TEMPERATURE DEPENDENCE OF SPIN DEPOLARIZATION OF DRIFTING ELECTRONS IN n-TYPE GaAs BULKS*

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The influence of temperature and transport conditions on the electron spin relaxation in lightly doped n-type GaAs semiconductors is investigated. A Monte Carlo approach is used to simulate electron transport, including the evolution of spin polarization and relaxation, by taking into account intravalley and intervalley scattering phenomena of the hot electrons in the medium. Spin relaxation lengths and times are computed through the D'yakonov–Perel process, which is the more relevant spin relaxation mechanism in the regime of interest ($10 < T < 300$ K). The decay of the initial spin polarization of the conduction electrons is calculated as a function of the distance in the presence of a static electric field varying in the range 0.1–2 kV/cm. We find that the electron spin depolarization lengths and times have a nonmonotonic dependence on both the lattice temperature and the electric field amplitude.

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1. Introduction

The processing of a high volume of information and world wide communication are, at the present, based on semiconductor technology, whereas information storage devices rely on multilayers of magnetic metals and insulators. Semiconductor spintronics offers a possible direction towards the

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development of hybrid devices that could perform logic operations, communication and storage, within the same material technology: electron spin could be used to store information, which could be transferred as attached to mobile carriers and finally detected [1–6].

Although these important potential advantages, the designers of spin devices have to worry about the loss of spin polarization (spin coherence) before, during and after the necessary manipulations. In particular, efficient injection, transport, control and detection of spin polarization must be carefully treated [2]. Electron–spin states depolarize by scattering with imperfections or elementary excitations such as phonons. Hence, for the operability of prospective spintronic devices, the features of spin relaxation at relatively high temperature jointly with the influence of transport conditions should be firstly understood [1, 7].

In recent years there was a proliferation of experimental works in which the influence of transport conditions on relaxation of spins in semiconductors has been investigated [8–14]. Even though for high speed transfer of information, high external electric fields must be used, up now only the influence of low electric fields ($F < 0.1$ kV/cm) on coherent spin transport has been investigated and very little is known about the effects of higher electric fields [10] or high lattice temperatures.

Despite of this great experimental interest, few theoretical works [13,15] and simulative studies [7, 16, 17], have been carried out. Theoretical approaches to describe spin dynamics and spin-polarized electron transport include the two-component drift-diffusion model [13], Monte Carlo techniques to solve the Boltzmann equation [7] and microscopic approaches solving the Bloch kinetic equations [18]. However, a comprehensive theoretical investigation of the influence of transport conditions on the spin depolarization in semiconductor bulk structures, in a wide range of values of temperature and amplitude of external fields, is lacking.

Inducing spin polarization in a semiconductor, such as GaAs and Si, can be done efficiently and at reasonable current levels by electrical transfer of spins from a ferromagnetic metal across a thin tunnel barrier, at low temperatures (5–150 K) [19, 20]. Very recently, electrical injection of spin polarization in n-type and p-type silicon at room-temperature have been experimentally carried out [21]. These promising experimental results for development of spintronic devices suggest that it is important to investigate the spin coherence up to room temperature. Earlier Monte Carlo simulation has revealed that the presence of an external electric field can accentuate spin relaxation in GaAs bulk materials [7]. In this work, solving the transport and spin dynamics stochastic differential equations by a semiclassical Monte Carlo approach, we estimate the spin lifetimes and depolarization lengths of an ensemble of electrons, for intermediate values of the electric field (0.1–2 kV/cm) and lattice temperatures in the range $10 < T < 300$ K.

The paper is organized as follows: in Sec. 2 the semiconductor physical model and the Monte Carlo approach are presented; in Sec. 3 the numerical results are given and discussed. Final comments and conclusions are given in Sec. 4.

