Negative differential resistance and spin filter effects in VS₂ monolayers

G. W. Peng, L. Zhu and K. L. Yao*

To determine the transport properties of VS₂ monolayers, we have calculated the current based on the bias voltage, band structure and transmission spectrum for VS₂ monolayers along the zigzag and armchair orientations by first-principles calculations combined with the non-equilibrium Green’s function method. A perfect spin filtering effect for the two directions and strong anisotropy have been found. Meanwhile, the zigzag orientation device shows obvious negative differential resistance around a bias voltage of ±0.55 V.

Previous research has shown the existence of strong anisotropy of transport in some layered TMD insulators, such as MoS₂ and MoSe₂, in which the resistance of the device with the armchair orientation is larger than that of the device with the zigzag orientation.²⁸ Due to it having the same structure, this may also occur in layered VS₂. To demonstrate the transport properties for spintronic applications, here we theoretically designed two kinds of devices based on VS₂ monolayers. The results show that the spin filtering effect is obtained in both devices, and negative differential resistance (NDR) exists in the VS₂ monolayer with the zigzag orientation, which makes the VS₂ monolayer a promising candidate for spintronics.

2. Computational methods

We established two kinds of hexagonal monolayer VS₂ devices which are placed along the z-direction with zigzag and armchair orientations, respectively. Based on first-principles calculations combined with the non-equilibrium Green’s function method (ATK code),²⁹–³¹ we have calculated the spin transport properties. The Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA) was used for the exchange–correlation potential.²² In the calculation, we used 

\[
I^{(i)}(E) = \frac{e}{h} \int_{-\infty}^{\infty} \{ T^{(i)}(E, V_b)[f_L(E, \mu_L) - f_R(E, \mu_R)] \} dE,
\]

where \( T^{(i)}(E) \) is the spin-dependent transmission function defined by \( T^{(i)}(E, V_b) = \text{Tr}[T_i G^{R}T_R G^{L}]^{(i)} \), \( f_{LR}(E) \) is the Fermi distribution function of electrons in the left (right) electrodes, and \( \mu_{LR} = E_F \pm eV_b/2 \) is the chemical potential of the left and right electrodes.
3. Results and discussion

The devices based on VS$_2$ monolayers in the zigzag orientation and armchair orientation are shown in Fig. 1. The spin-resolved currents as a function of bias voltage ($I$–$V$ characteristics) from $-1$ to $1$ V for both directions are shown in Fig. 2. For the device in the zigzag orientation, the spin-up current rises immediately and increases rapidly with a small bias, and becomes gentle when the bias is raised to $0.2$ V. Once the bias exceeds $0.4$ V, a significant NDR behavior appears, where the current reduces as the bias increases, and then increases approximately linearly after $0.55$ V of bias. Meanwhile, the spin-down current is neglected within the whole bias voltage range. For the armchair orientation device, the spin-down current is almost zero, while the spin-up one arises after the voltage rises to $0.6$ V for both positive and negative bias, which indicates a spin filtering effect. Therefore, the VS$_2$ of zigzag orientation shows metallic properties, while that in the armchair direction exhibits semi-conducting behavior. Meanwhile, the spin polarization ($SP = \frac{|I_\uparrow - I_\downarrow|}{|I_\uparrow + I_\downarrow|} \times 100\%$) also shows a perfect spin filtering effect. For the zigzag orientation device (inset of Fig. 2(a)), though the SP decreases very slightly as the voltage rises, it is still very close to $100\%$. For the armchair orientation device, the SP is nearly $100\%$ in the region where current appears. The spin filtering and NDR make the VS$_2$ monolayer useful for multi-function spintronic devices.

The spin filtering effect usually can be explained by the band structure. Here, we calculate the band structures of the electrodes along the transport direction, as shown in Fig. 3. It is very clear that both of them have half-metallic behavior: the spin-up band is metallic and the spin-down band has insulator character with a large energy gap. This result is consistent with previous research which was performed using VASP.$^{24}$ We know that the electrochemical potentials ($\mu_{L(R)}$) of the left (right) electrode will decrease (increase) when a positive bias voltage is applied. Therefore, the Fermi level will decrease (increase) with it and the band structure will shift with respect to the Fermi level. For the zigzag orientated VS$_2$ monolayer (Fig. 3(a)), the spin-down bands cannot cross the Fermi level after applying a positive or negative bias voltage, so there is no considerable current in the spin-down channel. Oppositely, the Fermi level crosses the bands of the spin-up state, resulting in an increase of the spin-down current with the bias voltage. Fig. 3(b) shows the band structure of the semiconducting behavior for the armchair orientated VS$_2$ monolayer. It is very clear that there is a gap for both the spin-up and spin-down band and no band crosses the Fermi level. So a current cannot be generated under low bias for both spin channels. When the bias increases, the Fermi level crosses the spin-up band due to the narrower gap, and therefore spin-up currents appear and increase with the bias. Accordingly, a spin filtering effect occurs in both of the devices.

