Monte Carlo simulation of spin injection and coherent transport in a heterostructure device with a Schottky source contact

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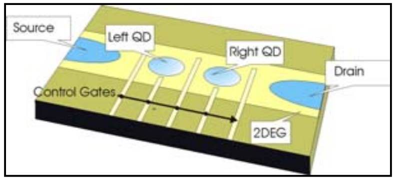
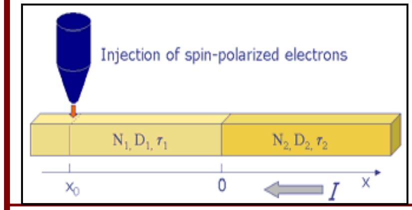
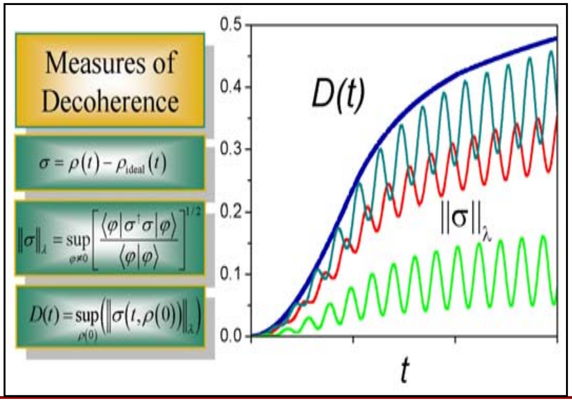
Research Objectives

The main objectives of our program have been to explore coherent quantum mechanical processes in novel solid-state semiconductor information processing devices with components of atomic dimensions. These include quantum computers, spintronic devices, and nanometer-scale logic gates.







Measures of Decoherence

$$\sigma = \rho(t) - \rho_{\text{ideal}}(t)$$

$$\|\sigma\|_\lambda = \sup_{\varphi \neq 0}\left[\frac{\langle\varphi|\sigma^\dagger\sigma|\varphi\rangle}{\langle\varphi|\varphi\rangle}\right]^{1/2}$$

$$D(t) = \sup_{\rho(0)}\left(\|\sigma(t,\rho(0))\|_\lambda\right)$$

Significant Results

Our achievements to date include:

- ✓ new measures of initial decoherence, and evaluation of decoherence for spins in semiconductors;
- ✓ evaluation of solid-state quantum computing designs;
- ✓ studies of transport associated with quantum measurement;
- ✓ investigation of spin-polarized devices and role of nuclear spins in spintronics and quantum computing;
- ✓ general contributions to quantum computing algorithms and to time-dependent and phase-related properties of open many-body quantum mechanical systems;
- ✓ novel analytical and numerical Monte Carlo approaches to studying spin-polarization control for spintronic device modeling;
- ✓ investigation of spin relaxation dynamics in two-dimensional semiconductor heterostructures.

Approach

Our approach has been truly interdisciplinary. For example, in developing new measures of decoherence for quantum computing, we have employed concepts from many-body quantum physics, computer error-correction algorithms, and nonequilibrium statistical mechanics. In our description of spintronic devices, we have utilized large-scale Monte Carlo simulations, knowledge from solid-state physics of semiconductors and from the microelectronics area of electrical engineering, as well as novel ideas of coherent control of quantum dynamics.

Our approach has been to design and evaluate architectures that allow implementation of many gate cycles during the relaxation and decoherence times. This requires development of techniques to evaluate all the relevant time scales: single- and two-quantum-bit gate “clock” times, as well as time scales of relaxation processes owing to the quantum bit (e.g., spin) interactions with environment, such as phonons or surrounding spins. We have also studied spin-control and charge carrier transport for spintronics and quantum measurement.

Broader Impact

We have extensive research *collaborations* with leading experimental and theoretical groups. The *educational impact* has included training undergraduate and graduate students, postdoctoral researchers, and development of three new courses to introduce quantum device and quantum algorithmic concepts to graduate and undergraduate students. Our program has contributed to *homeland security* and received funding from the National Security Agency.

Our outreach program has included sponsoring presentation events, and an international workshop series *Quantum Device Technology*, held in May of 2002 and May 2004, and sponsored by the Nanotechnology Council of IEEE and NSA (via ARO). We have worked with the REU site for students at SUNY Potsdam to guide several *undergraduate research projects* in the topics of quantum computing and quantum algorithms.

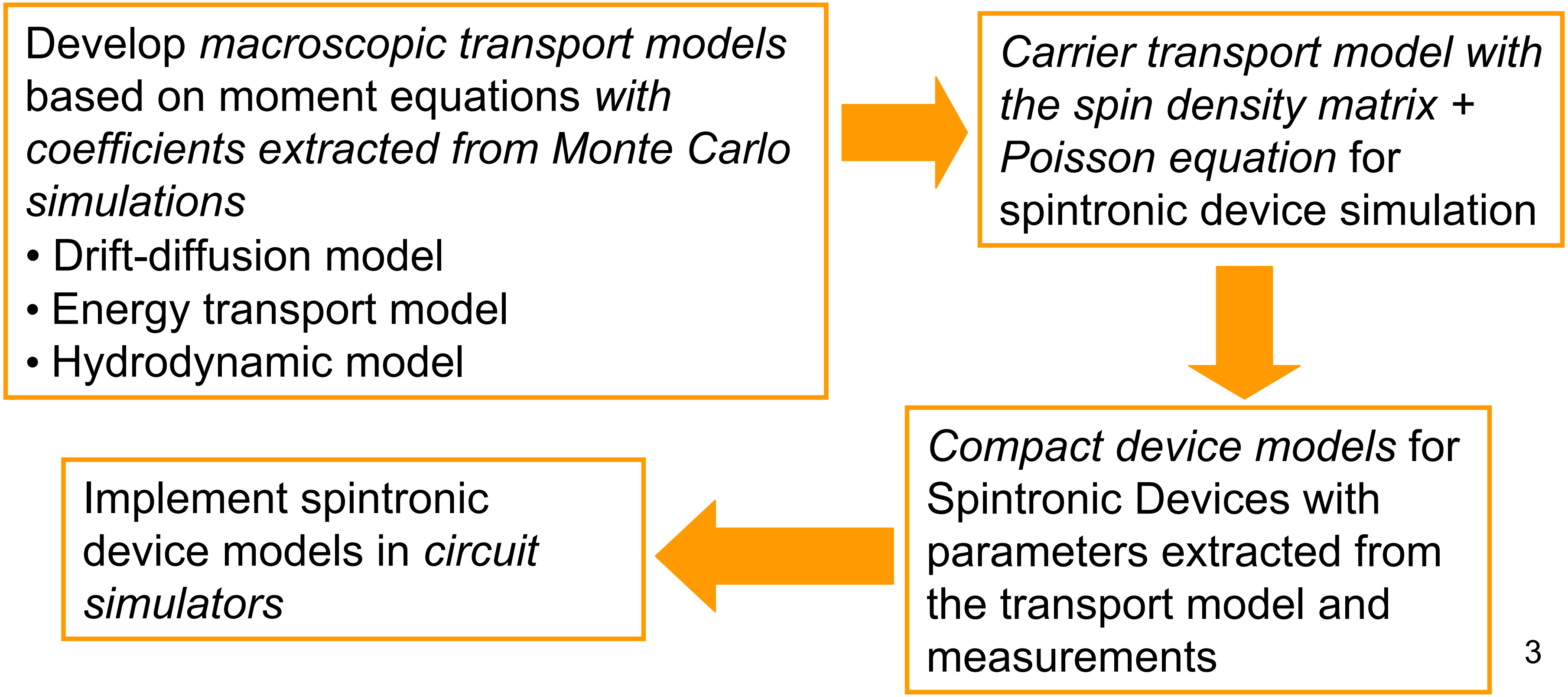
Semiconductor Spintronics Device Modeling

Center for Quantum Device Technology at Clarkson University

Short Term Goal:

Develop Monte Carlo methods for realistic spintronic device structures with unknown coefficients extracted from experimental measurements

Long Term Goal: to develop tools for engineering application



Develop *macroscopic transport models* based on moment equations *with coefficients extracted from Monte Carlo simulations*

- Drift-diffusion model
- Energy transport model
- Hydrodynamic model

Carrier transport model with the spin density matrix + Poisson equation for spintronic device simulation

Compact device models for Spintronic Devices with parameters extracted from the transport model and measurements

Implement spintronic device models in *circuit simulators*

Monte Carlo Simulation for Spin FETs

Charge transport

- $\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f - \frac{1}{\hbar} \frac{\partial V}{\partial \mathbf{x}} \nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t} \right)_C$
- $\nabla^2 V = -\frac{e^2}{\varepsilon_{\mathrm{s}}} \left(n(\mathbf{r}) - N_{\mathrm{d}} \right)$

Spin dynamics

- $\rho_i(t+dt) = e^{-iH_{\mathrm{SO}} dt/\hbar} \rho_i(t) e^{iH_{\mathrm{SO}} dt/\hbar}$
- $H_{SO} = H_{\mathrm{R}} + H_{\mathrm{D}}$

