, $\cdots$, NA, NB.

of the electronic and transport properties that are modified by the spin–orbit interaction as well as the perpendicular electric field in ASiNR systems is sparsely reported, and it is intriguing to investigate how these properties are modified by the spin–orbit interaction and the perpendicular electric field [22,23]. Here, we address this issue.

In this paper, we present a comprehensive investigation of the electronic and transport properties for a ASiNR system under effective SOC and potential energy. By using the non-equilibrium Green's function (NEGF) method combined with the tight-binding approximation, the dependence of energy band gap and conductance for the systems on the effective SOC λ_{SO} and the potential energy V_0 has been calculated. Further, the dependence of conductance on the Anderson disorder strengths has been examined. It is demonstrated that the energy gaps for semiconducting ASiNRs are sensitive to the effective SOC λ_{SO} and the potential energy V_0. With increasing λ_{SO}, the energy gaps for semiconducting 6-ASiNR and 7-ASiNR systems decrease, while the energy gap remains zero for metallic 8-ASiNR system. On the contrary, the energy gaps for 6-ASiNR and 7-ASiNR systems increase when V_0 increases. Interestingly, an energy gap appears in presence of V_0 for 8-ASiNR system, and it is dramatically enlarged with increasing the potential energy V_0. Furthermore, the conductance for three systems strongly depends on the effective SOC and the potential energy because the energy band structures can be effectively modulated by λ_{SO} and V_0. Moreover, the conductance plateaus for three systems can survive for small and moderate Anderson disorder strengths, but they can be strongly suppressed for larger disorder strengths.

2. Model and method

The device model considered here is an ASiNR divided into three regions (Fig. 1): the device region, the left lead and the right lead, where the armchair silicene sheet is located in the xy-plane and an electric field is perpendicularly applied to the plane. We use N, the number of $A(B)$-site atoms in a unit cell, to denote ASiNR with different width. The ribbon with N Si–Si chains is labeled by N-ASiNR. Here, the three typical numbers (6, 7 and 8) of N are chosen only to make N in the forms $3n$, $3n+1$ and $3n+2$ with positive integer n since the energy band structures of ASiNRs are highly sensitive to these typical ribbon widths [16], which is similar to that of armchair graphene nanoribbon [24]. The hard-wall condition is imposed on the edges of the ASiNR.

The total Hamiltonian for the system considered reads

$$H = H_C + H_L + H_R + H_{T\alpha}, \tag{1}$$

where H_C describes the device region, $H_{L(R)}$ is the Hamiltonian for the left (right) ASiNR lead, and $H_{T\alpha}$ ($\alpha = L/R$) for the coupling between central device region and leads. We assume that the electric field and the disorder exist only in the central device region. Here, the SOC are included for calculation of the self energies. In the tight-binding approximation, these partial Hamiltonians can be respectively written as following [6,7]:

$$\begin{aligned} H_C = &\sum_{is,i\in C}(\epsilon_C + w_i)c_{is}^\dagger c_{is} - t\sum_{\langle ij\rangle s(i,j)\in C} c_{is}^\dagger c_{js} \\ &+ \mathrm{i}\sum_{\ll ij\gg ss'(i,j)\in C}\frac{\lambda_{SO}}{3\sqrt{3}}v_{ij}c_{is}^\dagger \sigma_{ss'}^z c_{js'} \\ &- \mathrm{i}\frac{2}{3}\lambda_R\sum_{\ll ij\gg ss'(i,j)\in C}\mu_{ij}c_{is}^\dagger(\boldsymbol{\sigma}\times \boldsymbol{d}_{ij}^0)_{ss'}^z c_{js'} \\ &+ e\ell E_Z\sum_{is,i\in C}\zeta_i c_{is}^\dagger c_{is}, \end{aligned}$$

$$\begin{aligned} H_{\alpha=L,R} = &-t_\alpha\sum_{\langle ijs\rangle(i,j)\in\alpha} c_{is}^\dagger c_{js} + \mathrm{i}\sum_{\ll ij\gg ss'(i,j)\in\alpha}\frac{\lambda_{SO}}{3\sqrt{3}}v_{ij}c_{is}^\dagger\sigma_{ss'}^z c_{js'} \\ &- \mathrm{i}\frac{2}{3}\lambda_R\sum_{\ll ij\gg ss'(i,j)\in\alpha}\mu_{ij}c_{is}^\dagger(\boldsymbol{\sigma}\times\boldsymbol{d}_{ij}^0)_{ss'}^z c_{js'}, \end{aligned}$$

