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Tuning spin-filtering, rectifying, and negative differential resistance by hydrogenation on topological edge defects of zigzag silicene nanoribbons

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ABSTRACT

By first-principles calculations, we propose three heterojunction nanodevices based on zigzag silicene nanoribbons with different edge-hydrogenated topological line defects. The devices all present excellent spin-filtering properties with 100% spin polarization as well as remarkable rectifying effect (with rectification ratio around 10^2) and negative differential resistance behaviors. Our findings shed new light on the design of silicon-based nanodevices with intriguing spintronic applications.

1. Introduction

Silicene has been successfully fabricated on several substrate surfaces (Ag [1–3], Ir [4], ZrB_2 [5]), in which, silicon atoms compose two-dimensional (2D) honeycomb lattice, similar to the geometric structure of graphene. Interestingly, silicene has a slightly buckled geometric feature [6,7] originating from the mixing sp^2/sp^3 hybridizations due to the longer Si–Si bonding distance. However, silicene is expected to be more compatible with the conventional semiconductor industry than other Dirac materials. In particular, silicene nanoribbons (SiNRs), the one-dimensional derivative of silicene, have attracted extensive attention in both experiment and theory [8–11] because of their intriguing electronic properties as a function of nanoribbon width, chiralities, and edge structures. Increasing numbers of investigations have been focused on zigzag-edged silicene nanoribbons (ZSiNRs) owing to its potential applications in spintronics. Many intriguing phenomena were discovered in ZSiNR-based devices, such as spin-filtering effect (SFE) [12–14], negative differential resistance (NDR) [14–18], current rectification [12], and magnetoresistance [19].

Similar to bulk materials, silicene is grown with various imperfections, such as point defects [20,21] (vacancies and adatoms) and line defects [22–25]. These defects may severely affect the electronic, magnetic, and transport properties of the sheets or ribbons [26,27]. The line defects are of topological nature that is robust to the local geometrical rearrangements. Many efforts have been devoted to the modulation of topological line defects [28–31]. By generating the grain boundaries with strain (or other methods), one can make different kinds of line defects embedded in silicene, such as an octagon plus two paired pentagons (558 defect) or a pentagon plus a heptagon (57 defect) in each unit cell [32,33]. The defects do not change the geometric structure, but alter the electronic properties of the nanoribbons. As such, the design of line-defect-based electronic nanodevices is of practical importance for the development of nanoelectronics.

On the other hand, the edge states in SiNRs also play a critical role for the transport properties. Tuning the edge states can dramatically modify the electronic and magnetic properties of SiNRs [34–37]. It was demonstrated that edge hydrogenation represents an efficient method for tailoring the characteristics of

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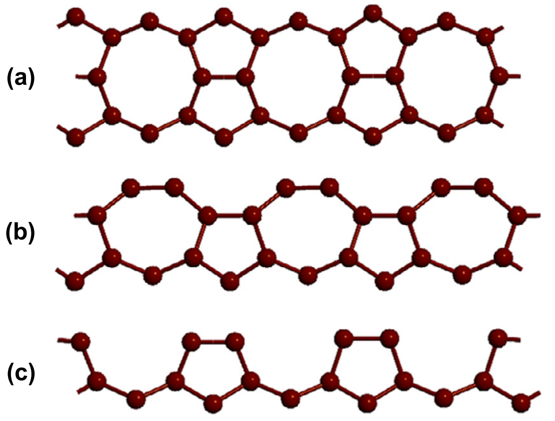

Fig. 1. (Color online.) Line defect structures for the 558-defect (a), 57-defect (b) and Klein (c) edges.

SiNRs, such as converting the system into spin-gapless semiconductors, ferromagnetic (FM) semiconductors or FM metals [37–39]. It is known that the silicon atoms at the edges of SiNRs is of sp^2 type when they are terminated by one hydrogen atom. This sp^2 type hybridization can be converted to sp^3 when the edge silicons adsorb two hydrogen atoms, and may exhibit exotic charge- and spin-transport properties [40].

In this Article, we report the design of nanodevices with mono-H-terminated and di-H-terminated ZSiNR heterojunctions with 558-defect edge, 57-defect edge, and Klein edge, as shown in Fig. 1(a)–(c), in the parallel [1, 1] and antiparallel [1, −1] magnetic configuration. According to our calculations, a nearly 100% spin-filtering effect and spin-rectifying effect are observed at low bias voltages. Moreover, remarkable negative differential resistance effect is also obtained in these devices.

2. Methods and computational details

Using the Atomistix Toolkit (ATK) package, we employ the density functional theory (DFT) for geometry optimization and electronic structures calculations, and the nonequilibrium Green's function (NEGF) method to simulate the electronic transport properties [41–44]. The exchange–correlation functional is treated in the local spin density approximation with the Perdew–Zunger (SLDA-PZ) parameters, and double-ζ polarized (DZP) basis set is adopted for electron wave functions. The cutoff energy is 150 Ry and the Monkhorst–Pack k-mesh is $1 \times 1 \times 100$. The convergence threshold of energy and force are set to be 1×10^{-5} eV and 0.05 eV/Å, respectively. The nonlinear current I_σ through the central scattering region is obtained by the Landauer–Büttiker formula [45],

$$I_\sigma(V) = \frac{e}{h} \int_{\mu_R}^{\mu_L} T_\sigma(E, V)\big[f_L(E - \mu_L) - f_R(E - \mu_R)\big]dE$$

Here $f_{L/R}(E) = 1/\{1 + \exp[E - \mu_{L/R}/K_B T]\}$ is the Fermi distribution function, k_B as the Boltzmann constant, T as the temperature and T_σ as the spin-dependent transmission.