Specific mechanisms in 2D III-V semiconductors

1. **Rashba term**

   Effect of quantum well asymmetry

   $$H_R = \eta \left(k_y \sigma_x - k_x \sigma_y \right)$$

   Linear spin orbit interaction

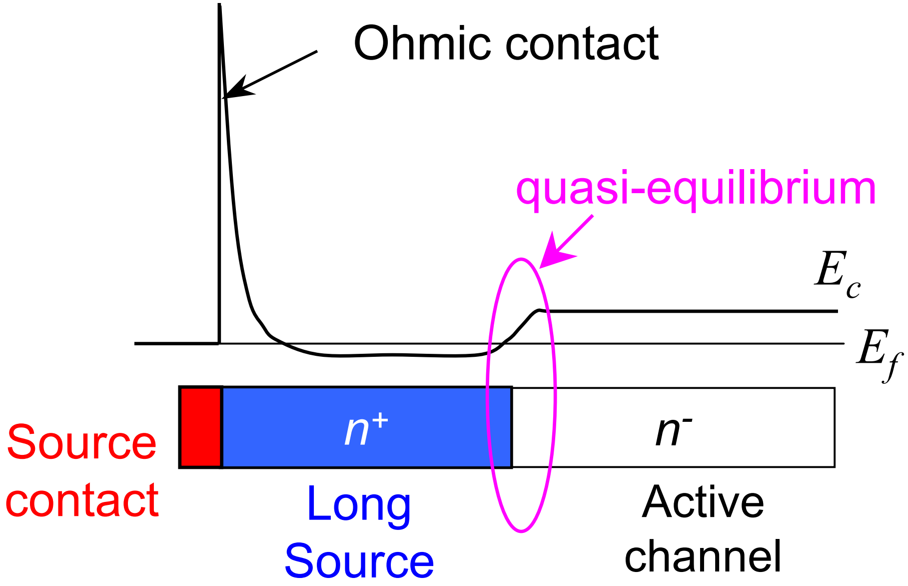
2. **Dresselhaus term**

   Effect of crystal inversion asymmetry

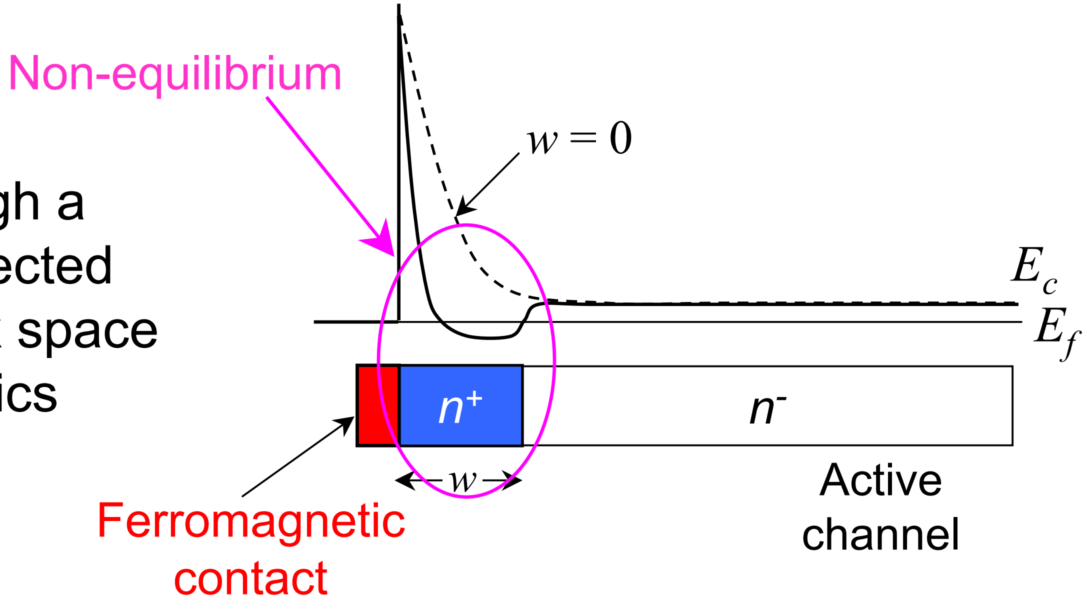
   $$H_{\mathrm{D}} = \beta [(\langle k_z^2 \rangle - k_x^2) \sigma_y k_y - (\langle k_z^2 \rangle - k_y^2) \sigma_x k_x]$$

   Include high order terms up to three order momentum

- In traditional electronic devices, the equilibrium boundary condition is always assumed

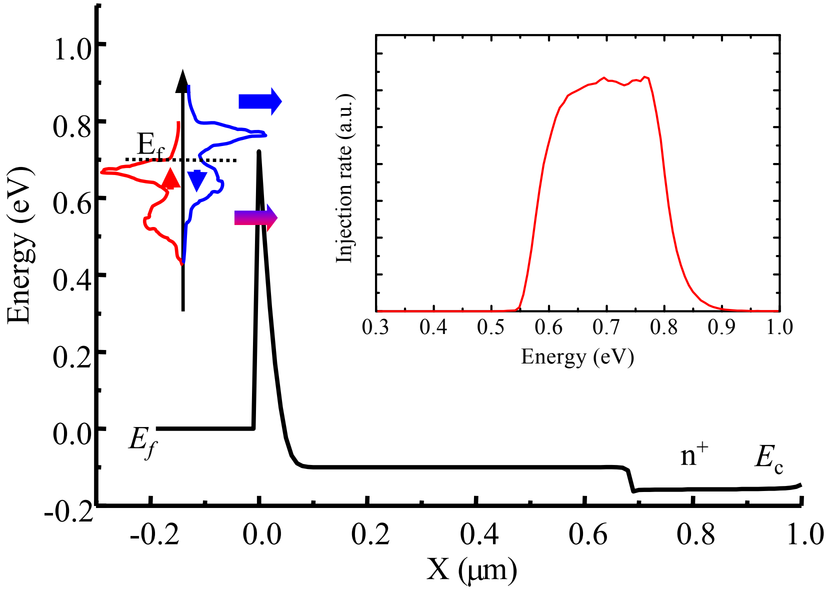


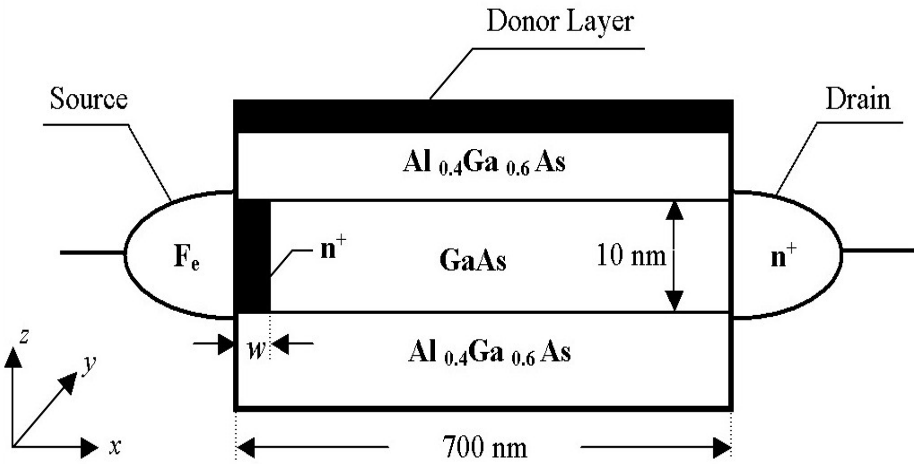
- For spin injection through a Schottky barrier, the injected electron distribution in **k** space is crucial to spin dynamics



Spin Injection Through a Schottky Barrier

Fe/GaAs 2DEG





Assumptions

- Spin polarization of electrons in the metal contact is determined by the densities of states for spin-majority and spin-minority carriers
- The tunneling probability of electrons is based on WKB approximation
- Electrons in the metal source contact are assumed thermalized
- Collection of electrons in the drain is assumed spin-independent.

