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Rapid Communication

Monte Carlo simulation of in-plane spin-polarized transport in GaAs/GaAlAs quantum well in the three-subband approximation*

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We develop a Monte Carlo (MC) tool incorporated with the three-subband approximation model to investigate the in-plane spin-polarized transport in GaAs/GaAlAs quantum well. Using the tool, the effects of the electron occupation of higher subbands and the intersubband scattering on the spin dephasing have been studied. Compared with the corresponding results of the simple one-subband approximation model, the spin dephasing length is reduced four times under 0.125 kV/cm of driving electric field at 300K by the MC tool incorporated with the three-subband approximation model, indicating that the three-subband approximation model predicts significantly shorter spin dephasing length with temperature increasing. Our simulation results suggest that the effects of the electron occupation of higher subbands and the intersubband scattering on the spin-dependent transport of GaAs 2-dimensional electron gas need to be considered when the driving electric field exceeds the moderate value and the lattice temperature is above 100K. The simulation by using the MC tool incorporated with the three-subband approximation model also indicates that, under a certain driving electric field and lattice temperature, larger channel widths cause spins to be depolarized faster. Ranges of the three components of the spins are different for three different injected spin polarizations due to the anisotropy of spin–orbit interaction.

Keywords: Monte Carlo, spin dephasing, spin-polarized transport, three-subband approximation model

PACC: 7210, 0365, 7320D

1. Introduction

Utilizing the carrier spin degree of freedom in hybrid semiconductor electric devices has received much attention of all.[1−3] Several devices including spin field effect transistors (FETs),[2] bipolar spin transistors[4] and spin battery device[5] have been proposed. To realize these devices, it is essential to be able to control spin dephasing in the conduction channel and learn about properties of the spin-dependent transport. In a spin FET, 2-dimensional electron gas (2DEG) formed at the heterostructure interface serves as the conduction channel, and its spin dynamics can be controlled only by an electric gate used to change the extent of the spin–orbit coupling. Up to date, most of the studies have focused on the spin relaxation of the 2DEG formed in the III–V group compound semiconductor quantum well in the one-subband approximation. [6,7] Carriers' spin states are depolarized by momentum scatterings such as ionized impurity scattering and intrasubband phonon scattering, but electrons will not stay in the first subband at all, and the one-subband approximation model neglects the influence of intersubband scattering on spin dephasing. Spin dephasing will even be stronger if the intersubband scattering is considered. What's more, the spin–orbit interaction constants are dependent upon subbands in quantum well. In our work, we investigate the 2DEG's in-plane spin-dependent transport

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in GaAs/GaAlAs quantum well in the three-subband approximation using the Monte Carlo method. Relevant momentum scattering mechanisms such as acoustic phonon scattering and polar optical phonon scattering are incorporated into our simulation.

2. Implementation of spin dynamics in Monte Carlo simulation

There are three mechanisms for causing spin dephasing of conduction electrons: the Bir–Aronov–Pikus mechanism[8] which involves a simultaneous flip of electron and hole spins due to electron–hole exchange coupling and is important in p-type GaAs or GaSb; the Elliot–Yafet mechanism[9,10] which is due to momentum relaxation and is important in the narrow-bandgap semiconductors such as InSb; and the D'yakonov–Perel (DP) mechanism[11] which is the main spin dephasing mechanism in undoped and n-type III–V semiconductors and n-type II–VI semiconductors. So the leading spin dephasing mechanism for our case is of the DP type. In our study, we consider a single GaAs/GaAlAs asymmetric quantum well grown in the (0,0,1) crystallographic direction, and assume that the in-channel electric field E_x is applied along the x crystallographic axis. The width of quantum well is 10 nm. We do not use the spin density matrix and spin–orbit interaction Hamiltonian[7] to characterize the spin dynamics. The precession description of the spin vector is incorporated into the Monte Carlo simulation to account for the spin evolvement. Under the influence of DP mechanism, the electron's spin precession can be described by the following precession equation:

$$\frac{\mathrm{d}\boldsymbol{S}}{\mathrm{d}t} = \Omega_{\mathrm{eff}} \times \boldsymbol{S}, \tag{1}$$

where $\boldsymbol{S}$ is the electron's spin polarization vector and Ω_{eff} is the so-called "precession vector". Ω_{eff} has two contributions $\Omega_{\mathrm{R}}(\boldsymbol{k})$ and $\Omega_{\mathrm{D}}(\boldsymbol{k})$ which are due to the structural inversion asymmetry (Rashba coupling interaction[12]) of the heterostructure and the bulk inversion asymmetry (Dresselhaus coupling interaction) of the III–V compound semiconductor respectively. $\Omega_{\mathrm{D}}(\boldsymbol{k})$ includes the linear Dresselhaus term $\Omega_{\mathrm{D}_1}(\boldsymbol{k})$ and the cubic Dresselhaus term $\Omega_{\mathrm{D}_3}(\boldsymbol{k})$. Their expressions are as follows:

