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Theoretical Study of Spin Lifetimes in [110] Strained GaAs

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We present first-principles studies of the zero field spin splitting of conduction band in [110] strained GaAs that determine spin lifetimes in semiconductors. Our calculations reveal strong anisotropy of the linear-$\boldsymbol{k}$ spin splitting in the (110) plane of the Brillouin zone and very minor in the (001) plane. This provides a qualitative understanding of the difference in the spin lifetimes in the GaAs/AlAs heterostructures grown along [100] and [110] crystallographic directions.

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1. Introduction

The present surge in interest for spin devices and spin relaxation effects calls for a detailed understanding of the spin dynamics in semiconductor nanostructures [1, 2]. The spin splitting of the bands caused by the spin–orbit coupling induces a coherent spin precession that is an essential factor, together with spin-dependent and spin-independent scattering rates, determining spin lifetimes in semiconductors and their heterostructures [2]. These spin-related effects have been studied extensively both theoretically and experimentally, yet there are still many open questions concerning the microscopic origin of the spin splitting of the energy bands, their dependence on material combinations, on quantum well widths, or external factors like strain and/or electric field [2]. For example, experimental studies have revealed that the spin lifetimes of conduction band electrons can be dramatically different in heterostructures grown along [001] and [110] crystallographic directions [3]. In this paper we attempt to explain these experimental findings by performing first-principles, relativistic local density calculations for biaxially strained GaAs. The biaxial strain in the (110) crystallographic plane causes that the bulk symmetry T_d is reduced to C_{2v}. The [110] grown GaAs/AlAs heterostructures possess also this symmetry, whereas the [001] heterostructures have

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higher D_{2d} one. Therefore, a comparison of the spin splitting in the (110) and (001) planes of the, respectively, orthorhombically and tetragonally strained GaAs should shed light on the physical mechanisms that lead to dramatic differences in the spin lifetimes in the heterostructures grown along [110] and [001] directions.

In the [110] and [001] strained bulks, the reduction of the cubic symmetry causes that linear-$\boldsymbol{k}$ spin splitting terms (not present in the conduction band of the cubic systems) appear in the conduction band. These linear-$\boldsymbol{k}$ terms cause a camel--back or Mexican-hat-type structure of the conduction band in the neighborhood of the Γ point. In systems of the symmetry C_{2v} the linear-$\boldsymbol{k}$ spin splitting is anisotropic and can be effectively described by two different interfering terms, bulk inversion asymmetry (BIA or Dresselhaus) and structural inversion asymmetry (SIA or Rashba) terms.

In this paper, we present a systematic study of the linear-$\boldsymbol{k}$ spin splitting through the Brillouin zone of the [110] strained GaAs by the mean of the *ab initio* relativistic calculations that are performed in the framework of the local density approximation to the density functional theory and pseudopotential method. This approach has been applied previously to various studies of the spin splitting in semiconductors and their heterostructures. It provides, for example, very accurate description of the valence band spin splitting Δ_0 in III–V bulks [4, 5]. The calculated linear-$\boldsymbol{k}$ spin splitting has been also mapped on the simple two-band effective Hamiltonian traditionally used to the analysis of this problem [4–6]. Owing to the nearly complete lack of experimental data concerning the linear-$\boldsymbol{k}$ spin splitting, the present calculations provide theoretical predictions for these quantities.

2. Results and discussion

2.1. Effective Hamiltonian for linear-$\boldsymbol{k}$ spin splitting around the Γ-point

As it was already mentioned in the introduction, the linear-$\boldsymbol{k}$ spin splitting in the conduction band around the Γ-point has two origins. This leads to the following effective Hamiltonian in the conduction band of the [110] strained bulk $\hat{H} = \boldsymbol{\sigma} \cdot \boldsymbol{\Omega}(\boldsymbol{k}) = \hat{H}_{\mathrm{BIA}}(\boldsymbol{k}) + \hat{H}_{\mathrm{SIA}}(\boldsymbol{k})$, where the components of the effective magnetic field $\boldsymbol{\Omega}(\boldsymbol{k})$ are given by $\Omega_x = \alpha_{\mathrm{SIA}} k_y$, $\Omega_y = -\alpha_{\mathrm{SIA}} k_x$, $\Omega_z = -\alpha_{\mathrm{BIA}} \frac{1}{\sqrt{2}}(-k_x + k_y)$, and $\boldsymbol{\sigma}$ is the vector of Pauli matrices. The components x and y of the vector $\boldsymbol{\Omega}$ originate from the SIA (Rashba) Hamiltonian, $\hat{H}_{\mathrm{SIA}} = \alpha_{\mathrm{SIA}} \boldsymbol{\sigma} \cdot \boldsymbol{k} \times \boldsymbol{\nu}$, where the vector $\boldsymbol{\nu}$ determines the direction of the axial symmetry [6]. For [110] strained bulk, the vector $\boldsymbol{\nu}$ is parallel to the [001] direction, leading to the above expressions for Ω_x and Ω_y components. The BIA Hamiltonian for [110] strained bulk (that originates from the Dresselhaus term) contributes only to the z-component of the vector $\boldsymbol{\Omega}$ [7]. The spin lifetime is proportional to the square of the vector $\boldsymbol{\Omega}(\boldsymbol{k})$ averaged over the angles. Therefore, the angular dependence of the vector $\boldsymbol{\Omega}(\boldsymbol{k})$ in the plane perpendicular to the growth direction will determine the spin lifetime in the heterostructure. The energy difference between two eigenvalues of the Hamiltonian, i.e., the spin splitting, is equal $\Delta E_{\mathrm{spin}}(\boldsymbol{k}) = 2|\boldsymbol{\Omega}(\boldsymbol{k})|$. Here, we

