Mathematical aspects of spin-related phenomena models and the associated criteria for spintronics

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Abstract

The mathematical aspects of spin-related phenomena models and the associated criteria for spintronics have been discussed in this short note, for giving an insight into the utility of the models for the particular applications of the subject. Drift-diffusion model, Monte Carlo approach, and the modeling of spintronics phenomena in magnetic nanostructures have been technically analyzed. The work on the novel application of the spin imbalance for improving the performance of the semiconductor lasers has been briefly reviewed and technically analyzed. The paper should be quite useful to the designers of spintronics for the applications including the recently evolving field of using the spin imbalance for improving the performance of the solid state lasers.*

Keywords: Drift-diffusion model, Monte Carlo approach, modeling of spintronics phenomena in magnetic nanostructures, spin imbalance in solid state lasers.

Resumen

Los aspectos matemáticos de los modelos de los fenómenos relacionados con el espín y los criterios asociados para la espintrónica se discuten en esta breve nota, para dar una idea de la utilidad de los modelos para las aplicaciones particulares de la asignatura. También son analizados técnicamente el modelo Drift-diffusion, el método de Monte Carlo y el modelado de fenómenos espintrónicos en nanoestructuras magnéticas. Se revisan brevemente trabajos sobre la nueva aplicación del desequilibrio del espín para mejorar el desempeño de los láseres semiconductores, y se analizan técnicamente. Este documento será muy útil para los diseñadores de aplicaciones de la espintrónica, e inclusive para el campo recién descubierto, de utilizar el desequilibrio del centrifugado para mejorar el rendimiento de los láseres de estado sólido*.

Palabras clave: modelo Drift-diffusion, método de Monte Carlo, modelado de fenómenos espintrónicos en nanoestructuras magnéticas, desequilibrio del espín en láseres de estado sólido.

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*.Some of the technical analysis presented in this paper is on the basis of the discussions with the various researchers in the Thin Film Group of Indian Institute of Technology, Delhi during the author's association with the group, in the year 2009, as the Research Scientist in the Project on "Spintronics" sponsored by the Department of Information Technology, Government of India.

I. INTRODUCCIÓN

It is now well understood that the newly evolving subject of spintronics is based on the spin of the electrons, which is the characteristic that differentiates it from the well established subject of electronics. Chopra [1, 2] has highlighted the fact that the subject has recently drawn the attention of various workers. Since the applications are of various forms, it is natural that many types of models of the spin-related phenomena have been put forward by the researchers, which are widely different from each other, each one having its merits for studying and analysing certain phenomena. The purpose of the present paper is to provide an overview of the various types of models, and also give their salient features, so as to enable the new entrants in the field to make a comparison of the models.

A. Drift-diffusion model

The drift-diffusion approximation is the easiest approach to spin involving process modeling, which is used to describe phenomena related to the charge degree of freedom. The drift diffusion models are subdivided into two classes: two-component drift-diffusion approximations and spin-polarization-vector or density-matrix based models.

Interestingly, both these approaches have been used successfully in the practical modeling of spin-related phenomena in semiconductors [3, 4]. These models are tecnically analyzed below:

B. Two-component drift-diffusion model

The salient features of this model are:
(i) the transverse spin coherence is not considered,
(ii) the spin relaxation processes are included phenomenologically, and
(iii) the electrons are considered to be of two types: having spin up and spin down. The drift-diffusion equations for the two cases, including the relaxation terms, can be written in the form:

$$e\frac{\partial n\uparrow(\downarrow)}{\partial t} = div j^{\rightarrow}\uparrow(\downarrow) + \frac{e}{2\tau_{sf}}\{n\downarrow(\uparrow) - n\uparrow(\downarrow)\} + S\uparrow(\downarrow)(r^{\rightarrow},t), \quad (1)$$

$$j^{\rightarrow}\uparrow(\downarrow) = \sigma\uparrow(\downarrow)E^{\rightarrow} + eD\nabla n\uparrow(\downarrow), \quad (2)$$

and

$$\sigma\uparrow(\downarrow) = en\uparrow(\downarrow)\mu, \quad (3)$$

Where:

