**SERBIAN JOURNAL OF ELECTRICAL ENGINEERING**
**Vol. 6, No. 3, December 2009, 461 - 469**

**UDK: 621.38.049.77**

# Influence of Strain on Band Structure of Semiconductor Nanostructures*

**Nevena Raičević[1], Milan Tadić[2]**

**Abstract:** The influence of the mechanical strain on the electronic structure of the asymmetric (In,Ga)As/GaAs quantum well is considered. Both the direct influence of strain on the orbital part of the electronic structure and an indirect influence through the strain dependent Rashba and Dresselhaus Hamiltonians are taken into account. The analyzed quantum well is taken to have a triangular shape, and is oriented along the <110> direction. For this direction, there exists both the intrinsic and strain-induced spin-orbit interaction. For all analyzed types of spin-orbit interaction, subband splittings depend linearly on the in-plane wave vector. On the other hand, the electronic structure for the Rashba type of the strain-induced spin-orbit interaction shows isotropic dependence in the k-space, while the electronic structure due to the Dresselhaus type shows anisotropy. Furthermore, the Rashba strain-induced spin-orbit interaction increases subband splitting, while the effect of the Dresselhaus Hamiltonian on the electronic structure is opposite to the intrinsic spin-orbit interaction for certain polar angles.

**Keywords:** Spin-orbit interaction, Strained structures.

## 1 Introduction

Devices based on spin transport, especially the ones made of nanometer layers, have lots of advantages compared to electronic devices, which is the reason for increased interest in (nano)spintronics. Good characteristics of spintronic devices are: improved operating speed, smaller dimensions and lower power consumption. Spintronic effect, giant magnetoresistance, is already used for production of great capacity hard disc heads. Realization of other suggested spintronic devices, such as Datta-Das transistor and magnetic resonant tunneling diode, will be possible if electron spin manipulation technique improves [1].

Very important spin manipulation technique is based on spin-orbit interaction (SOI), which leads to degenerate energy state splitting into electron energy states of different spin. Increase of different electron spin states

[1]Laboratory of Atomic Physics, Institute of Nuclear Science "Vinca", Beograd, Serbia; E-mail: nevenar@vinca.rs
[2]Department of Nanoelectronics, School of Electrical Engineering, University of Belgrade, Bulevar Kralja Aleksandra 73, 11120 Belgrade, Serbia; E-mail: tadic@etf.rs
*Award for the best paper presented in Section *Microelectronics and Optoelectronics*, at Conference ETRAN 2009, June 15-19, Vrnjačka Banja, Serbia.

difference is of critical importance for SOI application in suggested devices [1]. In unstrained structures one can recognize two types of SOI. The first one is a result of bulk of inversion asymmetry, called Dresselhaus effect, while the second one is due to structure inversion asymmetry, Rashba effect. Both types of SOI are denoted as intristic SOI, ISOI and represented as $H_{in}^{R}$ and $H_{in}^{D}$, for Rashba and Dresselhaus effect respectively.

Besides external fields which exist because of potential discontinuity at heterojunction or applied field, SOI can be changed by applying strain [2-4]. The influence on electronic structure is twofold. Change of crystal symmetry leads to the splitting of different electron spin states, which are split itself as a result of quantum confining. Second effect on electronic structure comes from strain-induced spin-orbit interaction (SISOI). Effectively, coupling coefficients between wavevector and electron spin depend on the strain [4, 5]. In quantum wells made of zinc-blende structure semiconductor, SISOI does not exist along <100> direction, but when structure is grown along <110> direction or <111> direction, it is not zero. Just like in a case of ISOI, SISOI can be Rashba like ($H_{st}^{R}$) and Dresselhaus like ($H_{st}^{D}$) [3-5].

Energy states splitting of different electron spin states depending on strain could be used for spin manipulation in nanostructures by *strain engineering*. It turns out that strain could be one parameter more for electron spin control. Strain influences spin precession and can be used for spin dephasing time increase [5].

We analyzed asymmetrical triangular quantum well made of (In, Ga) As/GaAs heterojunctions, where (In, Ga)As is used as a well material. Reason for choosing this structure is a relatively small energy gap of InAs, which is important because spin-orbit interaction in semiconductor increases with energy gap decreasing. Also, the strain among GaAs and (In, Ga)As layers has quite large value, which brings high strain-induced SOI. This system was used in experiment concerning spin Hall effect in paper [2]. We assumed structure growth in direction <110>. In this paper we compared influence of ISOI and SISOI and estimated importance of SISOI for application in spintronic devices.

## 2 Theoretical Consideration

Hamiltonian that describes electron energy in conduction band of semiconductor quantum well is defined as:

$$H = T + V_{off} + V_{hydro} + H_{in}^{R} + H_{in}^{D} + H_{s}^{R} + H_{s}^{D}, \tag{1}$$

where $T$ denotes kinetic part of Hamiltonian, $V_{off}$ represents conduction band offset potential and potential due to structure variation, $V_{hydro}$ is effective

potential due to hydrostatic strain in strained well layers. Rest of the terms in Hamiltonian determinates SOI. Hamiltonian of Dresselahus intrinsic spin-orbit interaction is defined by:

$$H_{in}^{D} = \gamma_D \left( k_x \sigma_x - k_y \sigma_y \right), \tag{2}$$

Rashba type ISOI Hamiltonian is given by the following relation:

$$H_{in}^{R} = \alpha_{BR} \left( k_x \sigma_y - k_y \sigma_x \right), \tag{3}$$

and $\alpha_{BR}$ refers to Rashba spin-orbit coupling strength, $y_D$ stands for Dresselhaus spin-orbit coupling strength, $\sigma_x$ and $\sigma_y$ are Pauli's matrix, and $k_x$ and $k_y$ denote components of the transversal wavevector:

$$\begin{aligned} k_x &= k_p \cos(\varphi), \\ k_y &= k_p \sin(\varphi), \end{aligned} \tag{4}$$

where $k_p = \sqrt{k_x^2 + k_y^2}$ represents the transversal wavevector of electron and $\varphi$ is a polar angle. When both of ISOI effects are present in the structure, anisotropy of energy splitting in $(k_x^2, k_y^2)$ plane occurs [1].