Electrons at the Ferromagnetic Contact

- Electron distribution function:

$$f(E) = \frac{1}{1 + e^{(E - E_{fm})/k_B T}} \sim e^{-(E - E_{fm})/k_B T}$$

- Equal average kinetic energy in *x*, *y* and *z* directions

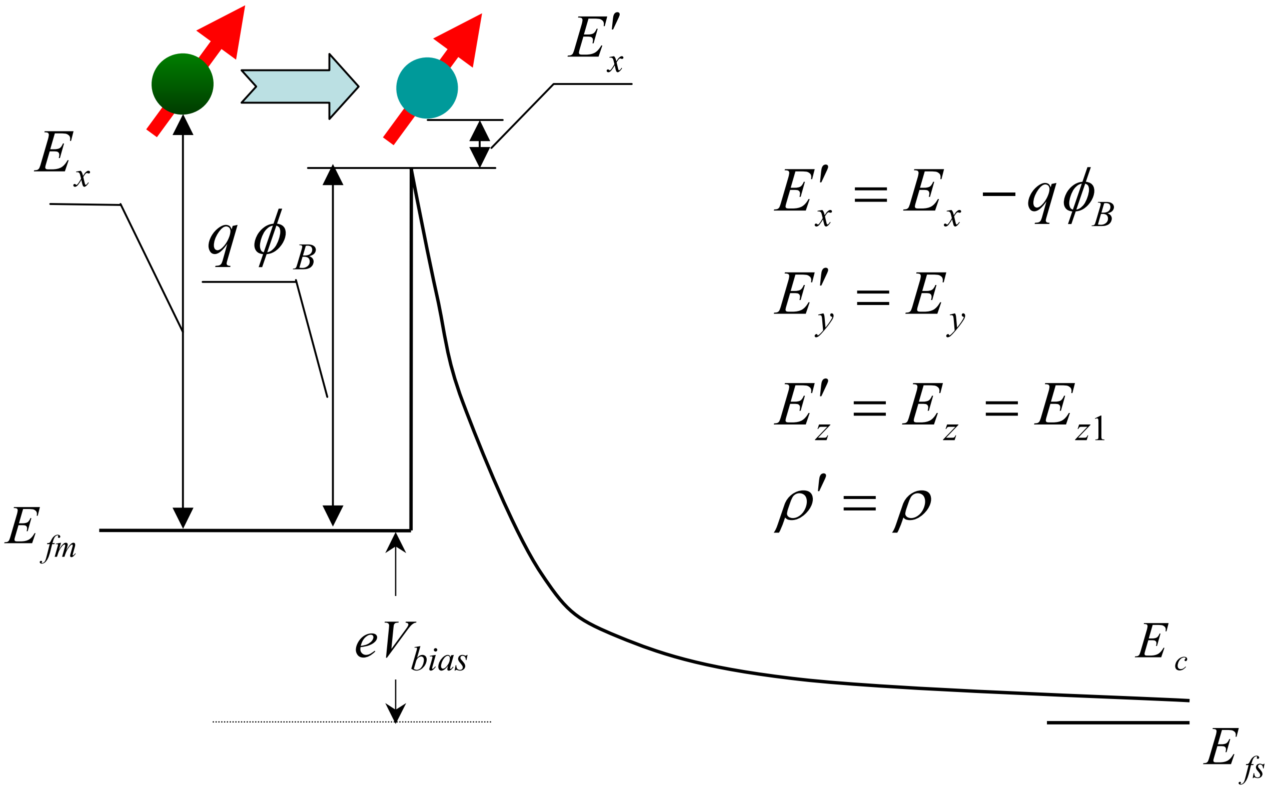
- Probabilities of spin states are based on the densities of states

$$P_{\uparrow}(E) = \frac{D_{\uparrow}(E)}{D_{\uparrow}(E) + D_{\downarrow}(E)} \quad \text{and} \quad P_{\downarrow} = 1 - P_{\uparrow}$$

Injection Mechanisms:

Thermionic Emission & Tunneling

- **Thermionic Emission:** $E_x > q\phi_B$ & spin is conserved



$$E'_x = E_x - q\phi_B \qquad k'_x = \sqrt{2m^* E'_x}\,/\,\hbar$$

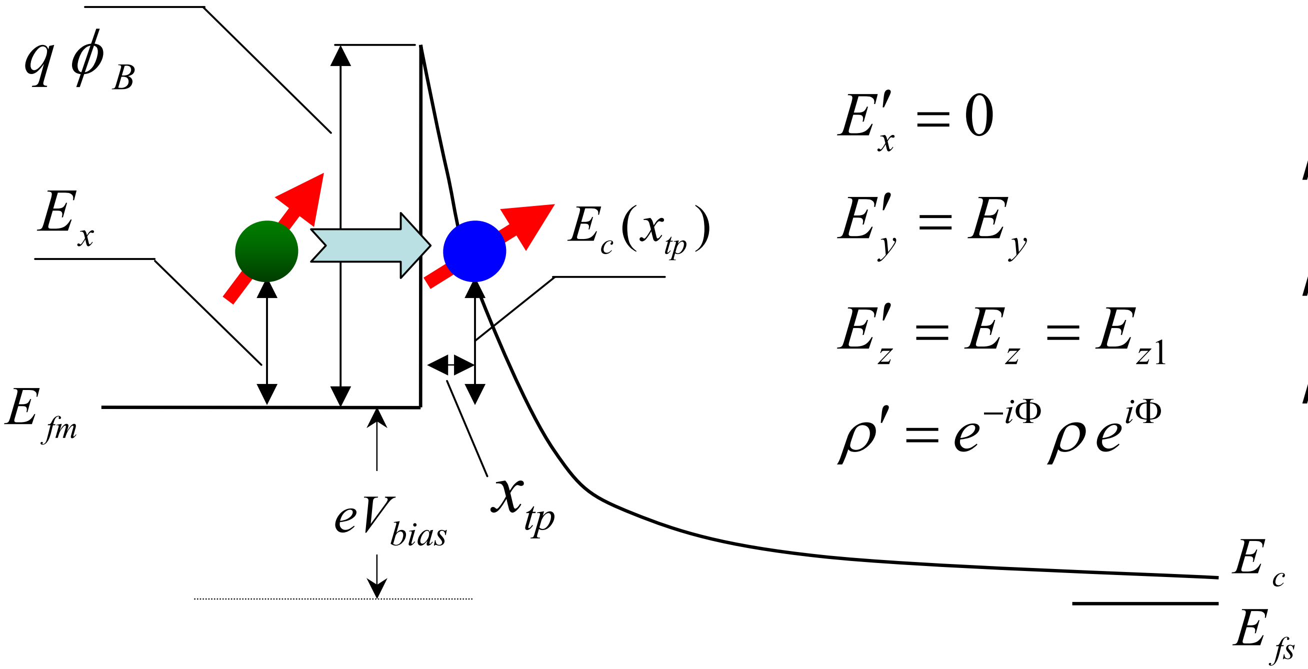
$$E'_y = E_y \qquad k'_y = \pm\sqrt{2m^* E'_y}\,/\,\hbar$$

$$E'_z = E_z = E_{z1} \qquad k'_z = k_{z1} = \pm\pi\,/\,d$$

$$\rho' = \rho$$

- **Tunneling through the Schottky barrier:** $E_x < q\phi_B$

Tunneling probability: $T_{\mathrm{tp}}(E) = \exp\left(-\frac{2}{\hbar}\int_0^{x_{tp}} \sqrt{2m^*[E_c(x) - E]}\, dx\right)$
(WKB approximation)