2. Semiconductor model and spin-polarized electron transport calculation

2.1. Semiconductor model and semiclassical Monte Carlo approach

The study of the transport properties and the spin relaxation process in a semiconductor in the presence of an external field is not simple, especially when the field is very strong. In this case, it is preferable to perform a numerical simulation of the process. The Monte Carlo method presents the remarkable advantage of giving a detailed description of the particles motion in the semiconductor taking into account the scattering mechanisms, and allows us to obtain all the needed information, such as average velocity of the electrons, temperature, current density, *etc.*, directly without the need of calculating the electron distribution function. The time of free flight (time interval between two collisions), the collisional mechanisms, the scattering angle, and all the parameters of the problem are chosen in a stochastic way, making a mapping between the probability density of the given microscopic process and a uniform distribution of random numbers.

The Monte Carlo algorithm, developed for simulating the motion of electrons in a GaAs semiconductor, follows the standard procedure described in Ref. [22]. Here, we incorporate the description of the electron spin dynamics by following a standard semiclassical formalism. We assume that the spatial electron transport is well described by the Boltzmann equation and that the electrons move along classical trajectories between two scattering events. The conduction bands of GaAs are the Γ-valley, four equivalent L-valleys and three equivalent X-valleys. The parameters of the band structure and scattering mechanisms are taken from Ref. [22]. In this work Monte Carlo simulations of electron transport and spin depolarization dynamics are limited to low-energy regime with the electric field amplitude varying in the range 0.1–2 kV/cm. In this energy range the electrons can be found only in the Γ-valley. Our computations include the effects of the nonparabolicity of the band structure and, among many different scattering mechanisms, electron scattering due to ionized impurities, acoustic, piezoelectric and polar optical phonons in the Γ-valley. The scattering probabilities are calculated by the Fermi Golden Rule and the scattering events are considered instantaneous. We assume field-independent scattering probabilities; accordingly, the influence of the external fields is only indirect through the field-modified electron velocities. Nonlinear interactions of the field with the lattice and bound carriers is neglected. We neglect also electron–electron interactions and consider electrons to be independent [27]. All simulations are performed

in a n-type GaAs bulk with a free electrons concentration $n = 10^{13}$ cm^{-3}. We have assumed that all donors are ionized and that the free electron concentration is equal to the doping concentration.

2.2. Spin relaxation dynamics

The spin depolarization of drifting electrons is analyzed for a lattice temperature T varying in the range $10 < T < 300$ K. For these values of T the D'yakonov–Perel process is the more relevant spin relaxation mechanism [14]. This mechanism, effective in the intervals between collisions, is related to the spin–orbit splitting of the conduction band in non-centrosymmetric semiconductors like GaAs [5, 15, 24] .

In a semiclassical formalism the effective single-electron Hamiltonian which accounts for the spin–orbit interaction term is

$$H = H_0 + H_{\mathrm{SO}}\,, \tag{1}$$

where H_0 is the self-consistent electron Hamiltonian in the Hartree approximation, including also interactions with impurities and phonons. The spin-dependent term H_{SO} may be written as

$$H_{\mathrm{SO}} = \frac{\hbar}{2}\vec{\sigma}\cdot\vec{\Omega}_{\mathrm{eff}}\,, \tag{2}$$

and can be viewed as the energy of a spin in an effective magnetic field that causes electron spin to precess. $\vec{\Omega}_{\mathrm{eff}}$ is a vector depending on the orientation of the electron momentum vector with respect to the crystal axes (xyz). Near the bottom of the Γ-valley, the effective magnetic field can be written as [25]

$$\vec{\Omega}_{\mathrm{eff}} = \beta_\Gamma\left[k_x\left(k_y^2 - k_z^2\right)\hat{x} + k_y\left(k_z^2 - k_x^2\right)\hat{y} + k_z\left(k_x^2 - k_y^2\right)\hat{z}\right]\,, \tag{3}$$

where k_i are the components of the electron wave vector, and β_Γ the spin–orbit coupling coefficient [15]. In particular,

$$\beta_\Gamma = \frac{\alpha\hbar^2}{m\sqrt{2mE_g}}\left(1 - \frac{E\left(\vec{k}\right)}{E_g}\frac{9 - 7\eta + 2\eta^2}{3 - \eta}\right)\,, \tag{4}$$

where $\alpha = 0.029$ is a dimensionless material-specific parameter which gives the magnitude of the spin–orbit splitting, $\eta = \Delta/(E_g + \Delta)$, with $\Delta = 0.341$ eV the spin–orbit splitting of the valence band, E_g is the energy separation between the conduction band and valence band at the Γ point and m is the effective mass. In Eq. (4), we consider the effects of nonparabolicity on the spin–orbit splitting in Γ-valley, estimated by Pikus and Titkov [26].