calculate $\Delta E_{\rm spin}(\boldsymbol{k})$ for the [110] strained GaAs directly employing *ab initio* calculations and then determine the constants $\alpha_{\rm SIA}$ and $\alpha_{\rm BIA}$ in effective Hamiltonian. Finally, the distribution of the effective magnetic field $\boldsymbol{\Omega}(\boldsymbol{k})$ through the Brillouin zone can be established.

2.2 Computational details

The elastic strain tensor for bulk cubic crystal biaxially strained in the (110) plane has the following components: $\varepsilon_{xx} = \varepsilon_{yy} = (a_{\parallel} + a_{\perp})/(2a_0) - 1$, $\varepsilon_{zz} = a_{\parallel}/a_0 - 1$, $\varepsilon_{xy} = (a_{\perp} - a_{\parallel})/(2a_0) - 1$, $\varepsilon_{xz} = \varepsilon_{yz} = 0$, where a_0, $a_{\parallel}$, and $a_{\perp}$ are equilibrium lattice constant, lattice constant in the (110) plane of the strained crystal, and lattice constants in the [110] direction, respectively. This implies that in addition to the tetragonal (diagonal) components, strain tensor possesses off-diagonal orthorhombic component just reflecting the C_{2v} symmetry. The external biaxial strain is defined by the relative difference of the lattice constants $a_{\parallel}/a_0 - 1$. The system can freely relax in the [110] direction, just to minimize the total deformation energy. This minimization has been performed in the *ab initio* total energy calculations for each value of $a_{\parallel}$ and the corresponding value of $a_{\perp}$ has been established. In strained bulk of C_{2v} symmetry, positions of atoms in the unit cell along the [001] direction are not determined by symmetry. Therefore, the geometry of the unit cell has been always optimized by requiring the vanishing of atomic forces. This allows one to find the so-called internal strain parameter ξ. The internal strain parameter is defined in a standard manner, i.e., in such a way that the position of the cation is equal to $\boldsymbol{\tau}_{\rm c} = (a_{\perp}/4, a_{\perp}/4, a_{\parallel}/4 - \xi(a_{\perp} - a_{\parallel})/4)$ (position of anion has been chosen as origin). For example, for the compressive strain corresponding to –0.5%, we find the value of $a_{\perp}/a_0 - 1$ to be equal to 0.0028 and the internal strain parameter $\xi = 0.5617$. Having the geometry of the unit cell determined, we are in position to calculate band structure with spin orbit coupling taken into account non-perturbatively, just employing previously developed pseudopotential formalism [5].

2.3. Linear-$\boldsymbol{k}$ spin splitting of conduction band in [110] strained GaAs

The calculated linear-$\boldsymbol{k}$ conduction band spin splitting in [110] strained GaAs for wave vectors lying in the (001) and (110) planes is depicted in Figs. 1 and 2, respectively. In these figures, the spin splitting has been normalized to the length of the in-plane vector. As one can see the spin splitting exhibits a small anisotropy for wave vectors lying in the (001) plane, whereas the anisotropy in the (110) plane is huge. The values of spin splitting obtained in the *ab initio* calculations perfectly agree with the angular dependence deduced from the effective Hamiltonian. The angular dependence of the spin splitting in the (110) plane is given by the formula $\Delta E_{\rm spin}^{(110)} = 2k_{\parallel}\cos\theta\sqrt{\alpha_{\rm BIA}^2 + \alpha_{\rm SIA}^2}$, where $k_{\parallel}$ is the length of the $\boldsymbol{k}_{\parallel}$ in-plane vector, and θ is the angle between vector $\boldsymbol{k}_{\parallel}$ and the cubic [–110] direction. For the spin splitting in (001) plane, we have the following expression $\Delta E_{\rm spin}^{(001)} = 2k_{\parallel}\sqrt{\alpha_{\rm BIA}^2\frac{1}{2}(1 - \sin 2\phi) + \alpha_{\rm SIA}^2}$, with $\boldsymbol{k}_{\parallel}$ vector lying now in (001) plane

