Simulation of Spin-polarized Transport in GaAs/GaAlAs Quantum Well Considering Intersubband Scattering by the Monte Carlo Method

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***Abstract*–Using the Monte Carlo method, we simulated the electrons' spin-polarized transport in GaAs/GaAlAs quantum well in the one-subband and three-subband approximation. The spin dephasing rate is larger for quantum well in the three-subband approximation than that in the one-subband approximation due to the intersubband scattering. The influences of in-channel driving electric field, lattice temperature and channel width on the spin dynamics are compared between the three-subband and the one-subband approximation model. At 300K, the spin vector relaxes slower for larger applied in-channel driving electric field. For lower lattice temperature, spin dephases slower. Under certain driving electric field and lattice temperature, larger channel width causes faster spin dephasing. These results are essential for design and fabrication of spintronic devices.**

I. INTRODUCTION

Up to date, many studies have been focused on the spin relaxation of the 2DEG formed in the III-V group compound semiconductor quantum well in the one-subband approximation [1]. However, electrons will not stay in the first subband entirely, considering only one subband will neglect the influence of the intersubband scattering on spin-polarized transport. The spin dephasing will even be stronger if the intersubband scattering is incorporated. Moreover, the spin-orbit interaction constants are larger for higher subbands of the quantum well. In our work, we use the Monte Carlo method to investigate the 2DEG's spin-dependent transport in GaAs/GaAlAs quantum well in the three-subband approximation for the first time. Properties of the spin-dependent transport such as spin scattering length are given.

II.SIMULATION METHOD

We use a variational technique to calculate each subband's energy and wave function.

$$V(Y)=\begin{cases}\infty & (Y\le 0)\\ -V_0\exp(-Y/Y_0) & (Y>0)\end{cases} \quad (1)$$

is chosen to express the shape of the quantum well which is shown in the inset of Fig.1. The width of quantum well is 10nm. The calculated energy of the first subband at 300K is about 0.069eV. The energy splitting between the first and second subband is calculated to be about 0.048eV and that between the second and third subband is approximately 0.036eV. The precession description of the spin polarization vector has been incorporated in the Monte Carlo method to account for the spin polarization dynamics. Polar optical phonon scattering and acoustic phonon scattering are included into the Monte Carlo simulator, because they are the main scattering mechanisms that influence electron's motion states in GaAs/GaAlAs quantum well. The driving electric field E_x is obtained self-consistently by solving the Poisson equation. The gate electric field E_y is also obtained by solving the Schrödinger and Poisson equations. Under the influence of D'yakonov-Perel (DP) mechanism [2] which includes Rashba interaction and Dresselhaus interaction, the electron's spin precession can be described by the following equation :

$$\frac{d\vec{S}}{dt}=\vec{\Omega}_{eff}\times\vec{S}. \quad (2)$$

As given by

$$\vec{\Omega}_{eff}=\vec{\Omega}_R+\vec{\Omega}_{D_1}+\vec{\Omega}_{D_3}, \quad (3)$$

$\vec{\Omega}_{eff}$ is the so-called "precession vector " and it has two contributions $\vec{\Omega}_R(k)$ and $\vec{\Omega}_D(k)$ both of which are given by

$$\begin{aligned}\vec{\Omega}_R&=\frac{2a_{46}E_y}{\hbar}(-k_z\vec{u}_x+k_x\vec{u}_z)\\ \vec{\Omega}_{D_1}&=\frac{2a_{42}}{\hbar}(\frac{n\pi}{W_y})^2(k_x\vec{u}_x-k_z\vec{u}_z)\quad,\\ \vec{\Omega}_{D_3}&=\frac{2a_{42}}{\hbar}(-k_xk_z{}^2\vec{u}_x+k_zk_x{}^2\vec{u}_z)\end{aligned} \quad (4)$$

where a_{46} and a_{42} are material parameters, $\vec{u}_{x(z)}$ the unitary vector along x(z)-axis, n =1,2,3 the subband index, and $\vec{k}=k_x\vec{u}_x+k_z\vec{u}_z$ the electron wave vector. $\vec{\Omega}_D(k)$ includes the linear Dresselhaus term($\vec{\Omega}_{D_1}(k)$)and the cubic Dresselhaus term($\vec{\Omega}_{D_3}(k)$). W_y is the width of the quantum well. From (2)-(4), we can see that during one free flight time, the magnitudes of the spin polarization vector and its components could be obtained.