The quantum-mechanical description of the evolution of the spin 1/2 is equivalent to the evolution of the classical momentum $\vec{S}$ under an effective magnetic field $\vec{\Omega}_{\text{eff}}$ with the equation of motion

$$\frac{d\vec{S}}{dt} = \vec{\Omega}_{\text{eff}} \times \vec{S}\,. \tag{5}$$

In Eq. (5), the scattering reorients the direction of the precession axis, making the orientation of the effective magnetic field random and trajectory-dependent, thus leading to spin relaxation (dephasing) [15]. The reciprocal effect of the electron spin evolution on the orbital motion through spin–orbit coupling can be ignored due to the large electron kinetic energy in comparison with the typical spin splittings and strong change of the momentum in scattering events [27]. In this modelization the scattering processes are considered spin-independent.

2.3. Calculation of spin depolarization times and lengths

The dependence of spin relaxation times and lengths on temperature and driving electric field has been investigated by simulating the dynamics of 5×10^4 electrons, initially polarized ($\langle\vec{S}\rangle = 1$) along the $\hat{x}$-axis at the injection plane ($x_0 = 0$). We calculate $\langle\vec{S}\rangle$ as a function of time by averaging over the ensemble of electrons. In Fig. 1 (a), we show the electron average polarization $\langle S_x\rangle$, calculated as a function of time in the presence of an electric field, with amplitude $F = 0.1$ kV/cm and directed along $\hat{x}$-axis, for three different values of temperature. In Fig. 1 (b), we show the same component of spin polarization $\langle S_x\rangle$, calculated at $T = 77$ K, as a function

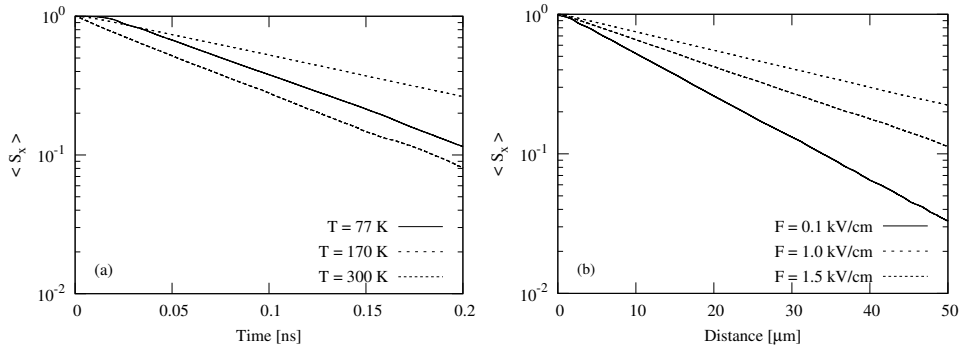

Fig. 1. (a) Spin polarization $\langle S_x\rangle$ as a function of time, with field amplitude $F = 0.1$ kV/cm, at three different values of temperature; (b) Spin polarization $\langle S_x\rangle$ as a function of distance at $T = 77$ K, for three different values of the electric field amplitude.

of the distance traveled by the center of mass of the electron cloud from the injection plane, for three different values of the external field amplitude. Since $\langle S_x \rangle$ is found to decrease with both time and distance by showing an almost linear trend in a semi-log plot, the spin relaxation times τ and lengths L are estimated by considering the spin depolarization as an exponentially process dependent on time and distance [7]. If $\langle S_x \rangle$ and $\langle x \rangle$ are the mean polarization along $\hat{x}$-axis and the mean position of the ensemble of the electrons as a function of time, τ and L are chosen to be characteristic time and distance such that

$$\langle S_x \rangle = A \times \exp(-t/\tau) = B \times \exp(-\langle x \rangle / L)\,, \tag{6}$$

with A and B normalization factors. L and τ satisfy the relation $L = v_{\mathrm{d}} \cdot \tau$, where v_{d} is the average drift velocity.