$$\begin{aligned}
\Omega_{\mathrm{R}} &= \frac{2a_{46}E_y}{\hbar}(-k_z\boldsymbol{u}_x + k_x\boldsymbol{u}_z) \\
\Omega_{\mathrm{D}_1} &= \frac{2a_{42}}{\hbar}\left(\frac{n\pi}{W_y}\right)^2(k_x\boldsymbol{u}_x - k_z\boldsymbol{u}_z), \\
\Omega_{\mathrm{D}_3} &= \frac{2a_{42}}{\hbar}(-k_xk_z^2\boldsymbol{u}_x + k_zk_x^2\boldsymbol{u}_z),
\end{aligned} \tag{2}$$

where a_{46} and a_{42} are material parameters, $\boldsymbol{u}_{x(z)}$ a unitary vector along $x(z)$ axis, $\boldsymbol{k} = k_x\boldsymbol{u}_x + k_z\boldsymbol{u}_z$ the electron wave vector, n=1, 2, 3 the subband index and W_y the width of the quantum well. Theoretically estimated values of a_{46} and a_{42} vary with the models and band parameters adopted. In GaAs, we take the value of a_{42} as 2.8×10^{-29} eV·m^3 that is close to the experimentally measured value[13] and a_{46} as 9.0×10^{-39} C·m^2.[14] We solve the Poisson equation to obtain the vertical electric field E_y self-consistently and its value is about 120kV/cm at the heterostructure interface. The driving electric field E_x is also obtained self-consistently by solving the Schrödinger and Poisson equations. Polar optical phonon scattering and acoustic phonon scattering are included in the Monte Carlo simulation, because they are the main scattering mechanisms that influence electron's final states in undoped GaAs.

3. Simulation results

In the simulation, we consider a triangle-like quantum well. The calculated energies of the first subband, the second subband and the third subband at 300K are about 0.069, 0.117 and 0.153eV respectively. In order to ensure that most of the electrons stay in the lowest three subbands at room temperature, we choose relatively low longitudinal electric field. At 77K, most of the electrons stay in the first subband, there is almost no difference in spin dephasing between the one-subband approximation model and the three-subband approximation model. Figure 1 shows the fraction of electron occupation of the first subband

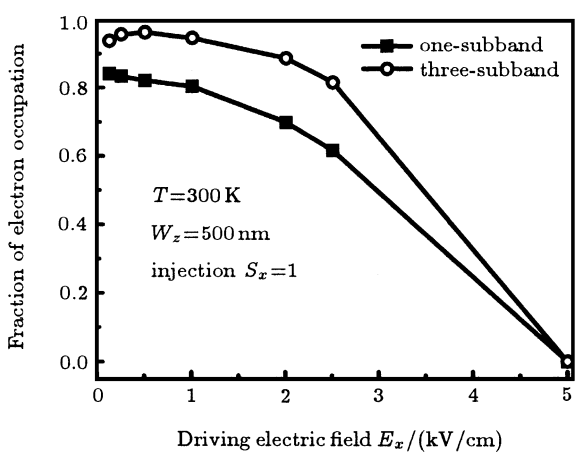


Fig.1. Fraction of electron occupation in the first subband for the one-subband approximation model and that in the lowest three subbands for the three-subband approximation model with the channel width W_z=500 nm, lattice temperature T=300K and the injected spin polarization being along the x-axis (S_x=1).

for the one-subband approximation model and that of the lowest three subbands for the three-subband approximation model at 300K with the channel width W_z being equal to 500 nm and the injected spin polarization being along the x axis (S_x=1). From this figure, we can see that more than 94% of the electrons stay in the lowest three subbands for driving electric fields E_x lower than 1.5kV/cm at 300K, while the number of the electrons that occupy the first subband cannot reach 85% in fraction. So considering just three subbands of the quantum well is more than sufficient.

The higher the lattice temperature is, the more random the electrons' motion states are. The change of electrons' wave vectors causes their spin "precession vector" to change and thus influence their spin dephasing. So at different lattice temperatures, electrons' spin relaxation rates will be different. The decay of the average (ensemble average over all electrons) spin vector $\langle \boldsymbol{S} \rangle$ is not simply exponential, however we define the spin dephasing length (L_s) as the distance (measured from the left end of the channel) where $|\langle \boldsymbol{S} \rangle|$ is decreased by the factor of e from its initial value of 1. This parameter is useful for rough estimation of a length scale within which spin-dependent transport is important. Figure 2 shows that in a constant driving electric field E_x, as the lattice temperature increases, the spin dephasing rate also increases and the spin dephasing length turns shorter no matter which energy band approximation model is adopted. Increasing the lattice temperature results in increasing phonon scattering, which randomizes $\boldsymbol{k}$ and $\Omega_{\rm eff}$ more rapidly. This results in faster rotation and dephasing of the spin vector. It is consistent with the theory that the more random the electron's motion is in space, the faster the spin dephasing will be. This figure also indicates that spin dephases faster in quantum well in the three-subband approximation than in the one-subband approximation. The spin dephasing length for the three-subband approximation model is about three times smaller than that for the one-subband approximation model at 300K. This is due to larger Dresselhaus interaction for higher subband and the influence of the intersubband scattering. Experiment[15] has also shown that intersubband scattering makes a contribution to faster spin dephasing. The higher the subband energy level is, the stronger the spin–orbit interaction is, thus the faster the spin depolarizes.