III.SIMULATION RESULTS AND DISCUSSION

Using the potential shape given by (1), we obtained the subbands' energies of quantum well. Fig.1 shows us with the calculated relation between $\lambda = \frac{\sqrt{2m^{*}eV_0}}{\hbar} Y_0$ and subband energies at 300K. Considering three subbands of the quantum well is enough because more than 94% of the electrons stay in the lowest three subbands for moderate driving electric field.

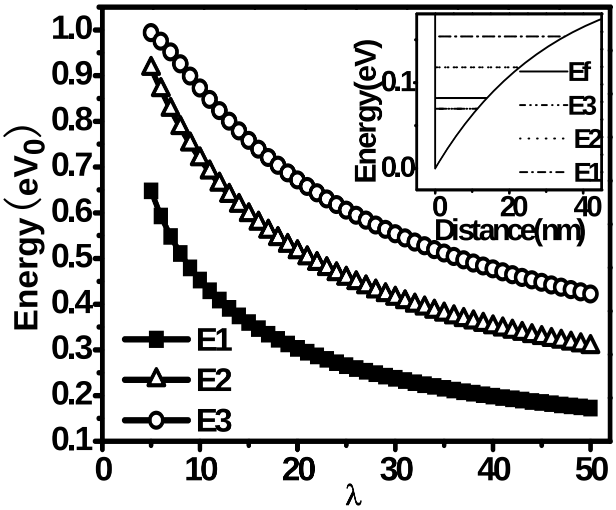

Fig.1.The calculated energy of the three subbands for different $\lambda = \frac{\sqrt{2m^{*}eV_0}}{\hbar} Y_0$ values. The inset gives us the schematic band model for GaAs/GaAlAs quantum well at 300K.

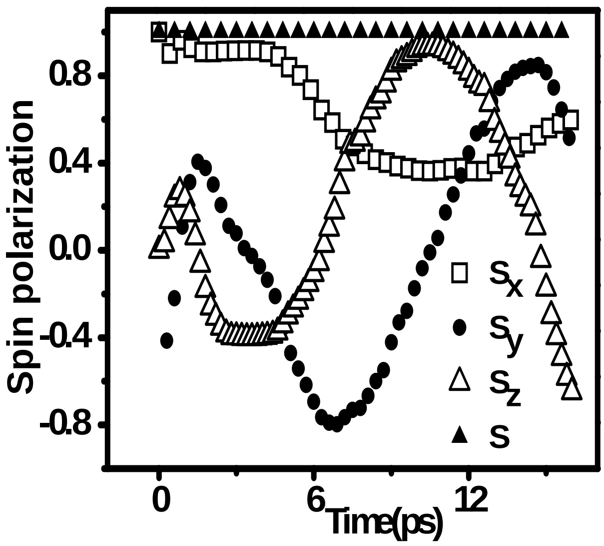

Fig.2. Precession of the components of single electron's spin polarization vector with time going in GaAs 2DEG. T=300K, E_x=0.5kV/cm, W_z=infinite.

As $\vec{\Omega}_{eff}$ depends strongly on $\vec{k}$, the moment scattering events randomize the $\vec{\Omega}_{eff}$ –direction. So, during the motion of single electron, its spin orientation becomes progressively incoherent as shown in Fig.2 This simulation result is for single electron, the electron's spin injected polarization is along the x axis. From this figure, we can see that all the three components S_x, S_y, S_z of the spin polarization vector oscillate with time going and the magnitude of the spin polarization vector equals to "1" all the time. The oscillation is due to the DP mechanism which is the most relevant spin relaxation mechanism for undoped GaAs 2DEG.

For narrow-band-gap semiconductors such as InAs, the Rashba term is the main spin dephasing mechanism; whereas for wide-band-gap semiconductors such as GaAs, the Dresselhaus term is dominant [3].Spin dephasing is simulated in the absence (Fig.3) and presence (Fig.4) of the Dresselhaus interaction. The influence of Dresselhaus effect on spin relaxation is larger than that of Rashba effect because of larger Dresselhaus spin-orbit coupling constant.