3. Numerical results and discussion

In Fig. 2 we show the spin electron relaxation length L (panel (a)) and the spin depolarization time τ (panel (b)) as a function of the lattice temperature, for different values of the electric field amplitude, namely $F = 0.1, 0.2, 0.3, 0.5, 1.0, 1.5, 2.0$ kV/cm. For a fixed electric field, the spin electron relaxation length is a monotonic decreasing function of the temperature. When $F = 0.5$ kV/cm, L shows its maximum value, remaining greater than 35 μm up to $T \simeq 80$ K. Furthermore, for field amplitudes greater than 1 kV/cm, the spin depolarization length remains almost constant for $T < 100$ K. At room temperature the maximum value of L (~ 6 μm) is obtained for F≥ 1 kV/cm.

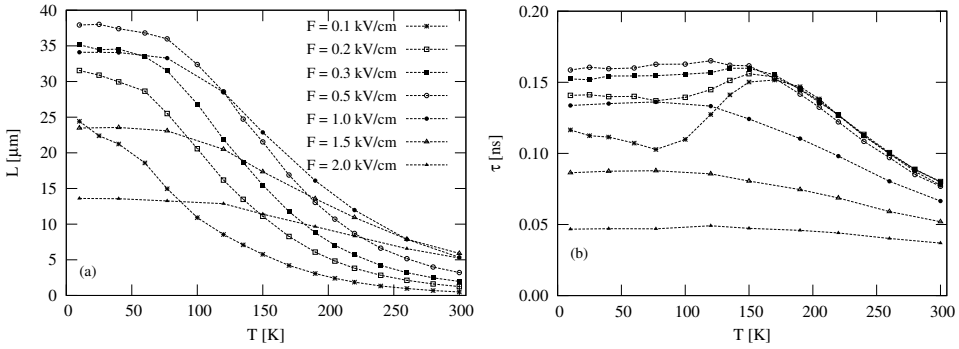

Fig. 2. (a) Spin depolarization length L and (b) spin depolarization time τ as a function of the temperature T, plotted for several values of the electric field amplitude F.

The relaxation time τ shows, instead, a nonmonotonic behavior with the temperature (see Fig. 2 (b)). In particular, the curves obtained with $F = 0.1$ and 0.2 kV/cm exhibit a minimum at $T \sim 80$ K and an increase in the range 100–170 K. For temperatures greater than 170 K, all curves with a field amplitude up to 0.5 kV/cm show a common decreasing trend. The longest value of spin coherence time is achieved for the field amplitude $F = 0.5$ kV/cm for almost the entire range of temperatures. For higher values of F, the spin depolarization time strongly decreases, becoming nearly temperature-independent for $F > 1.5$ kV/cm.

As the temperature increases, the scattering rate increases too, and hence the ensemble of spins loses its spatial order faster, resulting in a faster spin relaxation. This temperature dependence becomes less evident at higher amplitudes of the driving electric field, where, because of the greater drift velocities, the polarization loss is mainly due to the strong effective magnetic field. At very low electric fields, the spin dephasing is, instead, primarily caused by the multiple scattering events. The nonmonotonicity of τ can be ascribed to the progressive change, with the increase of the temperature, of the dominant scattering mechanism from acoustic phonons and ionized impurities to polar optical phonons [11]. Following the standard theory of D'yakonov–Perel, τ^{-1} is proportional to the third power of the temperature T and linearly depends on the momentum relaxation time τ_p [15]. An increase of the temperature initially leads to a slightly decrease of τ; for temperatures greater than ~ 100 K the electrons start to experience scattering by polar optical phonons. This switching on leads to an abrupt decrease of τ_p that, for lattice temperatures in the range 100–150 K, results more effective than the increase of T, giving rise to the observed increase of τ. For temperatures greater than 150 K this latter effect is no more relevant.

