Modeling of spin-polarized transport in semiconductor nanostructures

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Semiconductor Spintronics

Advantages

• Electric gate control
• Coupling to photons

Complications

• Electrical injection/detection
• Control for spin relaxation

Application

• Reprogrammable logic elements
• Photonic sources/detectors

SpinLED

Magneeto-optical modulator

Heterostructure Spin-FET

Hot electron Spin-FET

NRL, B. Jonker’s group

http://unit.aist.go.jp/nano-ele/spinics/

http://www.puretecmo.com/bob/

Outline

• Spin scattering in nonmagnetic semiconductors

• Spin transport in heterostructure spin-FETs
  
  Coherent precession vs. relaxation, anisotropy of spin transport, gate control

  Monte Carlo simulations

  Drift-diffusion model

• Schottky barrier devices, spin-LED
  
  Hot electron effects in electroluminescence spectra of spinLEDs

• Conclusions
Spin scattering

No direct interaction with phonons & non-magnetic impurities

Spin exchange with holes

Spin exchange with holes

\[ H_{\text{exch}} = AJ_S \delta(r) \]

p-doped semiconductors

Hyperfine interaction with nuclei

\[ H_{\text{Hf}}(r) = ASI \delta(r) \]

weak magnetic field

Spin-orbit (Elliott-Yafet)

SO mixes \( \uparrow \) and \( \downarrow \) states

\[ |k', \uparrow\rangle \]

\[ |k, \downarrow\rangle \]

impurity

narrow band-gap semiconductors

Spin-orbit (Dyakonov-Perel)

SO results in an effective magnetic field

\[ H_{\text{SO}} = -\mu B_{\text{eff}}(k)\sigma \]

no center of inversion
Precessional (Dyakonov-Perel) spin relaxation

Hamiltonian

\[ H = \frac{p^2}{2m} + V(r) + H_{SO} + \ldots \]

 Corrections to the effective mass model

Spin-orbit interaction

\[ H_{SO} = \alpha_T \left\{ \sigma_x k_x (k_x^2 - k_z^2) + \sigma_y k_y (k_y^2 - k_x^2) + \sigma_z k_z (k_x^2 - k_y^2) \right\} \]

Spins precess between the momentum scattering events

This scattering mechanism is important at high T limit
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Spin-orbit interaction in semiconductor layers

Spin-orbit interaction

\[ H_{SO} = kA\sigma \]

linear in an electron momentum

Effect of crystal inversion asymmetry (Dresselhaus term)

\[ H_D = \beta \{ \sigma_y k_y - \sigma_x k_x \} \]

Anisotropic with respect to crystallographic axes

Asymmetry of confining potential and strain effects (Rashba term)

\[ H_R = \eta(E) \left( k_y \sigma_x - k_x \sigma_y \right) \]

Can be controlled by an electric gate

Semiconductor heterostructures

donors are separated from the channel – high mobility

In$_{0.52}$Al$_{0.48}$As
n-doped In$_{0.52}$Al$_{0.48}$As
In$_{0.52}$Al$_{0.48}$As
10-20 nm

channel

In$_{0.53}$Ga$_{0.47}$As

Confining potential

\[ \Delta E_c \]

In$_{0.52}$Al$_{0.48}$As

In$_{0.53}$Ga$_{0.47}$As

Anisotropic with respect to crystallographic axes
Spin transport in semiconductor layers

**Ideal model**

1. **SO interaction**
   \[ H_{SO} \propto B_{eff}(k) \sigma \]

2. **Velocity**
   \[ v_j = \frac{1}{\hbar} \frac{\partial H}{\partial k_j} \]

**No dephasing due to k-distribution**

**Experiment, low field, low T**


**Dephasing/relaxation appears due to momentum scattering**
Heterostructure spin-FETs
Control magnetoresistance using an electric gate

Spin-FET


Controls spin precession

Non-ballistic spin-FET


Controls spin-relaxation
Would these devices be operational?
Monte Carlo device simulation scheme

Charge transport

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f - \frac{1}{\hbar} \nabla \cdot \mathbf{f} = \nabla \cdot \left( \mathbf{\nabla} f \right) + \frac{\partial f}{\partial t} \left( \frac{\partial f}{\partial t} \right)_C
\]

\[
\nabla^2 V = -\frac{e^2}{\varepsilon_s} \left( n(\mathbf{r}) - N_d \right)
\]

Spin dynamics

\[
\rho_i(t + dt) = e^{-iH_{SO}dt/\hbar} \rho_i(t) e^{iH_{SO}dt/\hbar}
\]

\[
H_{SO} = H_R + H_D
\]

Transition rate

\[
W_{k \rightarrow k'}^{i,j} = \frac{2\pi}{\hbar} |\langle \mathbf{k}' | T_j | \mathbf{k} \rangle|^2 \delta \left( E_k - E_{k'} \pm \hbar \omega \right)
\]

Sources of scattering

- acoustic phonon
- optic phonon
- charged impurity

Other momentum and spin scattering mechanisms can be added easily
Electron transport properties

