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Effect of Phase Inversion on Quantum Transport in Group IV Two-Dimensional U-shape Device

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Abstract

Quantum transport has been computationally investigated via non-equilibrium Green's function formalism in U-shape three-terminal system realized from zigzag nanoribbons of Group-IV materials for spin-separator application. The possibility of an efficient spin-separation, even in absence of magnetic field, is demonstrated. The effect of phase inversion from quantum-spin hall state to band-insulator state on output current and spin modulation is comprehensively examined. The material choice and device length are also shown to be vital for good device performance.

1. Introduction

Group-IV monolayers of Silicene (Si), Germanene (Ge), Stanene (Sn) and Plumbene (Pb), unlike graphene, have significant buckling due to sp^2-sp^3 bonds hybridization [1] leading to the large intrinsic spin-orbit coupling (λ_{SO}), which makes them accessible to spintronic applications [2]. Moreover, with two of the four elements' two-dimensional (2D) structures having being already synthesized (Si [3] and Ge [4]), the scientific community is greatly interested in the potential applications of these novel materials. One of the key goals of spintronics is to control spin in the devices without using magnetic field. It has been recently shown [5] that a three-terminal Y-shape device, operating in quantum spin hall (QSH) phase, works as an efficient spin-separator, producing nearly 100% spin polarized current with opposite polarizations at the two output contacts, without any magnetic field. The device is controlled via difference between top and bottom gate potentials which maneuvers the buckling in the material and referred as buckling field (λ_v) to distinguish it from phenomenological potential applied to shift the Fermi-level (E_F) in the device.

However, λ_v may drive the system from QSH state to band insulator (BI) phase [2]. Therefore, using Non-Equilibrium Green's Function (NEGF) formalism, the effect of λ_v on the quantum transport in a three-terminal U-shape device with zigzag edges (Fig. 1) based on monolayers of Si, Ge, Sn, and Pb has been thoroughly investigated in this work. Note that in contrast to Y-shape device, U-shape design suppresses Fano interference and provides a transition from spin-polarized (SP) states ($-\lambda_{SO}$ to λ_{SO} energy range) to unpolarized without decimating the transmission and is therefore more appropriate for the study of the effect of λ_v on transport. It is shown that phase inversion can sharply change the device behaviour even if operating in SP energy range, and is more severe for materials with smaller λ_{SO} (Si and Ge). Moreover, the device length is shown to be crucial to determine conductance modulation with phase change. The results are important for designing better spin-separators from Group-IV monolayers.

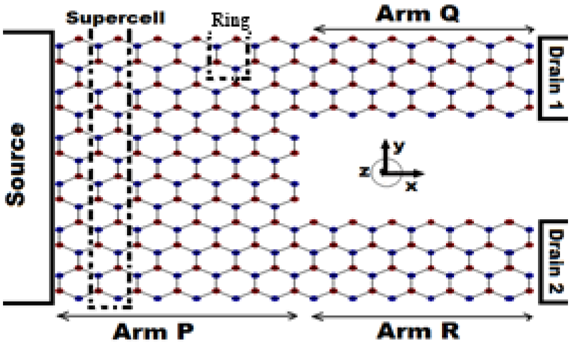

Fig. 1. U shape device structure. The out-of-plane buckled atoms in red ('A') and blue ('B') are at an offset of Δ_C along the z-axis.

2. Theory and Methodology

NEGF formalism is implemented to investigate the U-shape device with zigzag edges. Device has arm-P connected to a source and arms Q and R connected to two drain terminals. A four-band tight-binding model, that is fitted to ab-initio calculations as described in Ref.[2], has been used to model the Hamiltonian. The device Green's function is calculated by full inversion. The self-energies for the three contacts are computed from iteratively converged surface Green's function. The simulations are carried out at zero Kelvin because currently fabricated 2D-Group IV materials have small λ_{SO} (Ge λ_{SO} ~ 35meV). Future technological advances which increase the feasible energy window (Pb λ_{SO} ~ 200 meV) determined by $2^*\lambda_{SO}$ may make room temperature operation of U-shape device possible.

3. Results and Discussion

As a representative case for this work, the widths of arms P, Q and R are 14 rings, 6 rings and 6 rings respectively with length equivalent of 10 super-cells in each arm (Fig. 1). The E_F is set to 1 meV, and the voltage across contacts V_{PQ} (V_{PR}) to 1mV, unless specified otherwise.

The device acts as a spin separator with the current I_{PQ} flowing through the top edge atoms with +z spin-polarization (SP) (↑), and I_{PR} flowing through the bottom edge with opposite SP (↓). For zero buckling field when the width of arm P (nWp) is swept from 7 rings to 40 rings, with the width of arm Q and R set to (⌈nWp/2⌉- 1), conductance (G) of both arms is consistently above 99.5% and SP of equal magnitude but opposite polarity above 97.5% is observed. Change in the length of the arms results in no significant deviation in performance of the spin separator, and hence validates its robustness.