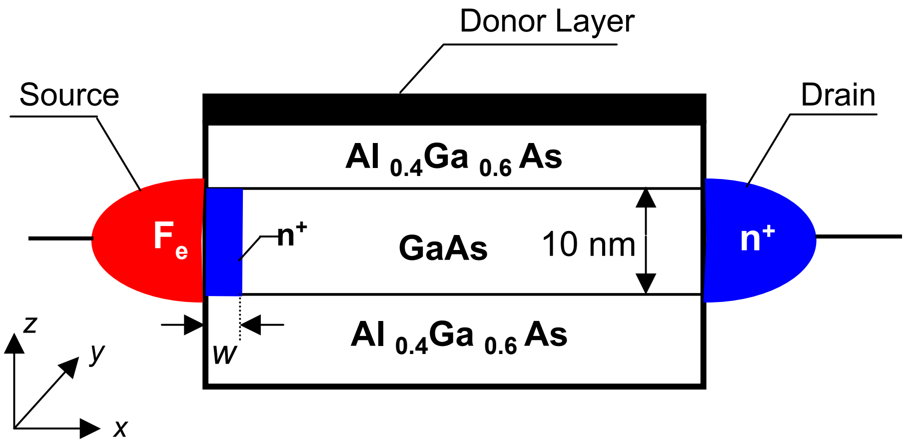


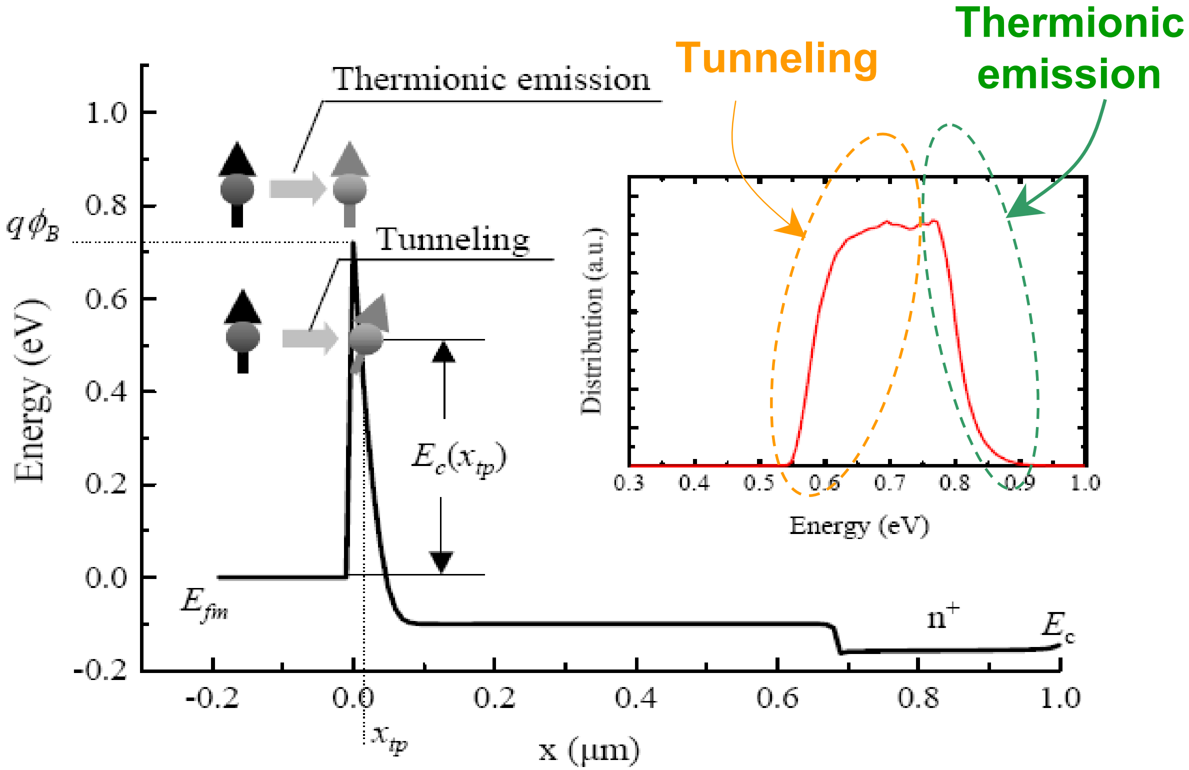
$$E'_x = 0$$
$$E'_y = E_y$$
$$E'_z = E_z = E_{z1}$$
$$\rho' = e^{-i\Phi}\rho\, e^{i\Phi}$$

$$k'_x = 0$$
$$k'_y = \pm\sqrt{2m^* E'_y}\,/\,\hbar$$
$$k'_z = k_{z1} = \pm\pi / d$$

$$\Phi = [\beta < k_{z1}^2 > (\sqrt{E_y / E_x}\sigma_y - \sigma_x) + \eta(\sqrt{E_y / E_x}\sigma_x - \sigma_y)]\frac{x_{tp} m^*}{\hbar^2}$$

Device Structure





$$w = 0$$

$$q\phi_B = 0.72\,(\mathrm{eV})$$

$$\eta = 0.005\ \mathrm{eV\AA}$$

$$\beta = 28\ \mathrm{eV\AA^3}$$

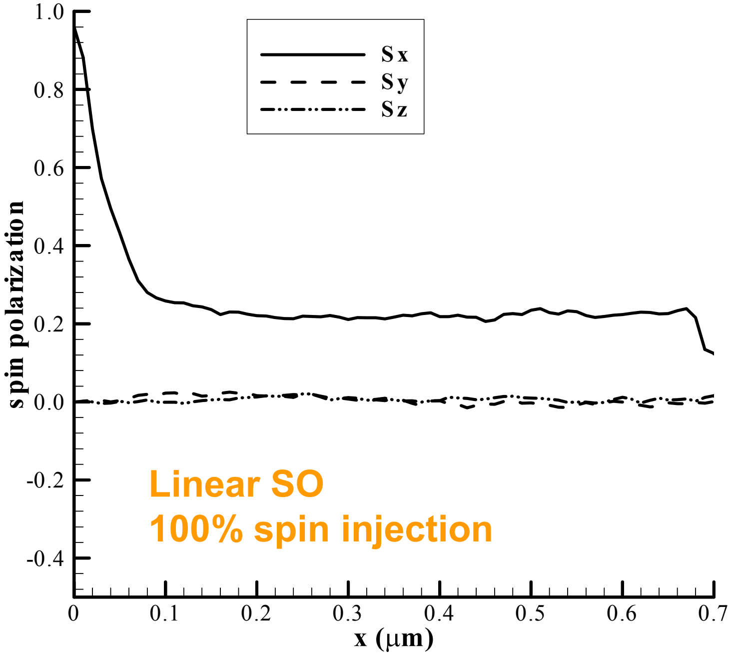
$$V_{bias} = 0.1\mathrm{V}$$

$$H_D >> H_R$$

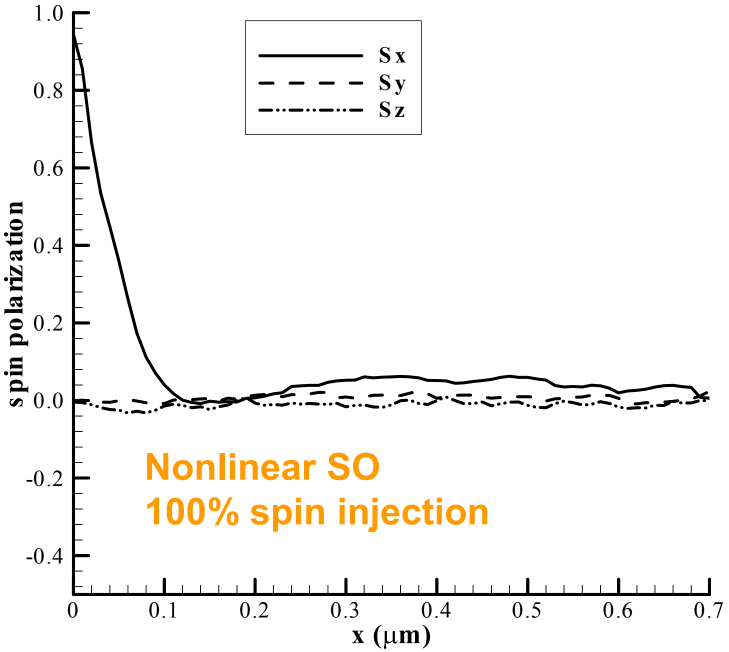
Spin Polarization

with injection in the *x* direction

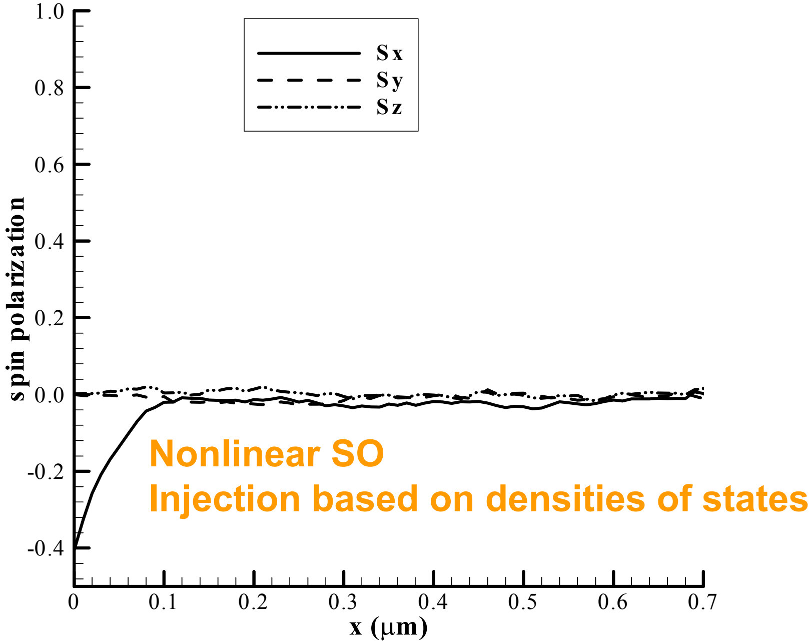
$w = 0$



Linear SO
100% spin injection



Nonlinear SO
100% spin injection



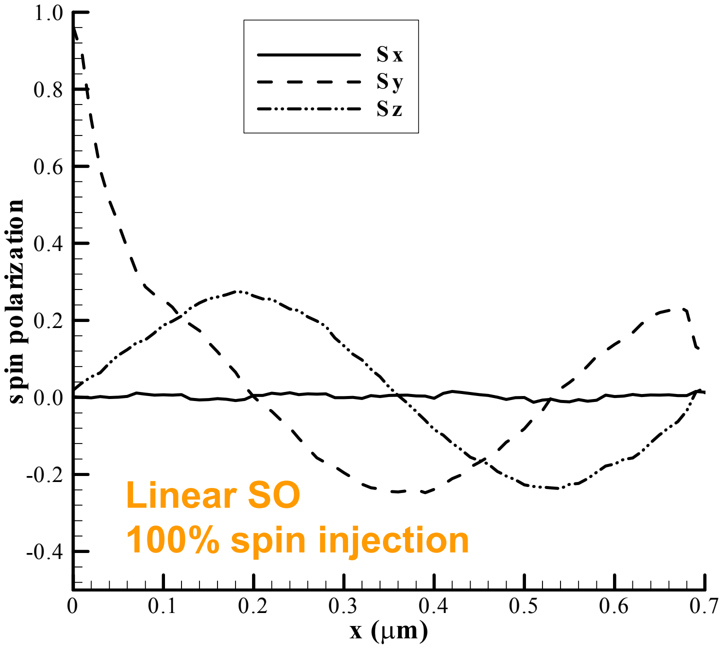
Nonlinear SO
Injection based on densities of states