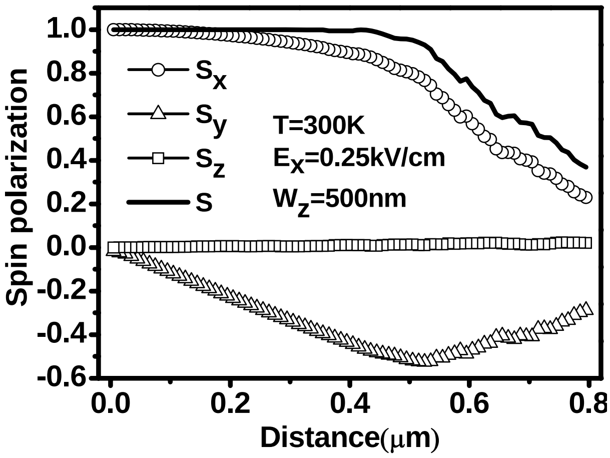

Fig.3. Spin relaxation of the GaAs 2DEG in the absence of the Dresselhaus interaction. T=300K, E_x=0.25kV/cm, W_z=500nm.

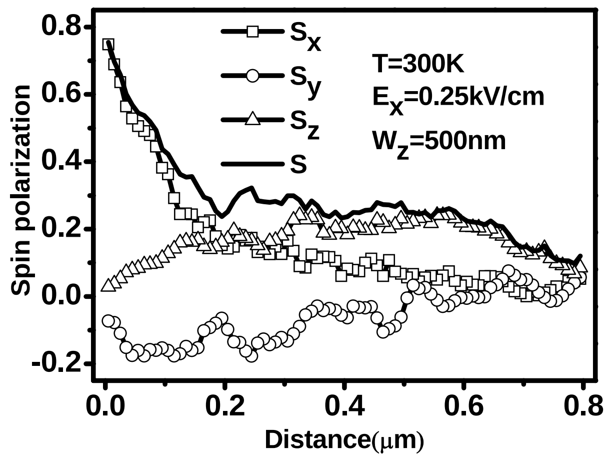

Fig.4. Spin relaxation of the GaAs 2DEG in the presence of the Dresselhaus interaction. T=300K,E_x=0.25kV/cm, W_z=500nm.

In order to check the difference of spin dephasing rates between the three-subband approximation model and the one-subband approximation model, we choose relatively lower longitudinal driving electric field which assures more than 94% of the electrons to stay in the lowest three subbands. As seen from Fig.5, the spin scattering length (L_s) becomes shorter for quantum well in the three-subband approximation than that in the one-subband approximation. This arises from the intersubband scattering and larger spin-orbit coupling constant for higher subband. Recent experiment [4] has also shown that scattering events between subbands may cause excessive spin dephasing.

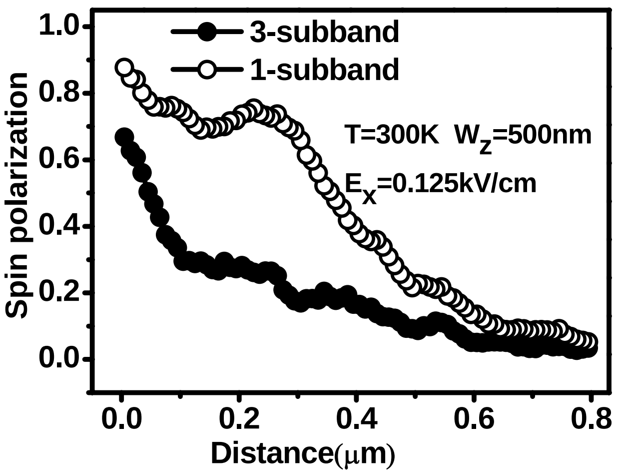

Fig.5. Comparison of the spin dephasing rates between the three-subband approximation model and the one-subband approximation model. T=300K, E_x=0.125kV/cm, W_z=500nm.

Fig.6 gives us the spin polarization distribution along the channel in quantum well in the three-subband approximation at 300K. The channel width we used in the simulation is 200nm and the driving electric field equals to 0.5kV/cm. Spin depolarizing rates will be different for different injected spin 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 equation (2).