e is the electron charge,
$n\downarrow(\uparrow)$ is the density of the spin-up (spin-down) electrons,
$j^{\rightarrow}\uparrow(\downarrow)$ is their current density,
τ_{sf} is the spin relaxation time,
$S\uparrow(\downarrow)(r^{\rightarrow},t)$ defines the source of the spin polarization,
$\sigma\uparrow(\downarrow)$ is the conductivity and
μ is the mobility,
related to the diffusion coefficient by the Einstein relation:

$$\mu = De / k_B T,$$

and defined as:

$$v_{drift} = \mu E.$$

Thus, it is necessary to optimize all these parameters by considering the specifications of the devices. It is also possible to bring the desired changes in the properties of the materials by doping [5]. In addition, various types of semiconductor materials [6] suitable for the particular applications can be chosen.

C. Spin polarization vector approach

The spin polarization vector approach is different from the above model, and it takes into consideration the transverse spin dynamics, which is important for the case, in which the time scales of processes studied are comparable with a characteristic decoherence/dephasing time for quantum-mechanical superposition of the two spin states: spin-up and spin-down; like the spintronic devices operating with analog logic.

Under the assumption, that the spin degree of freedom has no effect on the spatial motion, the dynamics of spin polarization density can be shown to be described by a vector drift-diffusion equation, which for the 1D case is given [7, 8] by:

$$\frac{\partial P}{\partial t} - D'\frac{\partial^2 P}{\partial x^2} - \mu'\frac{\partial P}{\partial x} + C'P = 0. \quad (4)$$

Where the coefficients D', μ', and C' are 3 by 3 matrices in the spin space, and P is the spin polarization density, which is a vector quantity, corresponding to a single-particle spin density matrix.

Thus, for the designing of the spintronic devices operating with analog logic, it is necessary to optimize the decoherence/dephasing time for quantum-mechanical superposition of the two spin states: spin-up and spin-down.

II. MONTE CARLO APPROACH

Monte Carlo simulation approach is very effective and useful for studying the characteristics of transport beyond quasi-equilibrium approximations (the drift-diffusion approximation or linear response approximation). This method is quite flexible and can be employed to investigate the different combinations details of scattering mechanisms, specific device design, material properties and boundary conditions in the simulation. However, the models designed for quantitative evaluations of transport parameters are very time consuming, which require a lot of programming and computational skills.

The Monte Carlo scheme used for the electronic device design describes transport of classical "representative" particles, in which each simulated particle describes a group of real electrons or holes with similar characteristics. In simulation, each particle is considered to propagate along a localized trajectory, and is affected by external fields. The electric field generated by the non-uniform charge distribution is recalculated at every sampling time step by using the Poisson equation, and the simulation is carried out step by step, by considering the free flight of a particle in constant external fields according to the classical equations of motion and instantaneous values of the external fields at sampling events or of the energy and momentum of a particle at scattering events.

The spin property can be included as an additional parameter-spin polarization vector [9] or spin density matrix [10] computed for each particle. The density matrix approach, during the free flight spin density matrix of the i^{th} particle evolves coherently, according to the equation given by:

$$\rho_i(t+\delta t) = e^{\frac{2i\pi H_S \delta t}{h}}\rho_i(t)e^{\frac{2i\pi H_S \delta t}{h}}, \quad (5)$$

where h is the Planck's constant, and H_S is the (spin-dependent) hamiltonian, assumed to be constant for short time steps, which changes instantaneously,

$$\rho_i(t) = \rho_i^{'}(t) \quad \text{at spin scattering events.}$$

As characteristic parameters, we can use spin polarization density,

$$P_\alpha = \sum_i Tr(\sigma_\alpha \rho_i) \, , \qquad (6)$$

and spin current densities [11]:

$$J_\alpha^\beta = \sum v^i \beta Tr(\sigma_\alpha + \rho_i) \cdot \qquad (7)$$

Where $v^i\beta$ is the β velocity component of i^{th} particle, and sums are taken over all the particles located in the grid element of volume dV, at the position r. Therefore, computations for the electric field generated by the non-uniform charge distribution for every sampling time step using the Poisson equation, have to be done, and the simulation has also to be carried out step by step, by considering the free flight of a particle in constant external fields according to the classical equations of motion, and instantaneous values of the external fields at sampling events or of the energy and momentum of a particle at scattering events. All this requires software skill, and good knowledge of the simulation techniques.