- Energy (meV) vs. distance (μm)
- Concentration (10^{12} cm^{-2}) vs. distance (μm)
- Velocity (10^5 m/sec) vs. distance (μm)

- **Boundary effects**
- **Drift regime**

- **Effective T?**
- **T = 300 K**

- Source drain
- \(V_{DS} = 0.05 \text{ V}\)
- \(V_{DS} = 0.1 \text{ V}\)
- \(V_{DS} = 0.15 \text{ V}\)
- \(V_{DS} = 0.2 \text{ V}\)
- \(V_{DS} = 0.25 \text{ V}\)

- **In0.52Al0.48As**
- **In0.53Ga0.47As**
- **n-doped In0.52Al0.48As**

- \(L = 550 \text{ nm}\)
- \(L_{Z} = 550 \text{ nm}\)
- \(Z \times X \times Y\)
Spin dynamics

(1 0 0) transport direction

Injection $P_x=1$

Spin polarization, $P$

Spin evolution

Spin scattering length

Injection $S_x=1$

Spin precession angle

$T = 77$ K

$\delta \phi_{end} \sim 90^\circ$

$X (\mu m)$

$P_x$

$P_y$

$P_z$

$V_{DS}=0.05 V$

$V_{DS}=0.1 V$

$V_{DS}=0.15 V$

$V_{DS}=0.2 V$

$V_{DS}=0.25 V$

$X (\mu m)$

$T, K$

$V_{DS}$

$V_{DS}$

$V_{DS}$

$V_{DS}$

$V_{DS}$

$V_{DS}$
Spin scattering anisotropy

Electron transport is isotropic
Spin scattering length depends on transport direction

(110) and (1-10) are not equivalent

Spin scattering length depends on transport direction

T = 300 K

(1 0 0) direction $\xi=0^\circ$
(1 -1 0) direction $\xi=-45^\circ$
(1 1 0) direction $\xi=45^\circ$
Monte Carlo simulation

- Flexibility
- High precision

vs.

- Time consumption
- Unclear physics

Simpler, but less precise model

Drift and diffusion
Quantum mechanical description

Hamiltonian

\[ H = \frac{\mathbf{p}^2}{2m^*} + V(\mathbf{r}) + H_{SO} \]

Spin-orbit interaction

\[ H_{SO} = kA\sigma \]

Effect of quantum well asymmetry (Rashba term)

\[ H_R = \eta(k_y\sigma_x - k_x\sigma_y) \]

Isotropic with respect to crystallographic axes

Effect of crystal inversion asymmetry (Dresselhaus term)

\[ H_D = \beta((k_y\sigma_y - k_x\sigma_x) \cos 2\xi + (k_y\sigma_x + k_x\sigma_y) \sin 2\xi) \]

Anisotropic with respect to crystallographic axes

Equation for density matrix

\[
\frac{i\hbar}{\partial t} \frac{\partial \rho}{\partial t} = -\frac{\hbar^2}{m^*} \sum_j \frac{\partial^2 \rho}{\partial R_j \partial \Delta r_j} + (V(\mathbf{R} + \Delta \mathbf{r}/2) - V(\mathbf{R} - \Delta \mathbf{r}/2))\rho + \frac{i}{2} \sum_{j,\alpha} A_{ja} \left\{ \sigma_\alpha, \frac{\partial \rho}{\partial R_j} \right\} + i \sum_{j,\alpha} A_{ja} \left[ \sigma_\alpha, \frac{\partial \rho}{\partial \Delta r_j} \right]
\]
Drift-diffusion equations

Wigner function eqn.

\[
\frac{\partial W}{\partial t} + \frac{1}{2} \left\{ v_j, \frac{\partial W}{\partial x_j} \right\} - \frac{1}{\hbar} \frac{\partial V}{\partial x_j} \frac{\partial W}{\partial k_j} + ik_j [v_j, W] = StW
\]

Wigner function \( W = \frac{1}{2} (W_nI + W_{\sigma_\alpha} \sigma_\alpha) \)  
Velocity \( v_j = (v_n^j I + v_{\sigma_\alpha}^j \sigma_\alpha) \)

Projections to the set of the basis matrixes \((\sigma_\alpha, \alpha=x,y,z \text{ and } l)\)

Particle density and current density definitions

\[
n_n = \int W_n d^2 k, \quad J_n^j = \int (v_n^j W_n + v_{\sigma_\alpha}^j W_{\sigma_\alpha}) d^2 k, \\
n_{\sigma_\alpha} = \int W_{\sigma_\alpha} d^2 k, \quad J_{\sigma_\alpha}^j = \int (v_n^j W_{\sigma_\alpha} + v_{\sigma_\alpha}^j W_{\sigma_\alpha}) d^2 k.
\]

\[
\frac{\partial n_n}{\partial t} + \frac{\partial J_n^j}{\partial x_j} = 0, \\
\frac{\partial n_{\sigma_\alpha}}{\partial t} + \frac{\partial J_{\sigma_\alpha}^j}{\partial x_j} - \frac{2m^*}{\hbar} [v_{\sigma_\alpha}^j \times J_{\sigma_\alpha}^j] = 0.
\]

\[
J_n^j = -\frac{\tau}{m^*} \left( kT \frac{\partial n_n}{\partial x_j} + \frac{\partial V}{\partial x_j} n_n \right), \\
J_{\sigma_\alpha}^j = -\frac{\tau}{m^*} \left( kT \frac{\partial n_{\sigma_\alpha}}{\partial x_j} + \frac{\partial V}{\partial x_j} n_{\sigma_\alpha} - \frac{2m^* kT}{\hbar} [v_{\sigma_\alpha}^j \times n_{\sigma_\alpha}] \right).
\]
Example 1