The spin-resolved transmission spectra, which are helpful for understanding the $I$–$V$ characteristics because the spin-polarized current is contributed by integrating in the bias window $[-V_b/2, V_b/2]$, were calculated and are shown in Fig. 4.
and 5 for both of the devices, where the Fermi levels are set to zero and the black dashed lines represent the bias window. Due to the symmetric behavior, we just discuss the transmission spectrum in the positive bias region. For the zigzag device, in Fig. 4, it is very clear that there is no transmission peak of the spin-down channel entering the bias window at all bias voltages, which means that the spin-down electron has no tunneling path. Thus, the spin-down current is nearly zero. At zero bias, the transmission of the spin-up channel crosses the

---

**Fig. 3** Band structure along the transport direction for the two devices: (a) zigzag direction; (b) armchair direction.

**Fig. 4** Spin-dependent transmission spectrum of the zigzag direction.

**Fig. 5** Spin-dependent transmission spectrum of the armchair direction.
armchair orientation, and why monolayer VS$_2$ shows distinct between the two devices can explain why the value of the current.

At the same time, the transmission coefficient appears at a bias of 0.55 V. As the bias increases, more transmission coefficients enter into the bias window, which results in an increase in the current.

Fig. 5 shows the transmission spectra of the armchair device. It is very clear, both for the spin-up and spin-down electrons, that no transmission coefficients appear in the bias window until the bias reaches 0.5 V, which means that the current is zero when the bias is below 0.5 V. Once the bias reaches 0.6 V, a tiny spin-up transmission coefficient enters into the window, and the integral area is significantly expanded with an increase in bias. At the same time, the transmission coefficient of the spin-down channel remains zero, which is consistent with the $I$-$V$ curve shown in Fig. 2. Meanwhile, the disparity in the transmission spectra between the two devices can explain why the value of the current for the zigzag orientation is 100 times higher than that for the armchair orientation, and why monolayer VS$_2$ shows distinct transport anisotropy along different orientations.

4. Conclusion

In this work, we have studied the electronic transport behavior of hexagonal monolayer VS$_2$ along the zigzag and armchair directions using density functional theory combined with the non-equilibrium Green’s function. A spin filtering effect has been obtained in both orientations, and strong anisotropy appears as expected: the zigzag direction has metallic behavior, while the armchair direction is a semiconductor. Meanwhile, NDR also exists in the zigzag orientation device, which is found in TMDs for the first time. Therefore, monolayer VS$_2$ can not only be used in spintronic applications as an electrode, but can also be applied in digital applications, amplification, and oscillators, which makes it a multifunction material.

Acknowledgements

This work was supported by National Natural Science Foundation of China under Grant No. 11274130 and No. 11374111.