From the spin precession equation, we can see that electrons' motion states determine their spin dephasing. However, lattice temperature and driving electric field have an influence on the change of electrons' motion states. So under different lattice temperatures and driving electric fields, electrons' spin dephasing rates will be different. As shown in Fig.7, at room temperature electrons' spin dephasing rate is slower for higher driving electric field. This originates from the smaller ratio of the electron thermal energy to its drift energy at higher voltages. The larger the ratio is, the larger the spin dephasing rate is at room temperature, and correspondingly the shorter the spin scattering length is.

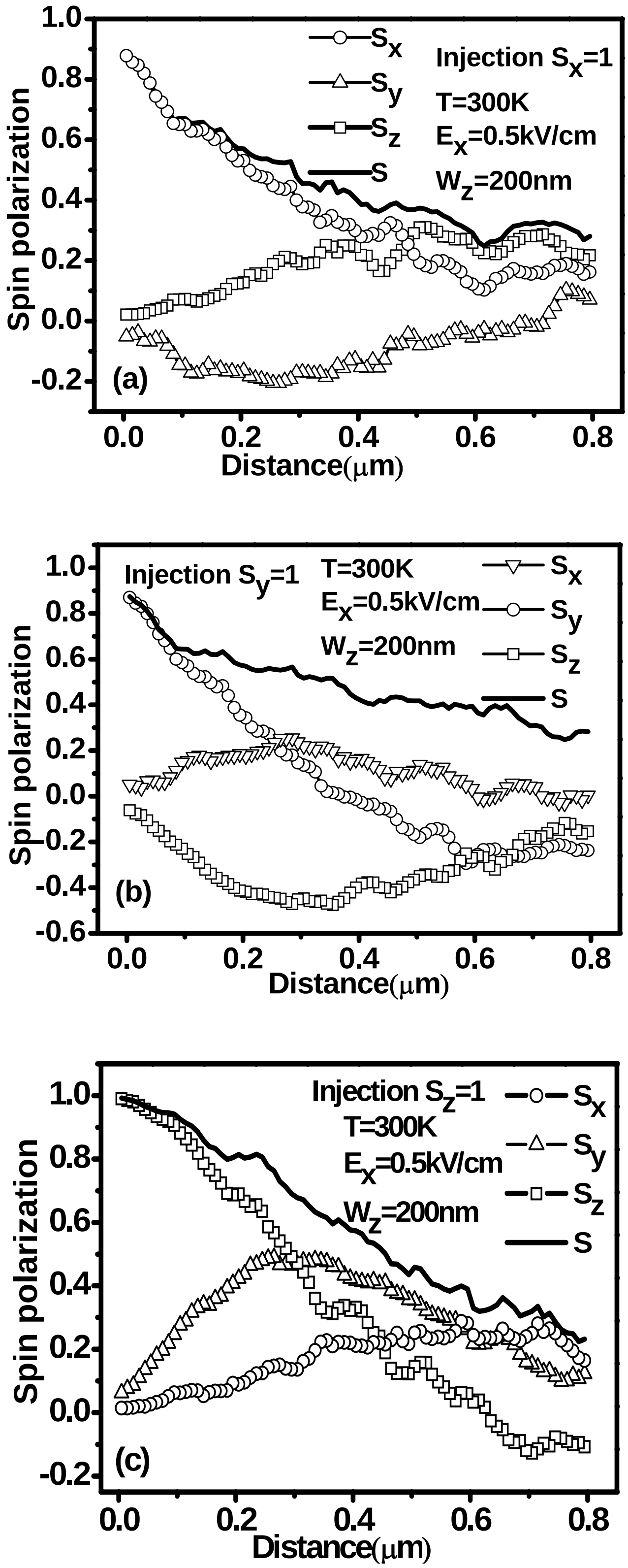

Fig.6.The spin polarization distribution in the channel for different injected spin polarizations. T=300K, E_x=0.5kV/cm, W_z=200nm.(a)-(c) correspond to injected polarization being along the x, y and z axes respectively.