$$\begin{aligned} H_{T\alpha} = &-t\sum_{\langle ij\rangle s(i\in C,j\in\alpha)} c_{is}^\dagger c_{js} + \mathrm{i}\sum_{\ll ij\gg ss'(i\in C,j\in\alpha)}\frac{\lambda_{SO}}{3\sqrt{3}}v_{ij}c_{is}^\dagger\sigma_{ss'}^z c_{js'} \\ &- \mathrm{i}\frac{2}{3}\lambda_R\sum_{\ll ij\gg ss'(i\in C,j\in\alpha)}\mu_{ij}c_{is}^\dagger(\boldsymbol{\sigma}\times\boldsymbol{d}_{ij}^0)_{ss'}^z c_{js'}, \end{aligned}$$

where $c_{is}^\dagger$ (c_{is}) create (annihilate) an electron with spin s at site i. $\langle ij\rangle$ stands for the nearest-neighbor pair, and $\ll ij \gg$ stands for the next-nearest neighbor pair. The effective SOC parameter and the Rashba SOC parameter are $\lambda_{SO} = 3.9$ meV and $\lambda_R = 0.7$ meV [7]. $\boldsymbol{\sigma} = (\sigma_x \quad \sigma_y \quad \sigma_z)$ is the Pauli matrix. ϵ_C is the on-site energy in the center region. The nearest-neighbor hopping energy is $t = t_\alpha = 1.6$ eV. v_{ij} is defined as $v_{ij} = (\boldsymbol{d}_i \times \boldsymbol{d}_j)/\mid \boldsymbol{d}_i \times \boldsymbol{d}_j \mid$ with $\boldsymbol{d}_i$ and $\boldsymbol{d}_j$ the two bonds connecting the next-nearest neighbors $\boldsymbol{d}_{ij}$, $\mu_{ij} = \pm 1$ for the A (B) site, and $\boldsymbol{d}_{ij}^0 = \boldsymbol{d}_{ij}/\mid \boldsymbol{d}_{ij} \mid$. $\zeta_i = \pm 1$ for the A (B) site and $2\ell = 0.46$ Å is buckling distance. When a perpendicular electric field E_Z is applied, a voltage energy $V_0 = 2e\ell E_Z$ is created between the two sublattices, so the dependence on E_Z is also referred to in the following as V_0 dependence. In the presence of Anderson disorder in the central region, the on-site disorder energy w_i, uniformly distributed in $[-W/2, W/2]$, is nonzero in the central region with the disorder strength W.

In what follows we show how to calculate the band structure and the conductance of the ASiNRs. Actually, the overall configuration of this system shown in Fig. 1 can be considered as a linear chain of iterative cells whose unit cell contains $2N$ silicon atoms. The cells forming the left lead are located at sites $-\infty, \ldots, -1, 0$ of the chain; likewise, those for the central device region are placed at $1, \ldots, M-1$ and for the right lead at $M, M+1, \ldots, \infty$. The electron wave vector k along the ribbon is a good quantum number if the bulk periodicity parallel to these armchair cells is preserved. This assumption provides a straightforward way to calculate the band structure within the tight-binding model. By applying Bloch's theorem, the k-dependent Hamiltonian can be written as [25]

$$H_0 = H_{0,0} + H_{0,1}e^{ika} + H_{-1,0}e^{-ika}, \tag{2}$$

where $H_{0,0}$ is a unit cell Hamiltonian matrix at site 0 of the chain, $H_{0,1}$ ($H_{-1,0}$) are the coupling matrices with the right-hand (left-hand) adjacent cells, and a is the length between two nearest-neighbor unit cells. The above Hamiltonian can be diagonalized to yield the energy band structure according to Schrödinger equation $H_0\psi_{nk} = E_{nk}\psi_{nk}$, where the Block state ψ_{nk} is a column vector in

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