The effect of spin-orbit interaction on the electron spin transport in inorganic semiconductors and the comparison of organic semiconductors

H Li, S Y Wu, X R Liang and M Y Zhou
Naval Aeronautical and Astronautical University Department of Basic Sciences,
Yantai, Shandong 264001, China
E-mail: 346521161@qq.com

Abstract. In theory, the influence of spin-orbit interaction on the electron spin transport in inorganic semiconductors was discussed, which was compared with that of organic semiconductors. Results reveal that the internal mechanism of spin precession in inorganic semiconductor is different from that of the organic semiconductor, while the influence of the spin-orbit interaction on the carrier spin transport is same.

1. Introduction
There are some spin-dependent interactions in the spin electronics. The first one is the classical interaction between a pair of electron magnetic dipoles usually in the intensity of 1K, which is very weak; The second one is the interaction between the spin and the external magnetic field, which is called the Zeeman effect[1-3]. Generally speaking, Only the magnetic field is in the order of tens of Tesla order can obvious spin level splitting appear; Third, spin-orbit interaction[4-7]; The fourth kind of interaction is the one between Heisenberg and Pauli; The fifth kind of interaction is the hyperfine interaction between the electron and the nuclear spins. Any one of these five interactions can cause the spin to be reversed. In accordance with different demands, the main task of the spin electronics is to control spin flip

Spin-orbit interaction is due to the asymmetric effects of electrons in motion. The spin moment will be affected effectively by the intrinsic magnetic field, which is spin-orbit interaction[8].

\[ H_{SO} = -\mu_s \cdot \vec{B} = \mu_s \cdot (\vec{v} / c^2) \times \nabla V(\vec{r}) = \frac{e\hbar}{4m_e c^2} \vec{\sigma} \cdot (\vec{v} \times \nabla V(\vec{r})) \]  

In this formula, \( e, m_e, c \) are the electronic power, the electron mass, and the speed of light, respectively. \( \vec{\sigma} \) is Pauli matrix, and \( \vec{v} \) is motion velocity of electrons. I analzsed the effect of the spin-orbit interaction on the spin transport of organic semiconductors, it found that the spin cycles would occur when the organic semiconductor carrier polaron moved along the polymer chain due to the spin-orbit interaction[9]. What is the difference between the spin-orbit interaction and the electron spin transport when we use the same model to describe the inorganic semiconductor? In this paper, we will discuss this problem.
2. Models and Formulas in the Organic Semiconductor

In the one-dimensional organic semiconductor with non-degenerate ground state, the Hamiltonian includes two parts, electronic partion and lattice partion[10-11]:

\[ H = H_e + H_{lattice} \]  \hspace{1cm} (2)

The electronic part is represented by the extended SSH model:

\[ H_e = -\sum_{n} t_0 (u_{n+1} - u_n) - \alpha (u_{n+1} - u_n) \left( \prod_{x=1}^{n} (e^{-i\delta x C_{n+1,x}^+ C_{n,x}^+} + e^{i\delta x C_{n,x}^+ C_{n+1,x}^+}) \right) \]  \hspace{1cm} (3)

in which \( t_0 \) is the transition integral of electrons in adjacent grid points \( n \) and \( n+1 \), \( \alpha \) the electron-phonon coupling constant, \( u_n \) the position deviation of the \( n \) lattice point(CH group), \( t_e \), \( \gamma = \frac{e a}{\hbar c} \). \( e, a, c \) the electronic power, the lattice constant and the speed of light respectively. Driving electric field \( E(x,t) = -\partial_t A(x)/c \), and \( A \) is vector-potential, which is a scalar in one dimensional system.

The crystal lattice is represented in the classical manner:

\[ H_{lattice} = \frac{K}{2} \sum_{n} (u_{n+1} - u_n)^2 + \frac{M}{2} \sum_{n} u_n^2 \]  \hspace{1cm} (4)

K is the elastic coefficient of the lattice, \( M \) represents the effective quality of a lattice point.

The spin-orbit interaction is introduced by the gate voltage perpendicular to the one-dimensional organic semiconductors. We assume that the one-dimensional organic semiconductor is along the \( x \) direction, the gate voltage points to the \( z \) direction, and the corresponding Hamiltonian is expressed as:

\[ H_{SO} = i\beta \left( \sigma_y \frac{\partial}{\partial y} - \sigma_x \frac{\partial}{\partial x} \right) \]  \hspace{1cm} (5)

in which \( \beta \) is the spin-orbit interaction strength, which is controlled by the gate voltage, and \( \sigma \) is the Pauli matrix. For the one-dimensional organic semiconductor along the \( x \) direction, only the second of the bracket is retained in equation (5). The one-dimensional tight binding model of spin-orbit interaction is obtained after the two quantization[12]:

\[ H_{SO} = -\tau_{SO} \sum_n \left[ C_{n+1,x}^+ C_{n,x} - C_{n+1,x}^+ C_{n,x}^+ + C_{n,x}^+ C_{n+1,x}^+ - C_{n,x} C_{n+1,x} \right] \]  \hspace{1cm} (6)

in which \( \tau_{SO} \) describes quantities of the Rashba spin-orbit coupling. \( \tau_{SO} = \beta / 2a \), \( a \) is a lattice constant, \( \beta = |e| \hbar^2 E_{SO} / 4m_e^2 c^2 \) [13], \( E_{SO} \) denotes Rashba electric field, \( m_e \) is electron mass, and \( C_{n,x}^+ (C_{n,x}) \) is the generation (disappearance) operator of an electron at a lattice point \( n \).

From the equation (6), we can see that this type of spin-orbit interaction is closely related to the movement of carriers. Due to the existence of driving electric field, the spin-orbit interaction Hamiltonian is correspondingly changed into the following form:

\[ H_{SO} = -\tau_{SO} \sum_n \left[ e^{iyA} C_{n+1,x}^+ C_{n,x}^+ - e^{-iyA} C_{n+1,x}^+ C_{n,x} + e^{iyA} C_{n,x}^+ C_{n+1,x} - e^{-iyA} C_{n,x} C_{n+1,x} \right] \]  \hspace{1cm} (7)

3. Effect of Spin-orbit Interaction on Electron Spin Transport in Inorganic Semiconductors

Contrary to the inorganic semiconductor, the organic one have a larger disorder[14-19], because of the strong electron-lattice interaction of organic materials, the structure is "soft". Any changes in the density of charge may cause restructure of system structure[20-22]. The injected electrons (or holes) are not in the form of an extended state like inorganic semiconductor, but form localized states such as soliton, polaron, etc. and at the same time, the local level is formed in the band gap, so the electron can not easily jump to the continuous conduction band. We know that the spin cycles will occur due to the
spin-orbit interaction in the organic semiconductor. Based on the analysis of the charge occupation in the eigen energy of polaron, the phenomenon of spin precession in organic semiconductors occurs only in polaron energy, which is also called internal level precession [23]. The internal mechanism of spin precession in inorganic semiconductor is different from that of the organic semiconductor, the electronic spin precession of inorganic semiconductor happened in different energy levels of electrons.

In order to compare the effect of spin-orbit interaction in organic semiconductors, we use a similar model to describe the inorganic semiconductors: one dimensional inorganic chain along the x direction, and electrons can only move in this direction, Rashba electric field point to the z direction, which is used to control the strength of the spin-orbit interaction ($t_{SO}$). Driving electric field is along the -x direction, which is introduced through the index terms of the transition integral in the electronic Hamiltonian. In the model, the biggest difference between the organic and inorganic semiconductors lies in the "soft" structure. The lattice points of organic semiconductors are movable, while the lattice points of inorganic semiconductors are fixed. In inorganic semiconductors, thus, the Vibronic coupling constant $\alpha = 0$, and the whole chain is rigid. The Hamiltonian of the inorganic semiconductor only has an electronic part:

$$ H_e = -\sum_{n,s} t_0 \left[ e^{-i\theta} C_{n+1,s}^+ C_{n,s} + e^{i\theta} C_{n,s}^+ C_{n+1,s} \right] $$

The Hamiltonian form of the spin-orbit interaction has not changed. We get the electron's energy eigen value by Fourier transformation:

$$ E(k) = E_0(k) \pm 2t_{SO} \sin(ka - \gamma A) $$

Rashba spin-orbit interaction causes the energy band of the spin in the inorganic semiconductor to split in the $\vec{y}$ direction and the $-\vec{y}$ direction. The split is different from that caused by the Zeeman effect, because it does not eliminate spin merger.

Due to the splitting of the energy level, the electrons of different wave vectors ($k_1$ and $k_2$) have the same energy, i.e. $E^+(k_1) = E^-(k_2)$. $k_1$ corresponds to spin intrinsic state $\left( \begin{array}{c} 1 \\ i \end{array} \right)$ in the $\vec{y}$ direction. $k_2$ corresponds to spin intrinsic state $\left( \begin{array}{c} 1 \\ -i \end{array} \right)$ in the $-\vec{y}$ direction. An electron pointing to the $\vec{z}$ direction (Spin intrinsic state is $\left( \begin{array}{c} 1 \\ 0 \end{array} \right)$) gets into to one dimensional inorganic semiconductor, and the electron will move in the $\vec{x}$ direction due to the driving electric field. Due to the Rashba spin orbit interaction, an effective magnetic field is generated in the $\vec{y}$ direction, and the electronic spin will rotate around the $\vec{y}$ axis.