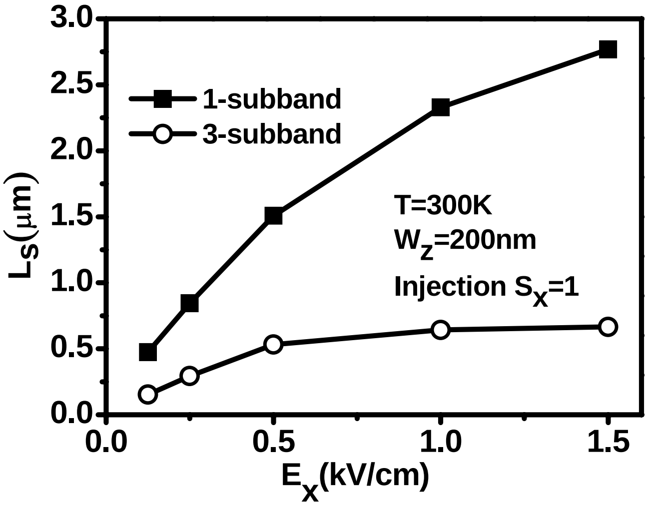

Fig.7. The spin scattering length (L_s) for different driving electric field E_x at 300K. The injected spin polarization is along the x axis. W_z=200nm.

Fig.8 tells us that at constant driving electric field , when the lattice temperature increases, the spin dephasing rate also increases and the spin scattering length becomes shorter. It is consistent with the theory that the more random the electron's motion state is in space, the faster the spin dephasing will be.

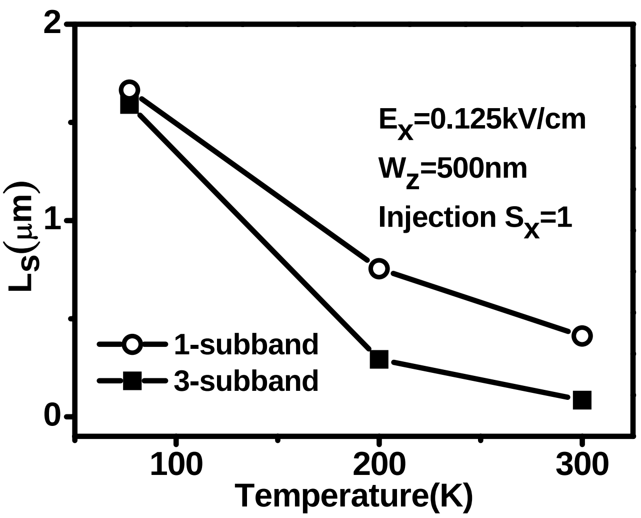

Fig.8. The spin scattering length(L_s) for different lattice temperature. E_x=0.125kV/cm, W_z=500nm. The injected spin polarization is along the x axis.

In Fig.9, spin scattering length as a function of the channel width is plotted. It is clear that the spin dephasing rate can be reduced by decreasing the channel width. When the spin injected orientation is along the x axis. the term proportional to k_x in $\vec{\Omega}_{eff}$ is the informative term and that proportional to k_z is the perturbing term. Spin dephasing is caused by the perturbing term, this term's magnitude depends on $< dz^2 >$, dz is the distance that one electron flies during one free flight time along the channel width direction.

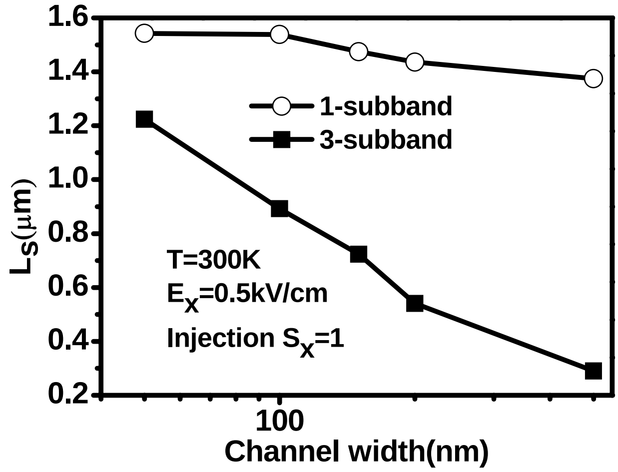

Fig.9. The spin scattering length (L_s) for different channel width. T=300K,E_x=0.5kV/cm. The injected spin polarization is along the x axis.

IV. CONCLUSION

Using the three-subband approximation model, spin-polarized transport is simulated in the 2DEG and the influence of intersubband scattering on it is considered. Our simulation results are in accordance with the conclusion made by the experiment [4].At room temperature, the larger the in-channel driving electric field is, the slower the spin polarization dephases. Higher temperature causes the magnitude of the spin polarization to decrease faster. Larger channel width will cause faster spin depolarization in the 2DEG.

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