3. Results and discussion

3.1. The mono-H-terminated and di-H-terminated ZSiNR heterojunction with 558-defect edge

The geometric structures of the model systems used in our calculations are depicted in Fig. 2(a) and (b). The monohydrogen-terminated and dihydrogen-terminated ZSiNR heterojunctions with 558-defect on the edge (denoted as 558-ZSiNR-H and 558-ZSiNR-H$_2$, respectively) serve as the central scattering region. The spin configurations on both electrodes can be designed as parallel (P) or antiparallel (AP) through setting simulate external magnetic fields, respectively. Fig. 2(a) and (b) also present the spin density distribution (SPD) of each spin configuration under zero bias, with pink (cyan) indicating up-spin (down-spin) distribution. The calculated spin-resolved currents as a function of the applied bias ranged from −0.5 V to 0.5 V for the P and AP configuration, results shown in Fig. 2(c) and (d). For P configuration, the up-spin electrons can smoothly flow through the system at positive bias, while it is nearly prohibited at negative bias from 0 V to −0.4 V. Meanwhile, the down-spin current is almost forbidden at the bias ranging from −0.1 V to 0.2 V and it arises gradually outside of this region.

On the other hand, the tendency of AP configuration is just reversed. The barrier of the down-spin channel is almost apparent under positive bias but prohibitive under negative bias from 0 V to −0.4 V. Inversely, the up-spin channel is open under the negative bias but closed between 0 V to 2.0 V. These phenomena are quantified precisely by the SFE as a function of bias in the inset of Fig. 2(c) and (d). In terms of the spin-resolved current, SFE is defined: $\mathrm{SFE} = (I_{\mathrm{up}} - I_{\mathrm{down}})/(I_{\mathrm{down}} + I_{\mathrm{up}})$, where I_{up} (I_{down}) denotes the up-spin (down-spin) current of the two spin configurations. The value of SFE can reach up to 100% whether at the positive or negative bias in both P and AP spin configurations. It reveals that the 558-ZSiNR-H/558-ZSiNR-H$_2$ heterojunction is promising candidate in fabricating dual-orientation spin-filtering devices. Another intriguing phenomenon, the rectifying effect, is also observed in devices constructed by 558-ZSiNR-H/558-ZSiNR-H$_2$ heterojunction. The rectifying ratio (RR) can be defined as $\mathrm{RR} = |I_{\mathrm{pos}}/I_{\mathrm{neg}}|$, where I_{pos} (I_{neg}) is the spin-resolved current at positive (negative) voltage. As shown in Fig. 2(e), the up-spin RR of P configuration presents a sustained increase until the bias reaches 0.4 V, and the maximum value is about 68. For the down-spin of P configuration, the valley value of RR is 1×10^{-1} at 0.2 V. After that it begins to increase to 1 at about 0.34 V and then greater than 1 as the bias continuing increasing. It suggests that the rectification reversal will appear in the down-spin I–V curve in P configuration. For AP configuration, the down-spin RR could be up to 130 at 0.2 V and the peak emerges at 0.23 V. And the valley ratio of up-spin is 3×10^{-2} at 0.2 V and then it increases larger than 1 with the bias increasing. So there is also rectification reversal in up-spin I–V curve in AP configuration. In addition, the up-spin current in AP configuration grows rapidly in negative bias before −0.2 V. But as the bias further increases, it starts to decrease gradually and an obvious NDR effect begins to emerge in the bias range of [−0.2 V, −0.4 V] as shown in Fig. 2(d).

To further rationalize the transport properties of 558-ZSiNR-H/558-ZSiNR-H$_2$ heterojunction, we plot the transmission spectra and band structures of magnetized left and right electrodes for P and AP configuration at finite bias in Fig. 3. In P configuration, when the positive bias is applied, the energy bands of left and right electrodes begin to shift downward and upward, respectively. Under a bias of 0.2 V as shown in Fig. 3(a), up-spin subbands of left electrode overlaps with those of right electrode in the bias window, leading to transmission peaks for up-spin channels. Nevertheless, we note that the transmission for the down-spin electrons is forbidden owing to lacking of down-spin subbands of the right electrode in the bias window. As a result, the up-spin current is much larger than the down-spin current at 0.2 V and a perfect spin-filtering occurs. Actually between 0 V and 0.2 V, the SFE can always maintain more than 80%. When negative bias is applied, the migratory direction of the left and right energy bands is just the reverse. Just as −0.2 V shown in Fig. 3(b), the up-spin channels close and partial down-spin channels open. Thus

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