Fig. 2 shows the results of the device transport for λ_v only being applied on arm-P. As the λ_v is increased (decreased)

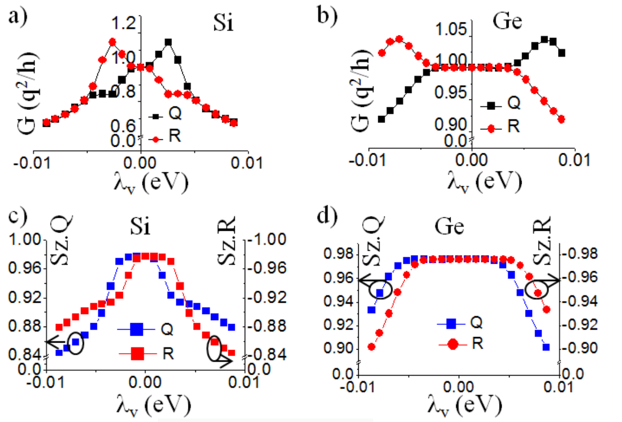

Fig. 2. Effect of λ_v, applied over arm-P, on Conductance (a, b) and Spin-Polarization (c, d) of current for Silicene (a, c) and Germanene (b, d) device.

from zero, a peak in conductance for arm-Q (arm-R) is observed, whereas the conductance through arm-R (arm-Q) degrades monotonically. The peak conductance (G_{max}) of arm-Q for Si is noted to be higher than that of Ge. The spin polarization for both the arms degrades with increasing magnitude of λ_v. To investigate the cause, energy dispersion for Ge zigzag nanoribbons (zNR) in presence of λ_v is illustrated in Fig. 3. Edge states and their spins are determined from the real-space eigenvectors distribution for each wave-vector. For small λ_v (Fig. 3(a)), the material is in QSH phase with forward moving states on 'A' and 'B' atoms on zNR edges being ↑ and ↓ polarized respectively. However, for large λ_v (Fig. 3(b)), the nano-ribbon undergoes phase inversion to band insulator phase in which energy-bands from 'A' ('B') atoms inverts from valence (conduction) to conduction (valence) band, resulting in unpolarized forward and backward states. The critical field (λ_c) at which phase transition triggers is the λ_v for which the system undergoes change from QSH to BI phase at an infinitesimally small wavevector offset to the left of the first minima (Dirac-point) for the first conduction band in energy-dispersion. For instance the phase transition for 14-Ring wide Ge nanoribbon occurs at λ_c of 9.56 meV, observed at $k_x.a_x$ of -3.911.

The increase (decrease) in modes for 'A' ('B') atoms on top (bottom) edge increases (decreases) the transmission, and hence conductance, for arm-Q (arm-R). It is observed that phase inversion is achieved at higher λ_v for higher λ_{SO} material. Since larger λ_v causes larger splitting of the bands (see eq. (1) of Ref. [2]), the momentum mismatch seen by electrons moving from arm-P to arm Q and R, where no field is

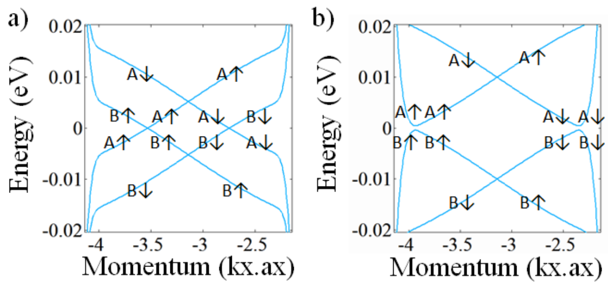

Fig. 3. Energy band for 14 rings wide Ge nanoribbon for λ_v = 5.2 meV (a) and 10 meV (b), illustrating spin-distribution on the edge states.

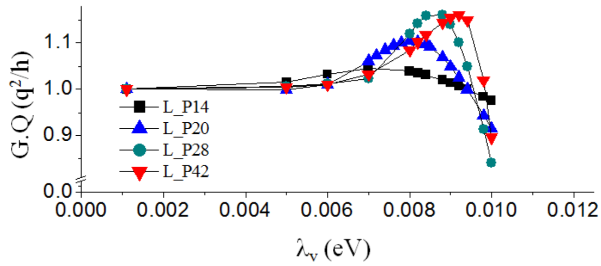

Fig. 4. Effect of λ_v, applied over arm-P, on the conductance of arm-Q, for 14, 20, 28 and 42 super-cells in arm-P (Germanene device).

applied, is higher for material with larger λ_{SO}. This results in smaller value of G_{max} for Ge than for Si. Beyond G_{max}, even arm-Q conductance starts to decrease because the bandgap created in tandem with phase inversion becomes increasingly prominent, in the concerned energy range, with increasing λ_v. There is SP degradation for both arms because of unpolarized states and subsequently absence of states in transmission window. Note that for the device with finite region under λ_v, the arm-P region is in meta-state between BI and QSH phase, while arm Q and R are in QSH phase which results in conductance much smaller than 2 as would have been expected from energy dispersion in Fig. 3(b). Fig. 4 appraises the meta-state by illustrating the effect of length of arm-P on G_{max}. It is indeed observed that G_{max} increases as the length is increased for arm-P as the arm properties increasingly mimic that of infinitely long nanoribbon which has dual 'A' channels in BI phase. Furthermore, the λ_v for G_{max} is observed to increase with the length of arm-P, tending towards critical field of 9.56 meV.

4. Conclusion

The U-shape device made of Group-IV zigzag nanoribbon has been computationally demonstrated to be an efficient spin separator in QSH phase, without the application of any magnetic field. The current (increase) and spin (decrease) modulation in band insulator phase through buckling field has been explained to result from additional channel created for in-plane atoms, as the device goes from QSH to BI phase. The materials with higher λ_{SO} should have smaller peak conductance. Furthermore, increasing the length of arm-P should increase the magnitude of the peak current and the buckling field for the peak current.

Acknowledgments

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