The electron wave function is expressed as

$$ \psi = \left( \begin{array}{c} 1 \\ i \end{array} \right) e^{i\bar{k}_1 L} + \left( \begin{array}{c} 1 \\ -i \end{array} \right) e^{i\bar{k}_2 L} $$

in which, $\bar{k}_1, \bar{k}_2$ are in the $\vec{x}$ direction, L is the distance of the electronic has gone through.

The projection of electron spin in the $\vec{z}$ direction:

$$ S_z = \frac{\left( \left| \langle 0, 1 | \psi \rangle \right|^2 - \left| \langle 0, 1 | \psi \rangle \right|^2 \right)}{2} = 4 \cos(k_2 - k_1)L $$

Owing to $E(k) = E_0(k) \pm 2t_{SO} \sin(ka - \gamma A)$, $E_0(k) = -2t_0 \cos(ka - \gamma A)$

When $E^+(k_1) = E^-(k_2)$, we get: $k_2 - k_1 = \frac{2}{a} \arctan \frac{t_{SO}}{t_0}$. 

So \( S_z = 4 \cos(k_x - k_y)L = 4 \cos \frac{2L}{a} \arctan \frac{t_{SO}}{t_0} \).

We see that in one dimensional inorganic semiconductors, electrons move along the \( \vec{x} \) direction, Affected by the Rashba spin-orbit interaction, the moving track of the projection of the electron spin in the \( \vec{z} \) direction satisfies the cosine law.

After the spin precesses in a cycle, i.e. \( S_z = 1 \), the distance that electrons have moved in this cycle:

\[
L = \frac{C}{\arctan \frac{t_{SO}}{t_0}} \quad (C \text{ is constant})
\]  

(12)

The bigger \( t_{SO} \) is, the smaller \( L \) will be, i.e. the faster the electron spin precesses, the smaller spin precession cycle will be, and vice versa. We can conclude that the electron spin precession cycle is inversely proportional to the strength of the Rashba spin orbit interaction.

4. Conclusion
After studying one dimensional organic semiconductor and one dimensional inorganic semiconductor, we find that the internal mechanism of spin precession in inorganic semiconductor is different from that of the organic semiconductor, while the effect of Rashba spin-orbit interaction on the spin evolution in the charge motion is same,i.e. the moving track of the projection of the electron spin in the \( \vec{z} \) direction meets the cosine law, the spin precession period is inversely proportional to the spin orbit interaction strength.

References

[1] Hichri A and Jaziri S 2004 Physica. 350 305
[2] Liu W W 2015 Physical Experiment of College. 6 15
[3] Peng Y H and Huang T T 2011 Journal of XiangNan University. 2 64
[4] Bychkov Y A and Rashba E I 1984 JETP Lett. 39 78
[5] Dresselhaus G 1955 Phys. Rev. 100 580
[6] Yang J, Da B F and Li X 2011 College physics. 8 65
[7] Chen G P 2015 Acta Physica Sinica. 3 203
[8] Sun Q F, Guo H and Wang J 2004 Phys. Rev. B. 69 054409
[9] Li H, Qu L S, Zhou M Y and Liang X R 2012 One dimensional spin precession of Polaron in organic polymer College Physics. 31 5
[10] Brazovskii S A and Kirova N N 1981 Sov. Phys. JETP. 33 4
[11] Su W P, Schrieffer J R and Heeger A J 1979 Phys. Rev. Lett. 42 1698
[12] Sun Q F 2005 Phys. Rev. B. 71 165310
[13] Hyun C L 2005 Phys. Rev. B. 72 245338
[14] Mastour N, Mejatty H and Bouchriha H 2015 Superlattice and Microstructure. 82 461
[15] Saidi H, Ridene S and Bouchriha H 2015 Int. J. Mod. Phys. B. 29 1550054
[16] Ridene R, Mastour N, Gammra D and Bouchriha H 2015 Int. J. Mod. Phys. B. 29 1550211
[17] Bai W F, Wu Y Q, Xin W and Eerdun C L 2014 Acta Physica Sinica. 17 329
[18] Mamat J, Dulat S and Hekim M 2015 Journal of Xinjiang University. 2 68
[19] Gong S J and Duan C G 2015 Acta Physica Sinica. 18 107
[20] Sun X, Fu R L, Yonemitsu K and Nasu K 2000 Phys. Rev. Lett. 84 2830
[21] Zhao H X, Zhao H and Chen Y G 2015 Journal of Nanchang Hangkong University. 4 31
[22] Zhang X M, Shigemi M, Takahide K, Ma Q L, Mikihi O, Hiroshi N, Yasuo A, Terunobu M and Shakin V A 2013 Nature communications. 50 4306
[23] Lei J 2009 Dynamics of spin injection and transport in organic polymer *JiNan: Shandong University press*. 46-48