References

1 N. Levy, S. A. Burke, K. L. Meaker, M. Panlasigui, A. Zettl, F. Guinea, A. H. Castro Neto and M. F. Crommie, Science, 2010, 329, 544–547.
2 S. Bai and X. Shen, RSC Adv., 2012, 2, 64–98.
3 L. Zhu, F. Zou, J. H. Gao, Y. S. Fu, G. Y. Gao, H. H. Fu, M. H. Wu, J. T. Lü and K. L. Yao, Nanotechnology, 2015, 26, 315201.
4 F. Zou, L. Zhu and K. L. Yao, Sci. Rep., 2015, 5, 15966.
5 G. Sansone, L. Maschio, D. Usyvat, M. Schütz and A. Karttunen, J. Phys. Chem. Lett., 2016, 7, 131–136.
6 D. Hanlon, C. Backes, E. Doherty, C. S. Cucinotta, N. C. Berner, C. Boland, K. Lee, A. Harvey, P. Lynch, Z. Gholamvand, S. Zhang, K. Wang, G. Moynihan, A. Pokle, Q. M. Ramasse, N. McEvoy, W. J. Blau, J. Wang, G. Abellan, F. Hauke, A. Hirsch, S. Sanvito, D. D. O’Regan, G. S. Duesberg, V. Nicolosi and J. N. Coleman, Nat. Commun., 2015, 6, 8563.
7 P. Yasaei, B. Kumar, T. Foroozan, C. Wang, M. Asadi, D. Tuschel, J. E. Indacoechea, R. F. Klie and A. Salehi-Khojin, Adv. Mater., 2015, 27, 1887–1892.
8 L. Chen, C. C. Liu, B. Feng, X. He, P. Cheng, Z. Ding, S. Meng, Y. G. Yao and K. H. Wu, Phys. Rev. Lett., 2012, 109, 056804.
9 B. Feng, Z. J. Ding, S. Meng, Y. G. Yao, X. Y. He, P. Cheng, L. Chen and K. H. Wu, Nano Lett., 2012, 12, 3507–3511.
10 H. Liu, A. T. Neal, Z. Zhu, Z. Luo, X. Xu, D. Tománek and P. Ye, ACS Nano, 2014, 8, 4033–4041.
11 B. Radišavljevic, A. Radenovic, J. Brivio, V. Giacometti and A. Kis, Nat. Nanotechnol., 2011, 6, 147–150.
12 Q. H. Wang, K. Kalantar-Zadeh, A. Kis, J. N. Coleman and M. S. Strano, Nat. Nanotechnol., 2012, 7, 699–712.
13 Z. Ni, Q. Liu, K. Tang, J. Zheng, J. Zhou, R. Qin, Z. Gao, D. Yu and J. Lu, Nano Lett., 2012, 12, 113–118.
14 M. Houssa, E. Scalise, K. Sankaran, G. Pourtois, V. O. Afanas’ev and A. Stesmans, Appl. Phys. Lett., 2011, 98, 223107.
15 F. Zhu, W. Chen, Y. Xu, C. Gao, D. Guan, C. Liu, D. Qian, S. Zhang and J. Jia, Nat. Mater., 2015, 14, 1020–1025.
16 M. Osada and T. Sasaki, Adv. Mater., 2012, 24, 210–228.
17 Y. Zhou, J. Dong and H. Li, RSC Adv., 2015, 5, 66852–66860.
18 B. Sipos, A. F. Kusmartseva, A. Akrap, H. Berger, L. Forro and E. Tutos, Nat. Mater., 2008, 7, 960–965.
19 J. A. Wilson, F. J. Disalvo and S. Mahajan, Adv. Phys., 1975, 24, 117–201.
20 A. H. Castro Neto, Phys. Rev. Lett., 2001, 86, 4382.
21 J. Feng, X. Sun, C. Wu, L. Peng, C. Lin, S. Hu, J. Yang and Y. Xie, J. Am. Chem. Soc., 2011, 133, 17832–17838.
22 Y. Ma, Y. Dai, M. Guo, C. Niu, Y. Zhu and B. Huang, ACS Nano, 2012, 6, 1695–1701.
23 T. Wang, Y. Li, C. Xia, X. Zhao, Y. An and X. Dai, J. Mater. Chem. C, 2016, 4, 8111–8120.
24 H. Pan, Sci. Rep., 2014, 4, 7524.
25 I. Galanakis and P. Mavropoulos, Phys. Rev. B: Condens. Matter Mater. Phys., 2003, 67, 104417.
26 J. Kübler, Phys. Rev. B: Condens. Matter Mater. Phys., 2003, 67, 220403.
27 J. E. Pask, L. H. Yang, C. F. Yong, W. E. Picket and S. Dag, Phys. Rev. B: Condens. Matter Mater. Phys., 2003, 67, 224420.
28 D. Çakır and F. M. Peeters, Phys. Rev. B: Condens. Matter Mater. Phys., 2014, 89, 245403.
29 J. Taylor, H. Guo and J. Wang, Phys. Rev. B: Condens. Matter Mater. Phys., 2001, 63, 245407.
30 M. Brandbyge, J. Mozos, P. Ordejón, J. Taylor and K. Stokbro, Phys. Rev. B: Condens. Matter Mater. Phys., 2002, 65, 165401.
31 J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón and D. Sánchez-Portal, J. Phys.: Condens. Matter, 2002, 14, 2745–2779.
32 J. P. Perdew, K. Burke and M. Ernzerhof, Phys. Rev. Lett., 1996, 77, 3865.