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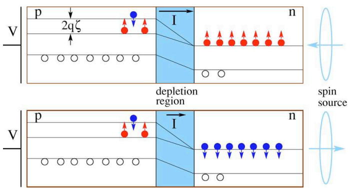
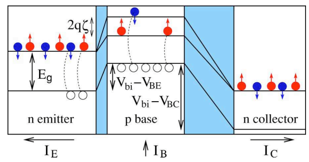
Semiconductor models with spin-polarization

Semiconductor spintronics

Semiconductor spintronic refers to the phenomena of spin-polarized transport in semiconductors. The goal is to find effective ways of controlling electronic properties such as current or accumulated charge, by spin or magnetic field as well as of controlling spin or magnetic properties by electric currents or gate voltages. From the technological point of view an efficient spin injection, slow spin relaxation and reliable spin detection are the important requirements. The aim is to develop practical device schemes what would enhance the functionality of the current charge based electronics. Examples are magnetic diodes, spin LEDs or a spin field effect transistor, which would change his logic state from ON to OFF by flipping the orientation of a magnetic field. Both figures below are taken from Zutic et al., [3]. Left: Scheme of a magnetic bipolar diode. The p region (left) is magnetic, indicated by the spin splitting $2q\zeta$ of the conduction band. The n region (right) is nonmagnetic, but spin polarized by a spin source: Filled circles. spin-polarized electrons; empty circles unpolarized holes. If the nonequilibrium spin in the n region is orientated parallel (upper figure) to the equilibrium spin in the p region, large forward current flows. If the relative orientation is antiparallel (lower figure) the current drops significantly. Right: Scheme of an n/p/n magnetic bipolar transistor with magnetic base B, nonmagnetic emitter E, and collector C. Conduction and valence bands are separated by the energy gap E_g. The conduction band has a spin splitting $2q\zeta$ leading to an equilibrium spin polarization $P_{B0} = \tanh(q\zeta/k_BT)$. Carriers and depletion regions are represented as in the left figure.





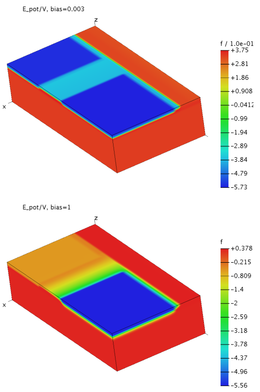
References

[1] I. Zutic and J. Fabian, *Bipolar spintronics*, Concepts in Spin Electronics (S. Maekawa, ed.), Oxford, 2006.

[2] I. Zutic, J. Fabian, and S. C. Erwin, *Bipolar spintronics: Fundamentals and applications*, IBM J. Res. & Dev. **50** (2006), 121–139.

[3] I. Zutic, J. Fabian, and S. Das Sarma, *Spintronics: Fundamentals and applications*, Rev. Mod. Phys. **76** (2004), 323–410.

Spin-polarized drift-diffusion model



3D simulation of a classical MOSFET. Electrostatic potential at equilibrium (top, gate wide strip in light blue); under operating conditions (bottom, drain blue, source orange).

Four continuity equations involving drift, diffusion, spin relaxation and generation/recombination reaction terms which are coupled with a Poisson equation

state equations

$$n_\lambda = \frac{N_c}{2}\exp[-(E_{c0} - q\psi - \lambda q\zeta_c - q\varphi_{n\lambda})/k_BT]$$

$$p_\lambda = \frac{N_v}{2}\exp[-(q\psi + \lambda q\zeta_c + q\varphi_{p\lambda} - E_{v0})/k_BT]$$

$$-\nabla\cdot(\varepsilon\nabla\psi) = f - n_\lambda - n_{-\lambda} + p_\lambda + p_{-\lambda}$$

evolution equations

$$\frac{\partial n_\lambda}{\partial t} - \nabla\cdot\frac{j_{n\lambda}}{q} = -\tilde R_{n\lambda}, \quad \frac{\partial p_\lambda}{\partial t} + \nabla\cdot\frac{j_{p\lambda}}{q} = -\tilde R_{p\lambda}$$

kinetic relations

$$j_{n\lambda} = \mu_{n\lambda} n_\lambda \nabla\varphi_{n\lambda}, \quad j_{p\lambda} = \mu_{p\lambda} p_\lambda \nabla\varphi_{p\lambda}$$

$$\tilde R_{n\lambda} = r(n_\lambda p - n_{\lambda 0} p_0) + \frac{n_\lambda - n_{-\lambda} - \lambda\tilde s_n}{2\tau_{sn}}$$

$$\tilde R_{p\lambda} = r(n p_\lambda - n_0 p_{\lambda 0}) + \frac{p_\lambda - p_{-\lambda} - \lambda\tilde s_p}{2\tau_{sp}}$$