III. MODELING OF SPINTRONICS PHENOMENA IN MAGNETIC NANOSTRUCTURES

Recently, interest has rapidly grown in studying the phenomena related with spintronics for the cases, when the size of the system is of the same magnitude as the spin relaxation length of the electrons ~ 1nm to 100nm. By using the suitable materials conductor /insulator thin films, and magnetic/nonmagnetic, with thickness ~1nm, these phenomena are observed, which are being used to build applications like field sensors, reading heads, magnetic MRAMs, and RF oscillators. Most of the models, both analytical and numerical, are based on taking into account the well-known interactions, *e.g.* exchange, anisotropy, and externally applied field. However, other kinds of effects have also to included for approaching the real behavior of the samples; which are: the dynamic dipolar coupling, mutual spin transfer, Rashba effect and spin Hall effect.

The impact of these types of effects on the magnetic behavior is studied by micromagnetic modeling, and the simulation is done together with the results of the experiments.

The control of the magnetization of nanostructures by the injection of a spin polarized current can be achieved only by reducing the size of the system below 100nm, and by associating the different kinds of materials in thin films.

The phenomena which are negligible at the macroscopic scale appear at the nanometer length scale, that are in the form of the dipolar coupling between ferromagnetic elements, mutual spin transfer, Rashba effect and spin Hall effect. A lot of work is going on the micromagnetic software for the integration of the Landau-Lifshitz-Gilbert equation enhanced by the spin transfer torque, which is of great interest for studying:

(i) magnetic nanopillars with a current flowing perpendicular to the plane, in which case, the dynamic dipolar coupling and mutual spin transfer play an important role; and

(ii) nanometric wires with magnetic domain walls inside, where the current flowing in the plane of the structure along with the spin-orbit coupling produces the Rashba effect and spin Hall effect with direct impact on the domain wall motion.

These effects are illustrated in the following figure:

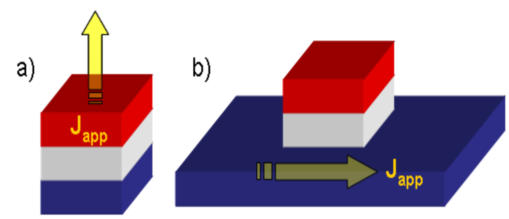

Fig1.a) nanopilier multicouches ; b) piste nanométrique

FIGURE 1 Magnetic nanopillars with a current flowing perpendicular to the plane (left), and nanometric wires with magnetic domain walls inside, where the current flowing in the plane of the structure (right). Figure courtesy Institut Nanosciences Et Cryogene, la recherché, ressource fondamentale (reseach a fundamental resource).

IV. SPIN IMBALANCE FOR UPGRADATION OF THE PERFORMANCE OF SEMICONDUCTOR LASERS

The spin lasers differ from the conventional lasers in many ways, notably:

(i) In the spin lasers, injected carriers are spin polarized. Based on this consideration, the spin lasers can be classified as unconventional lasers. Interestingly, the hole spin decays much faster as compared to the electron spin, and thus the electrons are considered as the spin carriers.

(ii) The light emitted from spin lasers is circularly polarized due to the spin-polarized carriers, and the output polarization is controllable by adjusting the injection polarization or the intensity.

(iii) The spin lasers are characterized by two lasing thresholds, each spin feeding one corresponding mode (polarization), the imbalance of spin-up and spin-down carrier injection leading to two separate thresholds for majority and minority spin carriers.