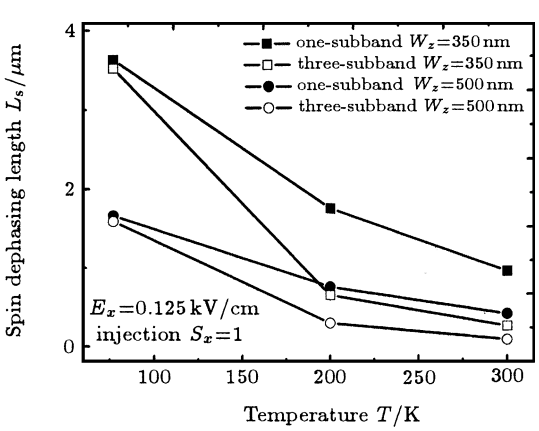


Fig.2. The spin dephasing length vs lattice temperature for the one-subband approximation and the three-subband approximation model. Driving electric field is E_x=0.125 kV/cm, and channel widths W_z are adopted to be 350 nm and 500 nm for each model. The injected spin polarization is along the x-axis (S_x=1).

In Fig.3, the spin dephasing length as a function of the channel width is plotted. The injected spin polarization is along the x-axis. It is clear that spin dephasing can be reduced with the decrease of the channel width W_z. This tendency can be explained as follows: as shown in Eq.(2), the term proportional to k_x appearing in $\Omega_{\rm eff}$ is the informative term and that proportional to k_z is the perturbing term to the spin in 2DEG. Spin dephasing is caused by the perturbing term. In a free flight time interval $t_{\rm f}$, the perturbation to the spin polarization vector varies roughly as $k_z t_{\rm f}$, which serves as the distance that an electron flies in $t_{\rm f}$. If scatterings are regarded as non-correlated events, the noise for the spin polarization during a great number of free flights is additive, and its magnitude depends on $\langle {\rm d}z^2 \rangle$ since $\langle {\rm d}z \rangle = 0$. So if we decrease the channel width, the spin dephasing rate will turn slower. From this figure, we also can see that at room temperature electrons' spin dephasing rate is slower at higher E_x. There are two contribution factors for this trend. First, at higher E_x, drift velocity is larger. This effect leads to slight increase in spin dephasing length. Second, because of the random effect of scattering, different electrons have different wave vectors $\boldsymbol{k}$ in the same free flight interval. However the precession vector $\Omega_{\rm eff}$ depends on $\boldsymbol{k}$, so the precession rates for different electrons will be different, ensemble average over the electrons therefore causes the magnitude of the spin vector $\langle \boldsymbol{S} \rangle$ to decay. Scattering will be stronger at higher E_x, and the difference between the precession rates becomes larger, resulting in faster spin dephasing. At room temperature, the former factor dominates over the latter one, leading to a larger L_s in the electric field range considered.

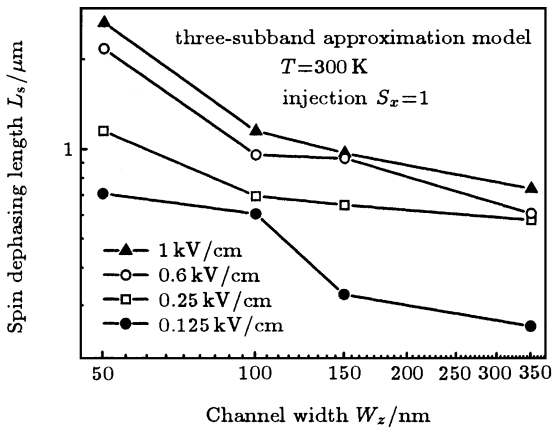


Fig.3. The spin dephasing length vs channel width under different driving electric fields E_x. The three-subband approximation model is used with lattice temperature T=300K and the injected spin polarization being along the x-axis (S_x=1).