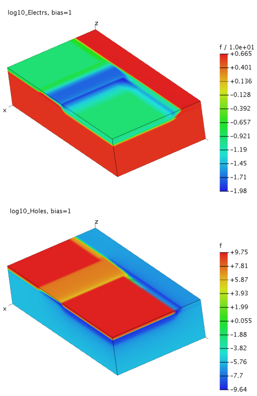
n_λ, p_λ	densities of electrons and holes with spin $\lambda = \pm 1$
$\varphi_{n\lambda}, \varphi_{p\lambda}$	electrochemical potentials
$\psi,\ T$	electrostatic potential, lattice temperature
$q,\ k_B$	elementary charge, Boltzmann's constant
$N_c,\ N_v$	effective densities of state
E_{c0}, E_{v0}	band edge energies
ζ_c, ζ_v	spin splitting of conduction and valence band due to magnetic impurities or an applied magnetic field
$\varepsilon,\ f$	dielectric permittivity, fixed charge density
$\mu_{n\lambda}, \mu_{p\lambda}$	mobility coefficients
$\tau_{sn},\ \tau_{sp}$	spin relaxation times
$n_{\lambda 0},\ p_{\lambda 0}$	equilibrium densities ($n_0,\ p_0$)
$\tilde s_n,\ \tilde s_p$	equilibrium spin densities

$$\tilde s_n = n\tanh(q\zeta_c/k_BT), \quad n = n_\lambda + n_{-\lambda}$$

$$\tilde s_p = p\tanh(q\zeta_v/k_BT), \quad p = p_\lambda + p_{-\lambda}$$

These model equations taken from [1-3] form an initial boundary value problem with mixed boundary conditions from device simulation which has to be treated in heterostructures. Its physical parameters may jump at interfaces.

Analytical results



Carrier densities $\log(n)$ (top) and $\log(p)$ (bottom), the holes beneath the gate carry the current.

References

[4] K. Gärtner, *Existence of bounded discrete steady state solutions of the van Roosbroeck system on boundary conforming Delaunay grids*, SIAM J. Sci. Comput. **31** (2009), 1347–1362.

[5] A. Glitzky, *Analysis of a spin-polarized drift-diffusion model*, Adv. Math. Sci. Appl. **18** (2008), 401–427.

[6] A. Glitzky and K. Gärtner, *Existence of bounded steady states to spin-polarized drift-diffusion systems*, SIAM J. Math. Anal. **41** (2010), 2489–2513.

Stationary spin-polarized drift-diffusion problem (see [6])

Continuous stationary problem

- A priori estimates for steady states
- Existence of weak steady state solutions
  - nested iteration scheme for Poisson equation and continuity equations,
  - Schauders Fixed Point Theorem in $L^2(\Omega)^4$
- Uniqueness result for Dirichlet data compatible or nearly compatible with thermodynamic equilibrium (i.e. uniqueness for small applied voltage)
  - formulation in a Sobolev-Campanato space setting
  - application of the Implicit Function Theorem

Discretized stationary problem

- Discretization
  - boundary conforming Delaunay grid
  - finite volume discretization of the Poisson equation and right hand side of the continuity equations
  - Scharfetter Gummel scheme for discretizing the flux terms in the continuity equations
- Existence of bounded solutions to the discretized stationary problem
  - establishing the same bounds as in the continuous problem
  - Brouwers Fixed Point Theorem
- Uniqueness for small applied voltages
- Qualitatively same behavior as van the Roosbroeck system (see [4])

Instationary spin-polarized drift-diffusion problem (see [5])

- Estimate of the free energy $F(u(t))$ along solutions
  - For general mixed boundary conditions

$$F(u(t)) \le (F(u(0)) + 1)\,e^{ct} \quad \text{for all } t \in \mathbb{R}.$$

  - If Dirichlet boundary conditions are compatible with thermodynamic equilibrium then the free energy decays monotonously and exponentially to its equilibrium value.
- Existence of global weak solutions to the spin-polarized drift-diffusion problem
  - regularization in state equations, reaction terms on finite time interval
  - time discretization, passing to the limit
  - a priori estimates
  - for sufficiently large regularization parameter each solution to the regularized problem is a solution to the original problem
- Uniqueness of the solution

Open questions

- Simulation tool for spin-polarized semiconductor devices based on existing simulation tools for classical semiconductor devices
- Mathematical modeling of optoelectronic devices in a spin-polarized drift-diffusion context
- Interaction between currents and magnetic field
- Extension to a spin vector approach

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