Nonlinear spin orbit interaction substantially reduces spin dephasing length (< 0.1 μm) with the injection in the *x* direction

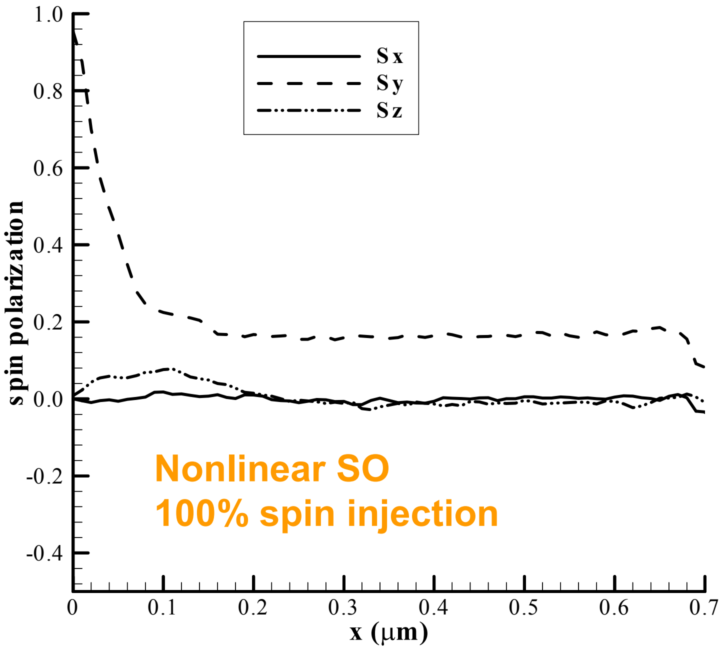
Spin Polarization

with injection in the *y* direction

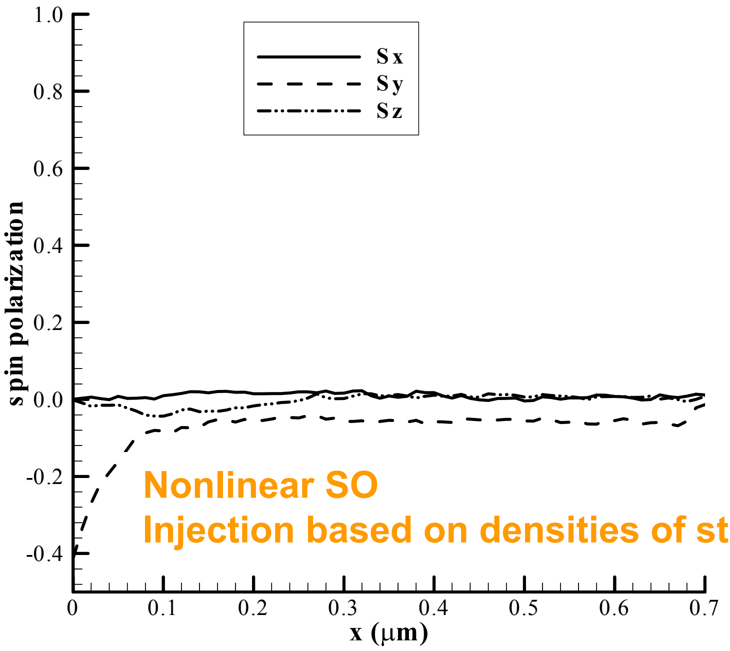
$w = 0$



Linear SO
100% spin injection



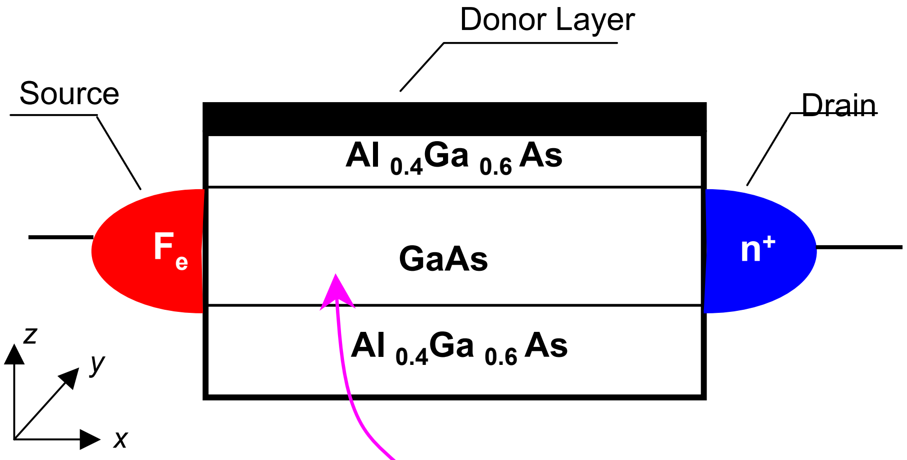
Nonlinear SO
100% spin injection



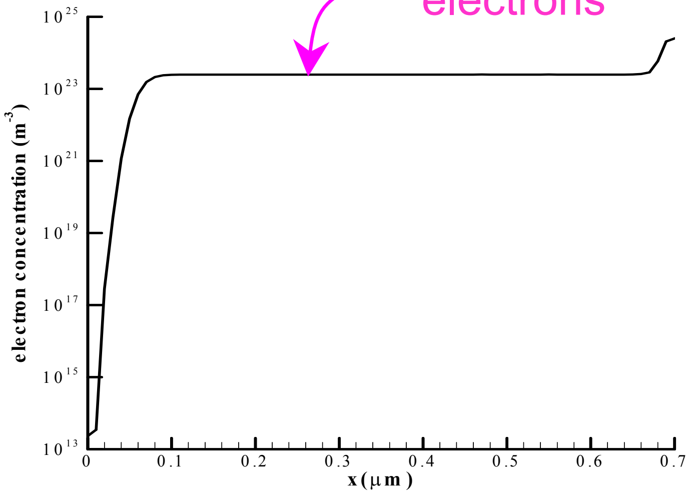
Nonlinear SO
Injection based on densities of states

Nonlinear spin orbit interaction reduces spin dephasing length (~ 0.1 µm) in the *y* direction

- Spin polarization was calculated only for injected electrons
- Inclusion of the existing non-polarized electrons ➔ spin dephasing length << 0.1 μm



A large number of non-polarized electrons



- Spin flux:

$$J_{S_\alpha} = \sum_i v_x^i Tr(S_\alpha \rho_i)$$

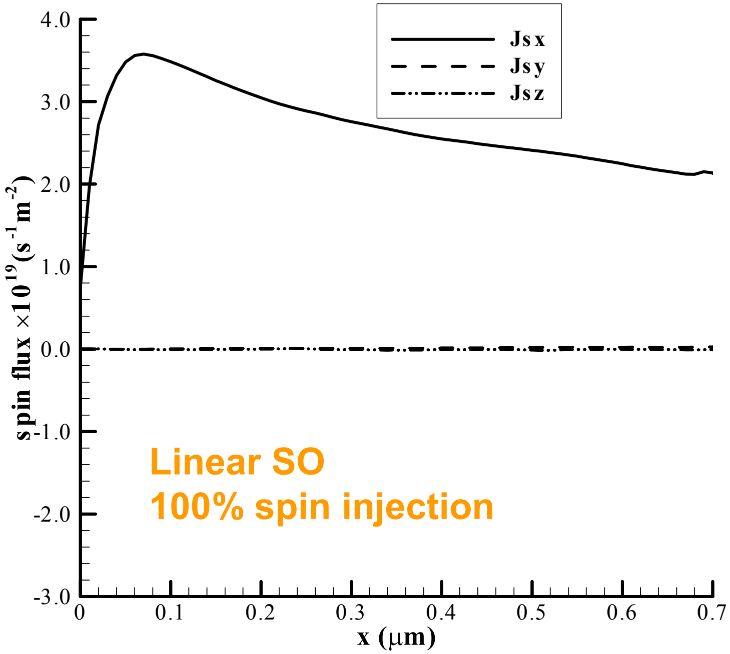
- Polarization of spin current:

$$P^J = \sqrt{\sum_{\alpha=x,y,z} J_{S\alpha}^2} \Big/ J$$

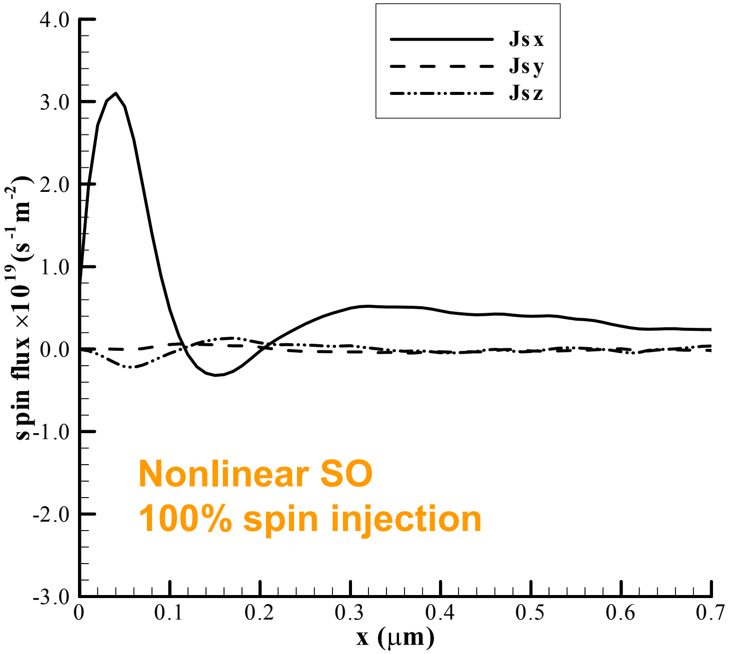
Spin Flux

with injection in the *x* direction

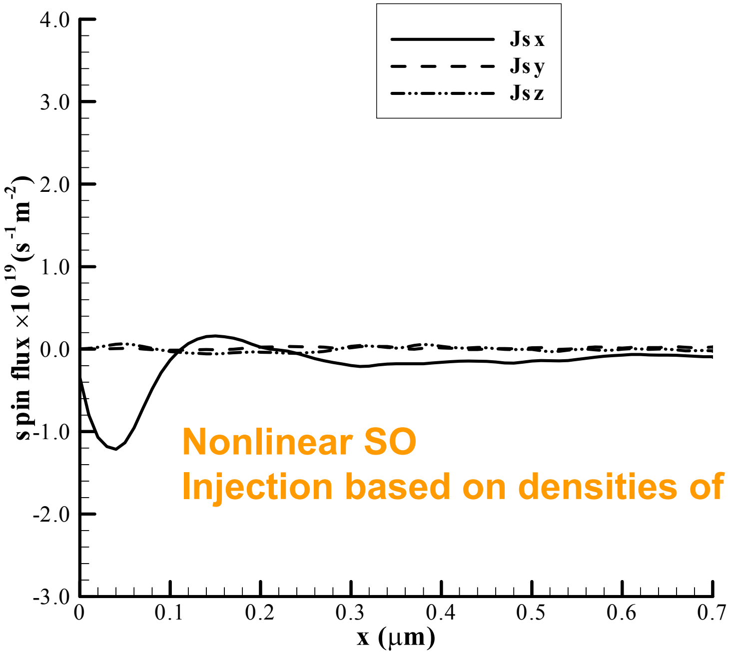
$w = 0$



Linear SO
100% spin injection



Nonlinear SO
100% spin injection



Nonlinear SO
Injection based on densities of states

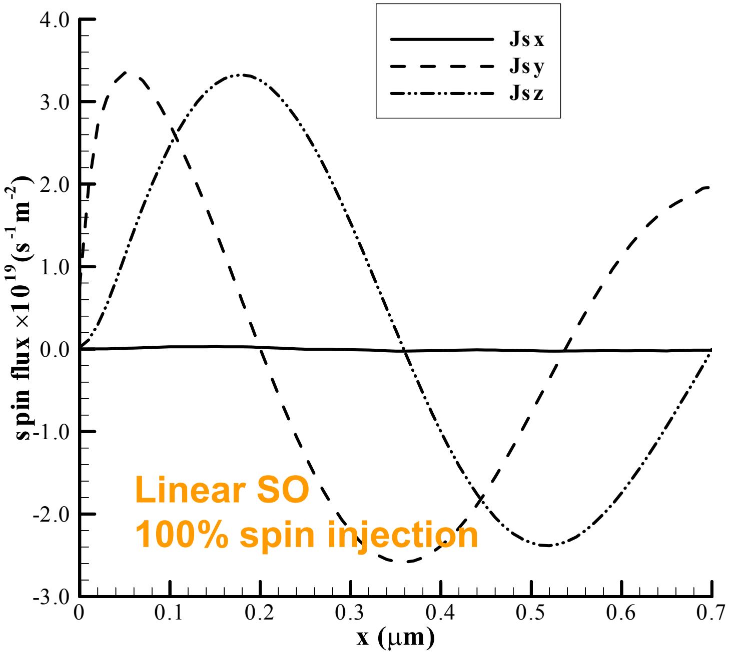
Linear SO: spin dephasing length > 0.7 μm

Inclusion of nonlinear SO interaction substantially reduces the spin dephasing length with the injection in the *x* direction