In Fig. 3 we plot the spin depolarization length L (panel (a)) and the spin depolarization time τ (panel (b)) as a function of the electric field amplitude, for different values of the lattice temperature. The spin relaxation lengths show a marked maximum that rapidly reduces its intensity, widens and moves towards higher electric field amplitudes with the increasing of the temperature. For temperatures $T \leq 150$ K the decoherence times plotted in Fig. 3 (b) show a nonmonotonic behavior. For $F > 0.5$ kV/cm, τ lightly depends on the temperature up to $T \sim 150$ K. At higher temperatures, the spin electron relaxation time becomes a monotonic decreasing function of the electric field intensity.

The presence of maxima in the spin depolarization length at intermediate fields can be explained by the interplay between two competing factors: in the linear regime, as the field becomes larger, the electron momentum and the drift velocity increase in the direction of the field. On the other hand, the increased electron momentum also brings about a stronger effective magnetic field, as shown in Eq. (3) [7]. Consequently, the electron precession frequency becomes higher, resulting in faster spin relaxation (*i.e.*, shorter

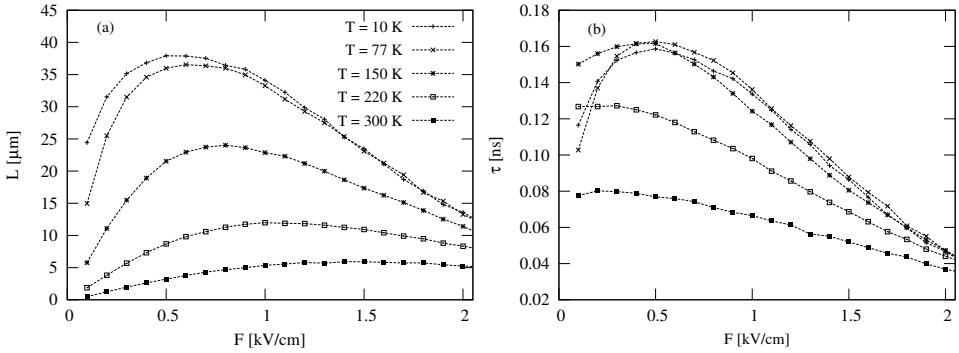

Fig. 3. (a) Spin depolarization length L and (b) Spin depolarization time τ as a function of the electric field amplitude F, plotted for several values of the temperature T.

spin relaxation time). For $F < 0.5$ kV/cm and $T \leq 150$ K the nonmonotonic behavior of the relaxation time reflects the complex scenario described above, caused by the triggering of scattering mechanisms having different rates of occurrence.

4. Conclusions

For the extensive utilization of spintronic devices, the features of spin decoherence at relatively high temperature, jointly with the influence of transport conditions, should be fully understood. In this work, by using a semiclassical Monte Carlo approach, we have estimated the spin mean lifetimes and depolarization lengths of an ensemble of conduction electrons in lightly doped n-type GaAs crystals, in a wide range of lattice temperatures ($10 < T < 300$ K) and field amplitudes ($0.1 < F < 2$ kV/cm). We have shown that, under particular conditions, also at temperatures greater than the liquid-helium temperature, it is possible to obtain very long spin relaxation times and relaxation lengths. These are essential for the high performance of spin-based devices, in order to extend the functionality of conventional devices to higher working temperatures and higher electric field amplitudes and to allow the development of new information processing systems. In particular, for $F = 0.5$ kV/cm we achieve the longer value of spin lifetime ($\tau > 0.15$ ns) up to a temperature $T = 150$ K. At room temperatures, we obtain a coherence length of about 6 μm, nearly independent from the intensity of the electric field.

Furthermore, depending on the interplay between the external electric field and the different collisional mechanisms with increasing electron energy, we find very interesting nonmonotonic behavior of spin lifetimes and depolarization lengths as a function of temperature and electric field amplitude. This point deserves further investigations.

Understanding these phenomena could lead to high temperature and high field improvement of the gating mechanisms engineering of spin-based devices.

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