The schematic of a spin laser structure with vertical cavity surface emitting laser (VCSEL) geometry is given below:

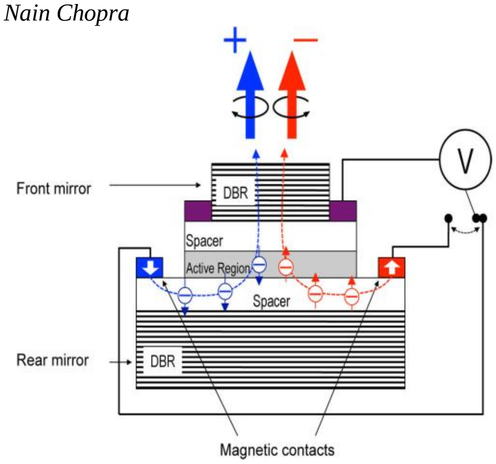

FIGURE 2 Schematic illustration of a spin laser structure with vertical cavity surface emitting laser (VCSEL) geometry. Figure courtesy spie.org.

The working principle is easy: the active region emits a beam of the coherent light through electron-hole recombination, which typically comprises of III-V quantum wells or quantum dots. Interestingly, a pair of distributed Bragg reflectors (DBRs) are used for amplification, as is done by the mirrors in case of the conventional laseres. The magnetic contacts shown have antiparallel orientation, which inject spin-polarized electrons (shown in the middle), and the emitted light is circularly polarized (shown as thick arrows on top). The computations show that the two thresholds delimit the three operational regimes, as compared to only two stages (on and off regimes, in case of the conventional lasers). This has been clearly illustrated in the figure given below:

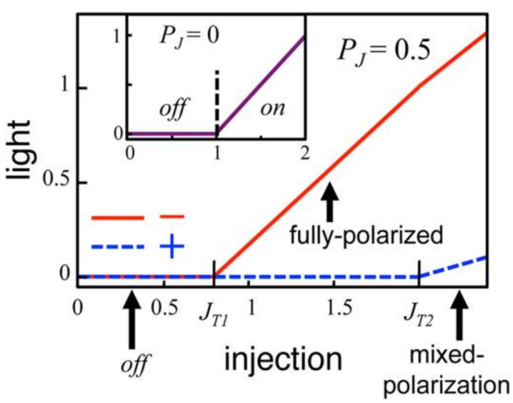

FIGURE 3. The variation of the emitted light intensity with the injection intensity for spin lasers ($P_J \neq 0.5$) and conventional lasers ($P_J=0$, inset). Figure courtesy Boéris G., Lee J., Výborný K., and Žutić I., *Tailoring chirp in spin-lasers*, Appl. Phys. Lett. **100**, 121111 (2012).

In this figure, P_J denotes the injection polarization. J_{T1} and J_{T2} denote the two lasing thresholds of the spin laser, delineating the laser's three operating regimes. And +/−: denote the right/left circular polarizations. It may be noted that depending on the strength of injection, a spin laser operates in three regimes (off, full) or mixed-polarization.

Also, it is observed that between the two thresholds, the emitted light is fully polarized, even with partially spin-polarized injection ($0 < |P_J| < 1$), which leads to the spin laser becoming a very good candidate for a spin-amplifier.

The two operations of spin lasers in steady-state:
(i) with enhanced light emission, and
(ii) spin filtering and amplification have already been demonstrated.

However, the most interesting applications of spin lasers are considered to be for their dynamic operation, where the spin lasers actually have better performance than the conventional lasers, while comparing the modulation bandwidth and chirp. The spin lasers can have two types of modulation: amplitude modulation (AM), and polarization modulation (PM). The former changing the injection intensity, and the latter modifying the polarization at a fixed injection intensity. In both cases, bandwidths in the range of the frequency response above -3dB are observed to enhance with increased polarization, which has been illustrated in the following figure:

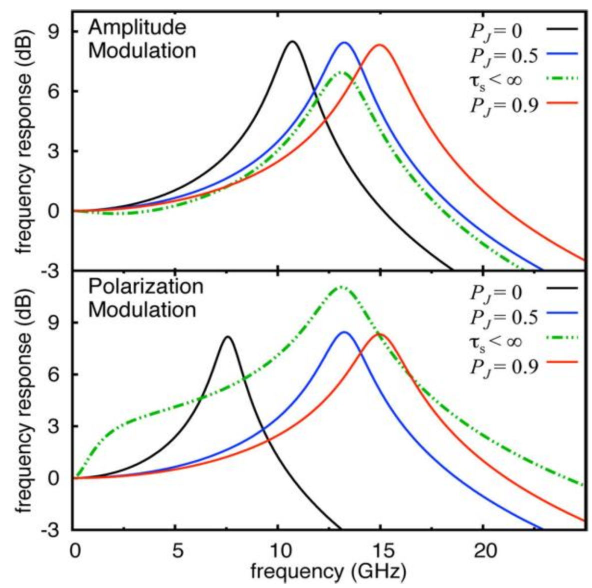

FIGURE 4 Frequency response with different polarizations. Figure courtesy Lee J., Falls W., Oszwałdowski R. and Žutić I., *Spin modulation in semiconductor lasers*, Appl. Phys. Lett. **97**, 041116 (2010).

As the polarization increases, the curves are shifted towards right side. All the curves except the central one (dash dots), are for infinite spin relaxation time τ_s.

The spin lasers are also characterized by the reduced frequency chirp, which is a parasitic frequency modification, due to dynamic change of the carrier-induced refractive index in the resonant cavity. Though for an ideal case like a vacuum, which gives no chirp, two sidebands are observed in the vicinity of the main peak corresponding to the resonance frequency for lasing. This can be easily seen in the following figure:

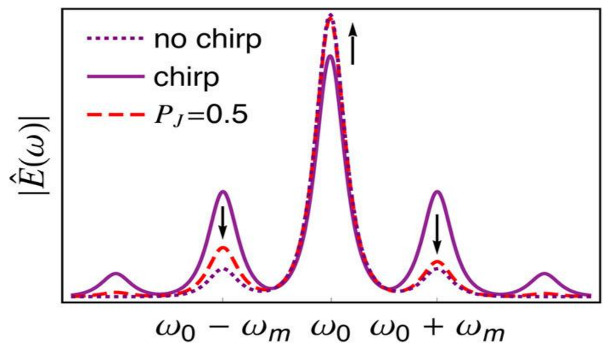

FIGURE 5. Broadened spectra of electric fields $|\hat{E}(\omega)|$, of a laser with optical frequency ω_0 where ω_m is modulation frequency. The conventional lasers with chirp and without chirp and a spin laser with spin injection are shown respectively by dotted line, solid line, and dashed line. Figure courtesy Boéris G., Lee J., Výborný K., and Žutić I., *Tailoring chirp in spin-lasers*, Appl. Phys. Lett. **100**, 121111 (2012).

It has been observed that when the chirp is switched on, the spectrum is modified. It is possible to reduce the signal distortion by injecting spin-polarized electrons. In this manner, the spin lasers provide an easy tool for reducing the chirp as compared to the other conventional methods, though the reduction is dependent on many factors like: injection intensity, modulation frequency and spin-resolved refractive index. Thus, the electron charge, the density of the spin-up (spin-down) electrons, their current density, the spin relaxation time, the source of the spin polarization, the conductivity and the mobility, related to the diffusion coefficient by the Einstein relation, have to be considered and optimized for achieving the desired results for the devices. This needs the designing experience and the software skills, for achieving the efficient improvement in the performance of the spintronics based devices.

Though the topic of spin imbalance in solid state lasers was explored by the researchers a decade back, a spurt in this has been noticed during the last five years or so, because of the various advantages. Lee *et al.* [12] have discussed the mapping between quantum dot and quantum well lasers: from conventional to spin lasers. Gøthgen *et al.* [13] have suggested an analytical model of spin-polarized semiconductor lasers, which is being usefully employed for the efficient designing of the semiconductor lasers. Iba *et al*. [14] have studied the room temperature circularly polarized lasing in an optically spin injected vertical-cavity surface-emitting laser with (110) GaAs quantum wells. Saha *et al.* [15] have discussed in detail the high-frequency dynamics of spin-polarized carriers and photons in a laser.

Gerhardt *et al*. [16] have done interesting investigations on the ultrafast spin-induced polarization oscillations with tunable lifetime in vertical-cavity surface-emitting lasers.

Thus, it is clear that the subject of spintronics modeling is evolving fast, especially for the newly growing field of spin imbalance.

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