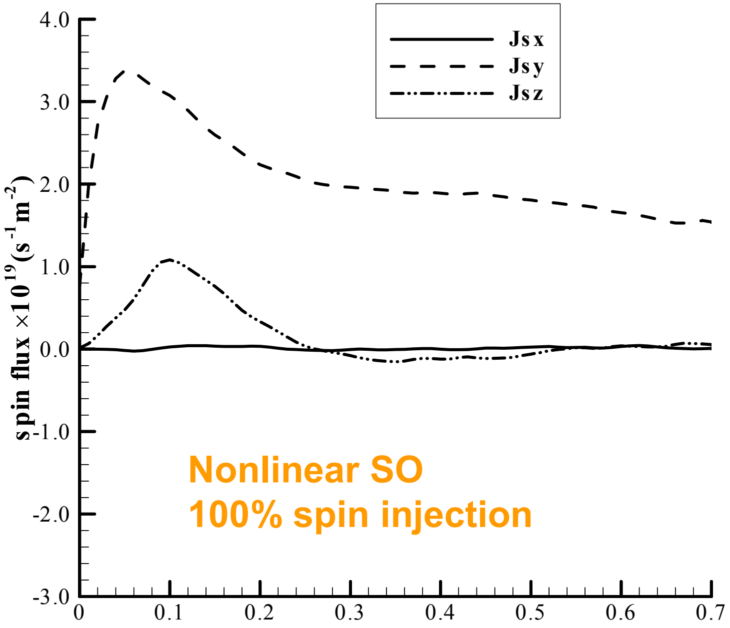
Spin Flux

with injection in the *y* direction

$w = 0$



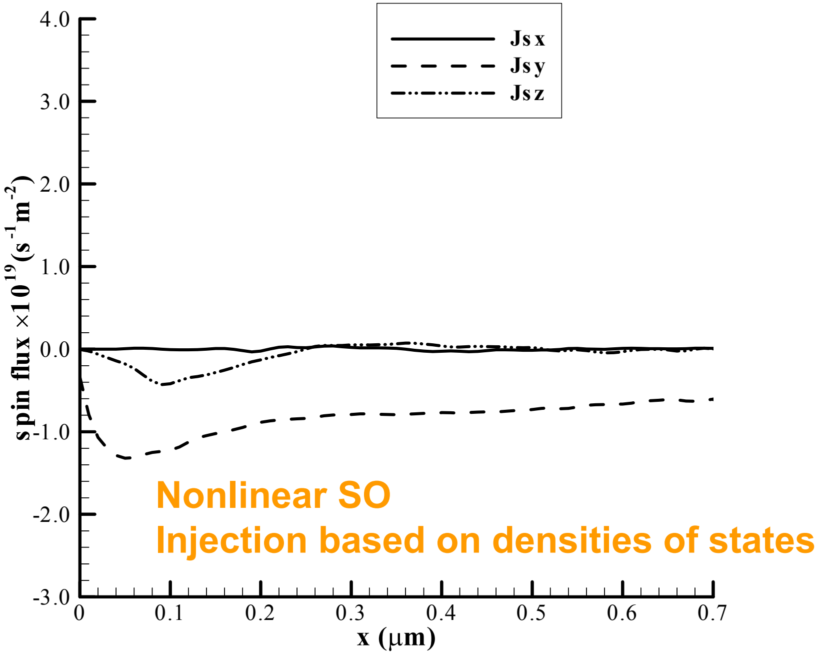
Linear SO
100% spin injection



Nonlinear SO
100% spin injection

Spin dephasing length > 0.7 μm

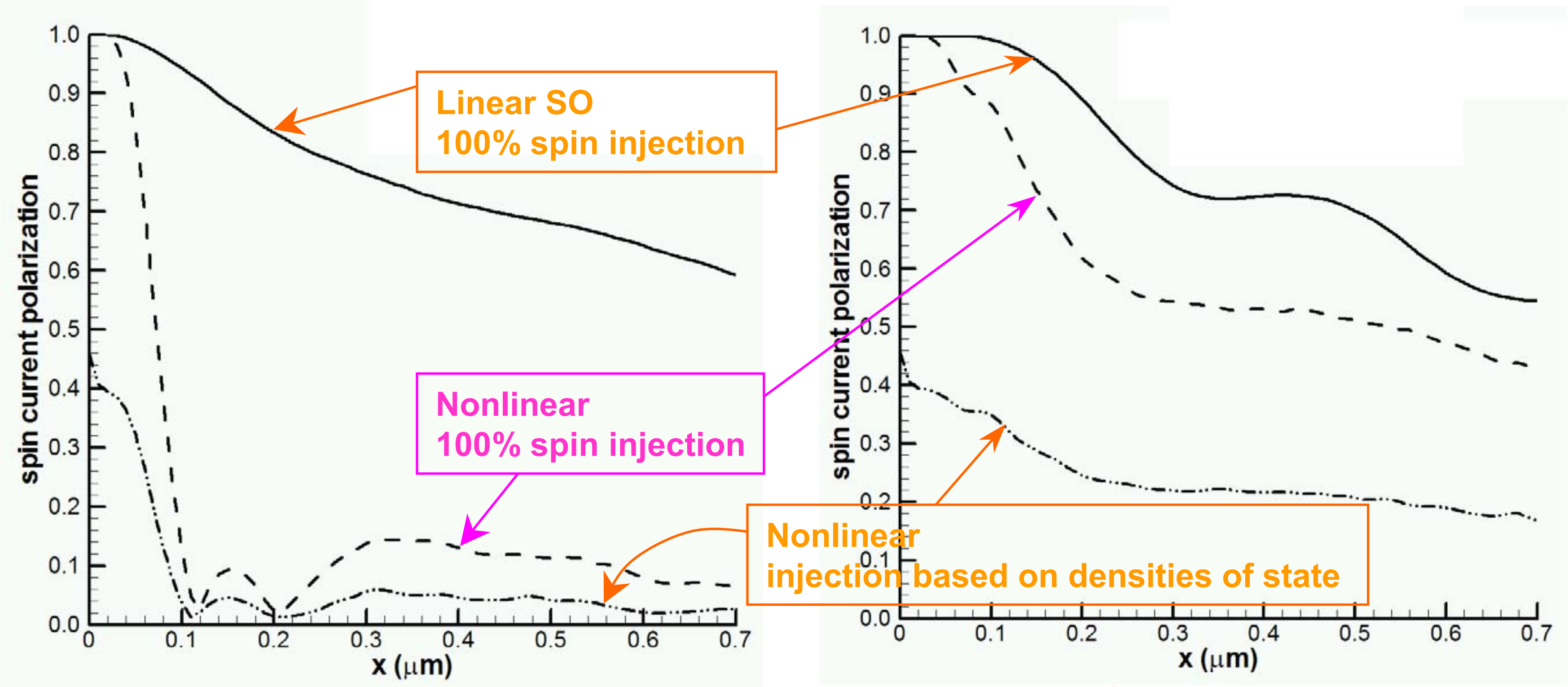
Inclusion of nonlinear SO interaction only slightly reduce the dephasing length with spin injection in the *y* direction



Nonlinear SO
Injection based on densities of states

Polarization of spin current

$w = 0$



Linear SO
100% spin injection

Nonlinear
100% spin injection

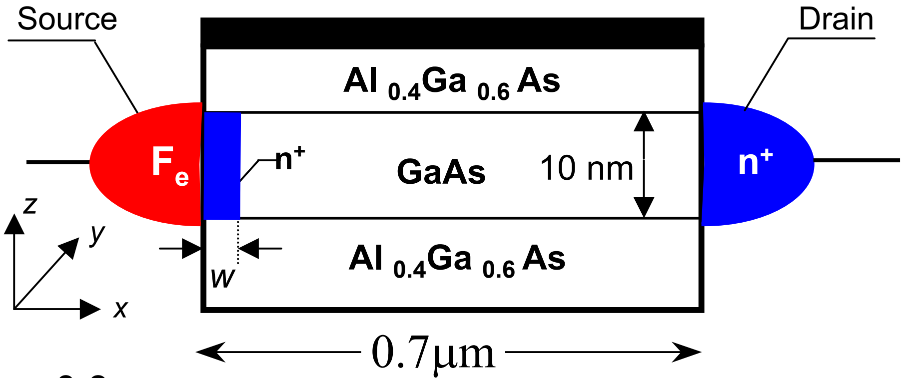
Nonlinear
injection based on densities of state

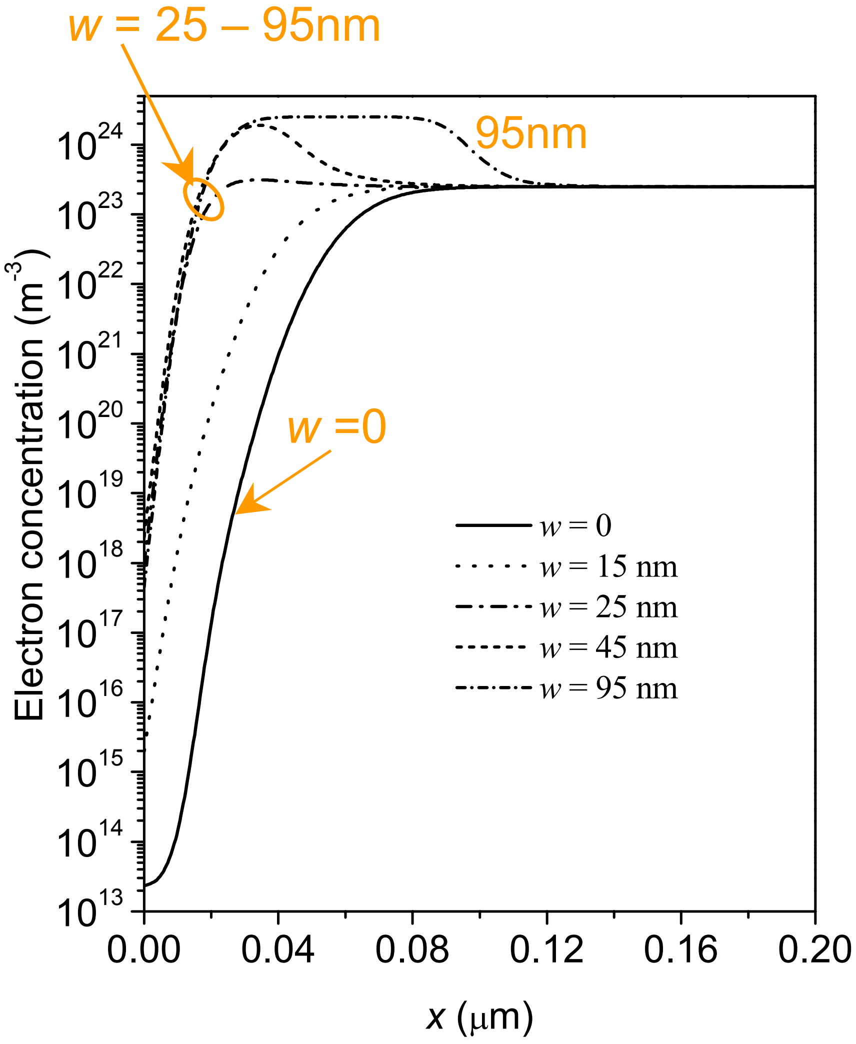
S_x injection

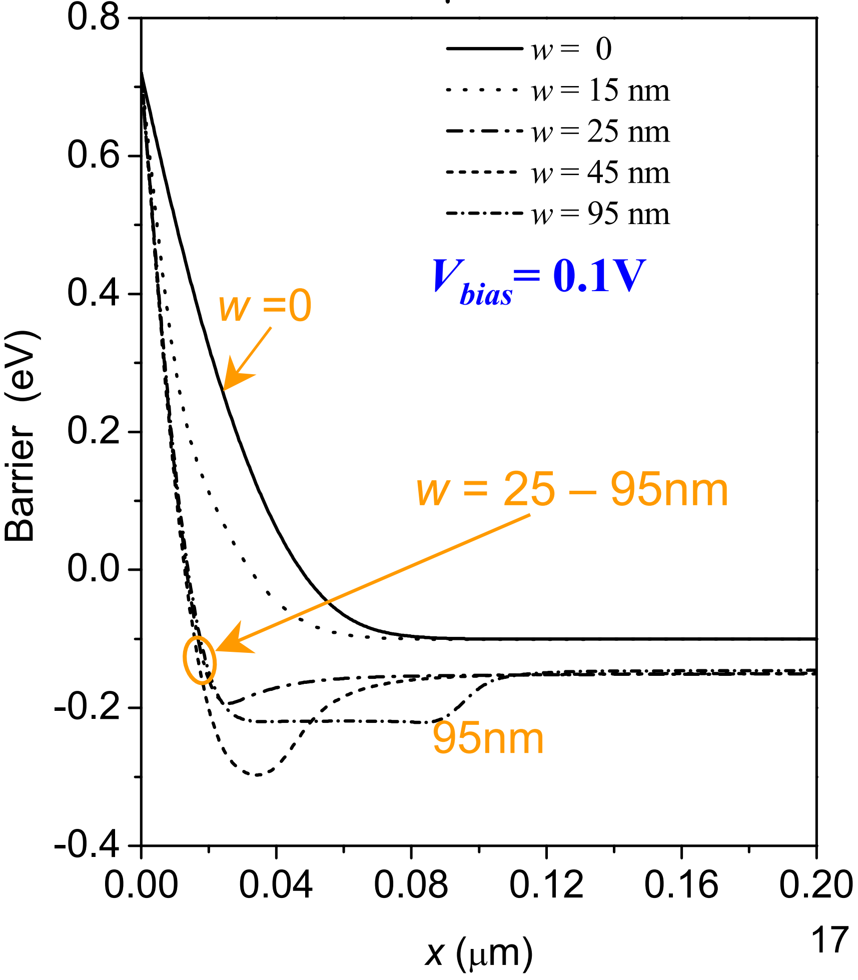
S_y injection

Even with nonlinear SO interaction included, spin current can maintain its polarization for a distance > device length (0.7 μm), with spin injection in the *y* direction