Case $\eta(E) = \beta$, anisotropy of spin transport

Spin dephasing length

$$L_\perp = \left( \frac{\mu E}{2D} + \sqrt{\left( \frac{\mu E}{2D} \right)^2 + B_{yz}^2} \right)^{-1}$$

Spin precession length

$$L_p = \frac{2\pi}{B_{xz}}$$

where

$$B_{xz} = \left( \frac{2m^*}{\hbar^2} \right) \sqrt{\eta^2 + \beta^2} - 2\eta \beta \sin 2\xi$$

$$B_{yz} = -\left( \frac{2m^*}{\hbar^2} \right)^2 2\eta \beta \cos 2\xi / B_{xz}$$
Example 2
Can we control spin relaxation using an electric gate?

Device structure

Spin density

\[ n_{\sigma}(x,V_g) = n_{\sigma}(0,V_g) e^{-\frac{x}{L(V_g)}} \]

Spin scattering length

\[
L(V_g) = \left( \frac{\mu E_\parallel}{2D} + \sqrt{\left( \frac{\mu E_\parallel}{2D} \right)^2 + \left( \frac{2m \times (\gamma - \eta_R)}{\hbar^2} \right)^2} \right)^{-1}
\]

field dependent parameters

Modulation

\[
\Gamma_{\sigma,n} = \frac{n_{\sigma,n}(a,V_{g}^{\text{off}})}{n_{\sigma,n}(a,V_{g}^{\text{on}})}
\]

Spin polarization

\[ \Lambda = (1 - \frac{\Gamma_{\sigma}}{\Gamma_n}) \times 100\% \]

\[ \Lambda \approx 15\% \]

at room temperature
Partial conclusion

- There is a number of issues related to functionality of heterostructure spin-FETs, but the physical phenomena of polarization precession and gate control of spin relaxation in semiconductor heterostructures could be observable at room temperature.
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Electron injection through a Schottky barrier

Injection mechanisms

- Thermionic injection
- Field injection

Modified Schottky barrier Fe/GaAs

Field injection is weak unless strong bias is applied

$V_{SB} \quad eV_{bias} \quad E_{c} \quad E_{fs}$

$n$-doped SC

$w = 0 \quad w = 15 \text{ nm} \quad w = 25 \text{ nm} \quad w = 45 \text{ nm} \quad w = 95 \text{ nm}$

$V_{bias} = 0.1 \text{V}$

$w = 25 - 95 \text{nm}$

$n+$ doped interface
Spin-light-emitting diode

**Electroluminescence (1,0,0)**

Sample 1
T = 6 K

- EL Spectra
- $X$
- a
- $X_{bulk}$

Sample 1
T = 6 K

- EL Spectra
- $X$
- a
- $X_{bulk}$
Spin-LED

Electroluminescence (1,0,0)

ΔE~84 cm⁻¹ = TA phonon at X

Simulated device structure

Monte Carlo simulation accounts for transport in \( \Gamma, L, \) and \( X \) valleys

Potential profile

- \( V = 1.0 \) V
- \( V = 1.2 \) V
- \( V = 1.5 \) V
- \( V = 2.5 \) V
- \( V = 3.0 \) V

Potential profile:

\[ V = 1.0 \text{ V} \]
\[ V = 1.2 \text{ V} \]
\[ V = 1.5 \text{ V} \]
\[ V = 2.5 \text{ V} \]
\[ V = 3.0 \text{ V} \]
Transport near Schottky barrier

Electrons redistributed into upper valleys

Spin polarization decays faster in upper valleys due to stronger SO int.
Spin-LED

**Electroluminescence (1,1,0)**

Sample 3
T = 6 K

- EL Spectrum
- X
- a
- X_{Bulk}
- Bulk feature

\[ \Delta E \approx 105 \text{ cm}^{-1} \sim \text{phonon at K} \]

Brillouin zone GaAs

K point is along (1,1,0) direction

Model

AlGaAs \((p)\)  \(\Delta\)

AlGaAs \((n)\)  \(\Sigma\)

GaAs  \(\Gamma\)  \(L\)

Electron transition schematic:

- \(e_1\) to \(\Delta\)
- \(h\omega\) to \(A^0\)

- \(h\omega\) to \(A^-\)
Conclusions

• Gate control for spin relaxation and spin precession in semiconductor heterostructure devices is feasible at room temperature.

• Hot electron effects are important in spintronic devices utilizing Schottky barriers for spin injection.

• Spin transport simulation is an important tool to study functionality of novel spintronic devices.
Thank you