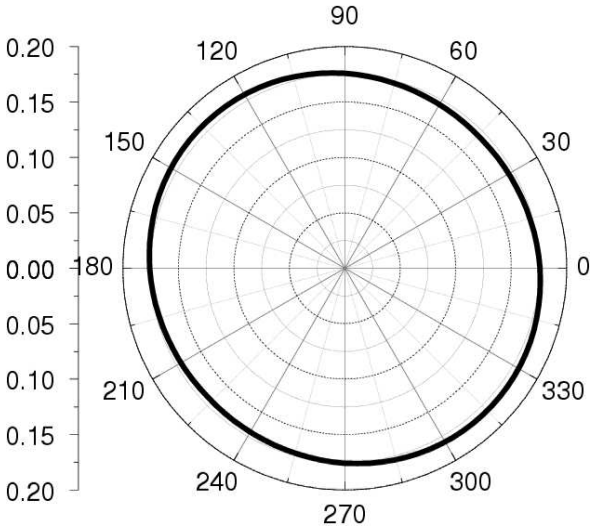

Fig. 1. The angular dependence of the conduction band spin splitting for the wave vectors lying in the (001) plane. The angles 0° and 90° correspond to the directions [100] and [010], respectively.

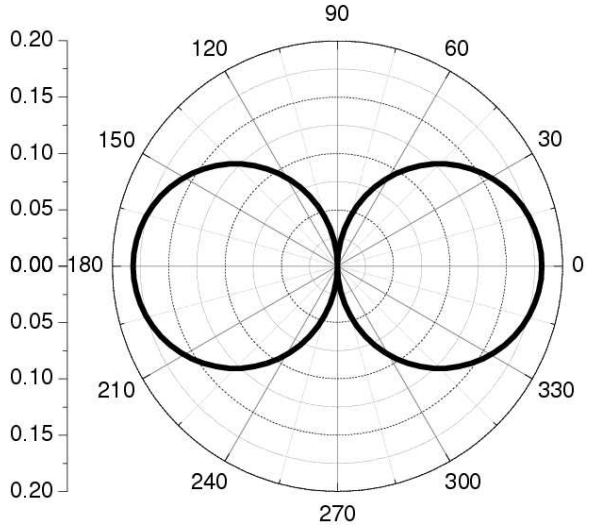

Fig. 2. The angular dependence of the conduction band spin splitting for the wave vectors lying in the (110) plane. The angles 0° and 90° correspond to the directions [–110] and [001], respectively.

and ϕ being the angle between $\boldsymbol{k}_{\|}$ and cubic [100] axis. The linear-$\boldsymbol{k}$ spin splitting disappears only along the [001] axis, being not zero in the rest of the Brillouin zone. This together with the direct dependence of the $\Delta E_{\mathrm{spin}}^{(110)}$ on the $\cos\theta$ is the

reason of the strong anisotropy of the linear-$\boldsymbol{k}$ spin splitting in the (110) plane. A comparison of the spin splitting from *ab initio* calculations (for small length of the wave vectors) with the analytic formulae gives the BIA and SIA constants. For example, in the case of –0.5% compressive strain α_{BIA} and α_{SIA} are equal to 0.032 and 0.085 eV Å, respectively.

The angular dependence of the spin splitting for in-plane wave vectors from the (001) plane strongly resembles spin splitting of the no-common-atom heterostructures grown along [001] direction (also with symmetry C_{2v}). It is worth noting that for wave vectors parallel to [110] direction only Rashba term contributes to the linear-$\boldsymbol{k}$ spin splitting in the [110] strained bulk, whereas in the no-common-atom heterostructures one has both, i.e., BIA and SIA contributions [7]. In the case of the symmetric heterostructures grown along [001] direction (e.g., [001] GaAs/AlAs), the linear-$\boldsymbol{k}$ spin splitting in the (001) plane is isotropic; because of D_{2d} symmetry only BIA term contributes and SIA Rashba term disappears [6]. The (110) plane of the [110] strained GaAs is a prototype of this plane in the [110] grown GaAs/AlAs heterostructures. The strong anisotropy of the linear-$\boldsymbol{k}$ spin splitting in the (110) plain contrasts with the isotropic in-plane spin splitting in the symmetric [001] GaAs/AlAs heterostructures. In the [001] and [110] GaAs/AlAs heterostructures, two-dimensional electron gas forms in the crystallographic planes (001) and (110), respectively. The large difference in the angular dependence of spin splitting in planes (001) and (110) might be the origin of the large discrepancy in the lifetimes in the [001] and [110] heterostructures. The further calculations for the [110] heterostructures are under way and will be published elsewhere.

3. Conclusions

We have performed *ab initio* calculations of the zero field linear-$\boldsymbol{k}$ spin splitting of the conduction band in the [110] strained GaAs. We have found that the spin splitting exhibits very strong anisotropy in the (110) plane, whereas the spin splitting shows only weak anisotropy in the (001) plane. For tetragonally strained cubic crystals or symmetric [001] heterostructures, the linear-$\boldsymbol{k}$ spin splitting is isotropic. Since the angular average of the spin splitting determines the spin lifetime, this explains qualitatively the huge difference in the spin lifetimes in the [110] and [001] heterostructures as observed in experiment. It opens also new opportunities in tuning the spin lifetime of electrons through the growth of heterostructures onto suitable crystallographic plane.

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