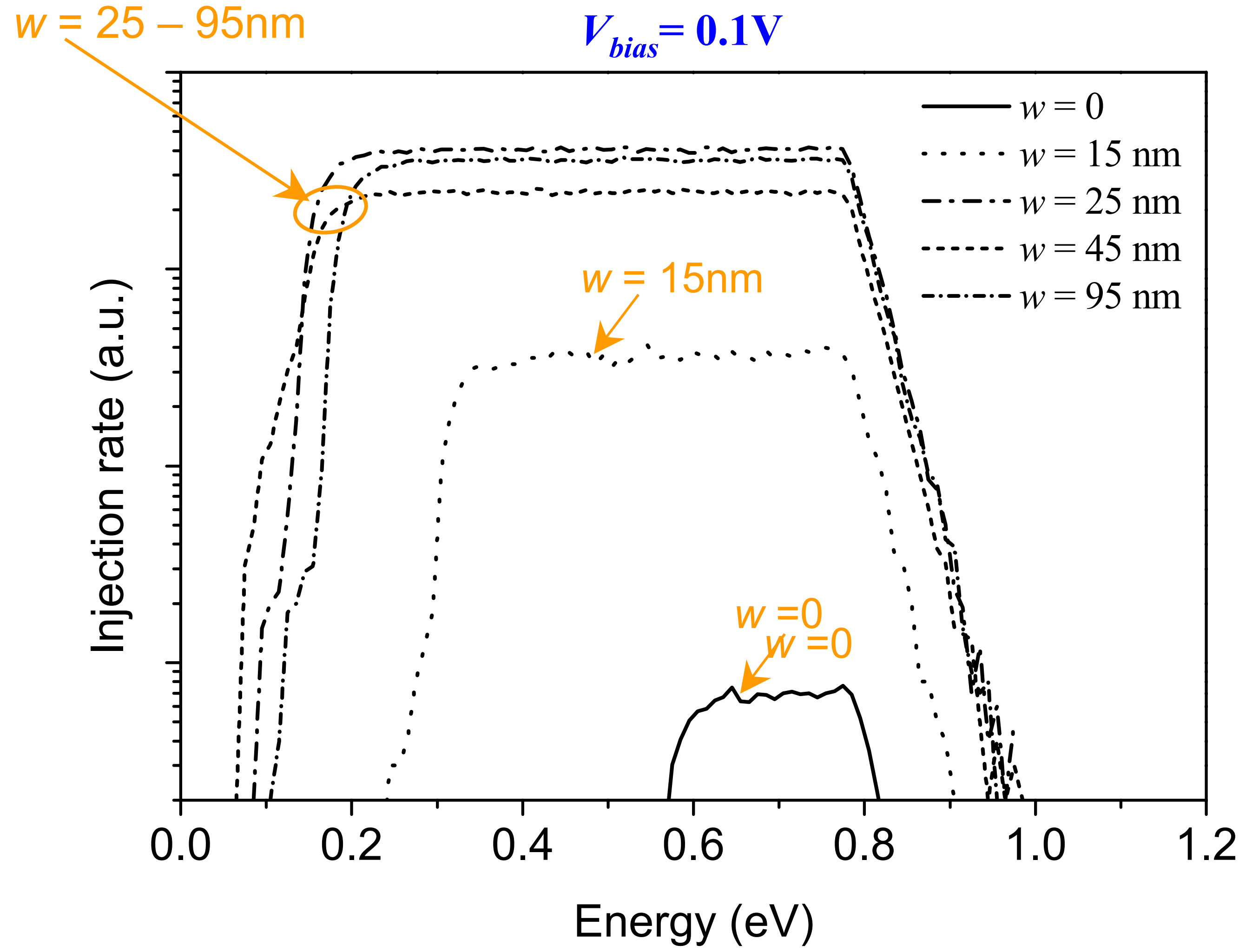
Enhancement of Spin Current Injection







Distribution of Injected Electrons



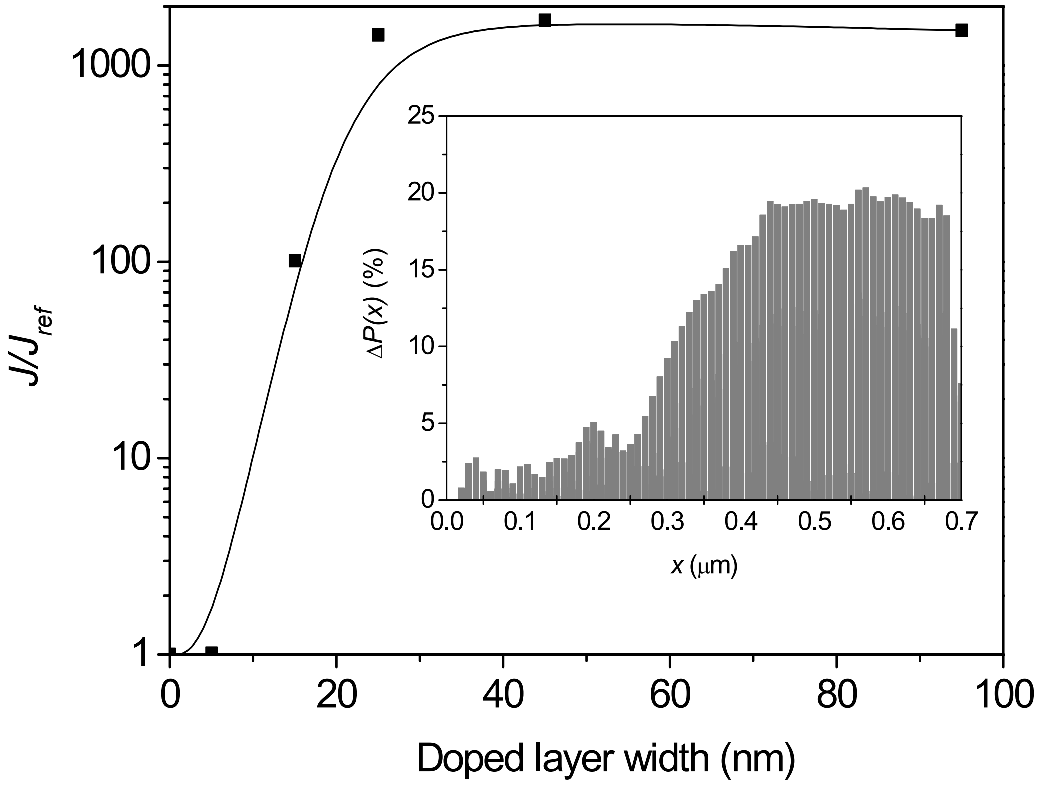
Spin Current Density

Total current densities:

$J = J(w);\ \ J_{ref} = J(w=0)$

$$\Delta P(x) = \max_w \left| \frac{P^J(w,x) - P^{Jref}(x)}{P^{Jref}(x)} \right|$$

$$\Delta P(x) < 20\%$$



- $J(w)$ is 3 orders of magnitude greater than J_{ref} for w > 30nm
- Effect of *w* on the spin current polarization is small.
- In addition to the total current density, spin current density is also substantially enhanced by the heavily doped layer

Summary

- Models for spin injection and spin-polarized transport have been implemented in Monte Carlo simulation, accounting for thermionic emission and tunneling
- Injected current can maintain its spin polarization to a length much longer than the electron spin dephasing length.
- Polarization of spin current may be a better measure for semiconductor spin FETs
- A thin heavily doped layer can be used to enhance the spin injection

References:

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5. S. Saikin, M. Shen, M.-C. Cheng and V. Privman, “Semiclassical Monte Carlo model for in-plane transport of spin-polarized electronics in III-V heterostructures,” *J. Appl. Phys.*, Vol.94 pp. 1769-1775, August 2003