Using the three-subband approximation model, we can obtain the distributions of the x-components of the spins in the electron ensemble at 300K for three different injected polarizations being along the x-, y- and z-axes which are shown in Figs.4(a), 4(b) and 4(c) respectively. The channel width is 500 nm and E_x equals 0.125kV/cm. Spin depolarizing rates will be different for different injected polarizations. This is due to the precession characteristic of the spin vector and the anisotropy of the spin–orbit interaction terms as can be seen in Eq.(2). Because of difference in spin dephasing rate, the distributions of the spin components in the channel will be different for these three cases too. When electrons are injected with their initial spin polarization being aligned along the x-direction, there is a slight accumulation at one extremity of the distribution function, this is due to the fact that an electron whose x-component of spin equals +1 is emitted at the emission boundary whenever there is an electron absorbed at the collection boundary. So more spins in the ensemble will have values close to +1 than have any other intermediate value. When the spins are initially polarized along the y direction, the x-component shows a U-shaped distribution weighted towards the extreme values of –1 and +1. This U shape is a consequence of the oscillatory nature of the decay characteristic for x-component. It is can be explained by Eqs.(1) and (2). When the injected spin polarization is along the z-axis, the x-component shows a Gaussian-type distribution with zero mean. Some spread about the zero value is due to the influence of the z-component of the "precession vector". It is expected that the x-components of the spins should be ideally zero (the distribution would be a delta function at zero) in the absence of the z-component of the "precession vector". We can also explain this result from Eqs.(1) and (2).

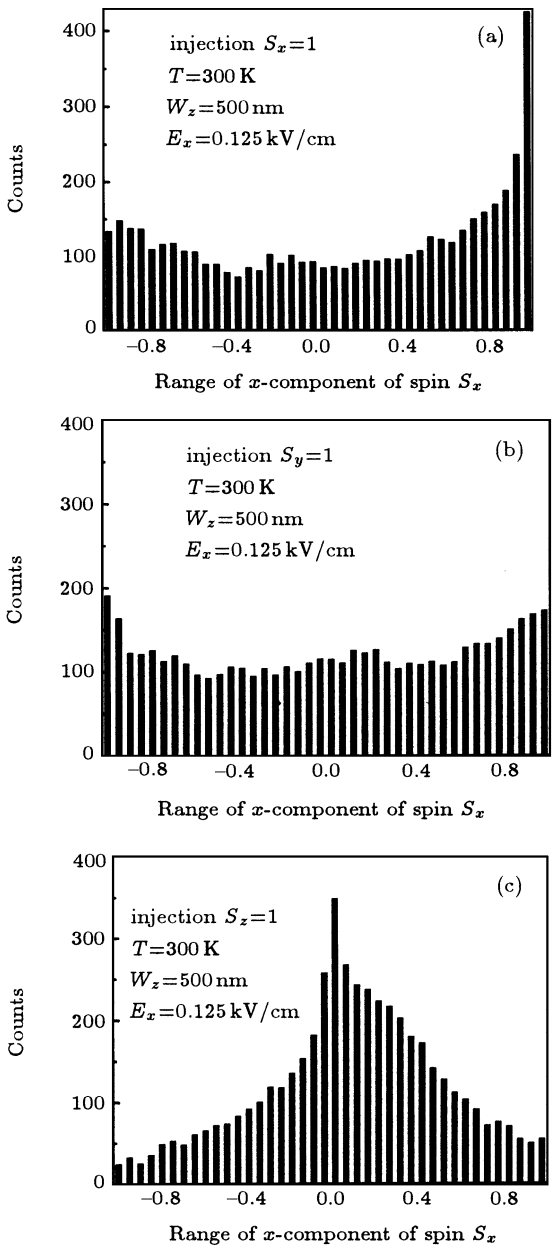


Fig.4. Range of the x-components of the spins in the channel for three different injected polarizations. The three-subband approximation model is used with lattice temperature T=300K, driving electric field E_x=0.5kV/cm and channel width W_z=500 nm. Figs.4(a)–4(c) correspond to the injected polarization being along the x-(S_x=1), y-(S_y=1) and z-(S_z=1) axes respectively.

4. Conclusion

By using the MC tool incorporated with the three-subband approximation model, we have demon-

strated that the electron occupation of higher subbands and the intersubband scattering will cause faster spin dephasing in GaAs/GaAlAs quantum well. Higher lattice temperature makes electron's motion state more random in space, thus causing the magnitude of the spin vector to decrease faster. Because the perturbing variation of the spin polarization vector along the channel width direction is additive, larger channel width will cause faster spin depolarization in the 2DEG channel. At room temperature, the larger the driving electric field is, the more slowly the spin dephases. Ranges of the three components of the spins are different for three different injected spin polarizations. With the increase of driving electric field and lattice temperature, the effects of the electron occupation of higher subbands and the intersubband scattering on in-plane spin-polarized transport of GaAs 2DEG will become significant and the three-subband approximation model is needed to replace the one-subband approximation model.

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