Mechanical strain is a consequence of lattice misalignment between the substrate and thin well layers. We assumed that the analyzed structure is pseudomorphic, i.e. strain energy is confined in elastic deformation, and there are no defects at interface or in well or barrier materials. Condition for pseudomorphic growth of Frank-van der Merve mode are satisfied until reaching critical thickness, which depends on heterojunction materials. Electronic structure of pseudomorphic structures is described by electron deformation potential and strain tensor.

Values of strain tensor components depend on nanostructure growth direction. For <110> structure orientation strain tensor components are [6]:

$$\begin{aligned} \varepsilon_{xx} = \varepsilon_{yy} &= \frac{(2C_{44} - C_{12})\varepsilon_{\|}}{C_{11} + C_{12} + 2C_{44}}, \\ \varepsilon_{zz} &= \varepsilon_{\|}, \\ \varepsilon_{xy} = \varepsilon_{yx} &= -\frac{-(C_{11} + 2C_{12})\varepsilon_{\|}}{C_{11} + C_{12} + C_{44}}, \\ \varepsilon_{xz} = \varepsilon_{zx} = \varepsilon_{yz} &= \varepsilon_{zy} = 0. \end{aligned}$$

Here $C_{12}$, $C_{11}$ and $C_{44}$ denote elasticity constants, $\varepsilon_{\|}$ represents biaxial strain in $xy$ plain, while $\varepsilon_{\|} = (a_0 - a)/a$, where substrate lattice constant is $a_0$,

and $a$ denotes lattice constant of a layer. Mechanical strain leads to potential energy increase of conduction band. Mathematically it is described by:

$$V_{hydro} = a_c \left( \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} \right). \tag{5}$$

This term forms effective potential, together with discontinuity potential.

Classification of SISOI Hamiltonians on Dresselhaus type and Rashba type is based on similarities between forms of ISOI and SISOI. Form of Dresselhaus SISOI is [3]:

$$H_{st}^{D} = D\left(\varepsilon_{zz}(z) - \varepsilon_{xx}(z)\right)(\sigma_x k_x - \sigma_y k_y). \tag{6}$$

This Hamiltonian depends only on diagonal components of the strain tensor, while Rashba SISOI depends on the shear strain [1]:

$$H_{st}^{R} = \frac{1}{2} C_3 \varepsilon_{xy} (\sigma_x k_y - \sigma_y k_x). \tag{7}$$

In last equations $C_3$ and $D$ are material constants.

Hamiltonian in (1) consists of four types of spin-orbit interaction. For the sake of simplicity, we are taking into consideration only intrinsic Rashba spin-orbit interaction. Effectively we will compare only two types of SOI, $H_{so}^{R+R} = H_{in}^{R} + H_{st}^{R}$ and $H_{so}^{R+D} = H_{in}^{R} + H_{st}^{D}$. It actually means that we are going to compare $H_{st}^{R}$ and $H_{st}^{D}$ when intrinsic Rashba SOI is taken into account in asymmetric triangular quantum well. Hamiltonian has a matrix form in both analyzed cases. For $R+R$ combination, Hamiltonian is defined as

$$H_{so}^{R+R} = \begin{bmatrix} 0 & H_{12} \\ H_{12}^{+} & 0 \end{bmatrix}, \tag{8}$$

where:

$$H_{12} = \left( \alpha(z) + \frac{1}{2} C_3 \varepsilon_{xy} \right) \left( k_y + i k_x \right). \tag{9}$$

Eigenproblem:

$$H\chi = E\chi, \tag{10}$$

is solved by spinor discretization of anvelope functions $\chi$ using the finite difference method on adequate net.

## 3 Numerical Results

For numerical calculations we used material parameters that define the analized structure [6]:

$m(x) = (0.067 - 0.04)m_0$;

$E_g(x) = (1.42 - 1.06x)$ [eV];

$C_{11}(x) = (1221 - 388.1x)$ [GPa];

$C_{12}(x) = (566 - 113.4x)$ [GPa];

$C_{44}(x) = (600 - 204.1x)$ [GPa];

$a_c(x) = (-7.17 + 2.09x)$ [eV];

$\alpha(x) = (4.72 + 107.7x) \cdot 10^{10}$ [meV];

$C_3(x) = 0.52$ [eV nm];

$D = 1.59 \cdot 10^4$ [m/s];

$a(x) = (0.56532 + 0.04051x)$ [nm].

Here $x$ denotes InAs fraction in the layer and $m_0$ represents free electron mass.

Analyzed structure is presented on Fig. 1a. We assumed well thickness to be 20 nm, and for the sake of simplicity we assumed that there are infinitely high barriers 5 nm distant from the well. Thin barrier is a good approximation for the lowest energy states whose wavefunctions decrease very quickly in the barriers. Fraction of InAs in (In,Ga)As alloy grows linearly, from zero on the left well interface to one on the right well border. The potential energy of the unstrained structure is presented with doted line in Fig. 1a. Dashed line stands for the potential profile in a strained structure.

Splitting energies as a result of intrinsic Rashba effect are plotted on Fig. 1b. It is important to notice that energy splitting linearly grows with the increase of the wavevector, which is consequence of linearly dependence SOI Hamiltonian on the wave vector. Energy splitting decreases with the increase of subband number, i.e. it is lower for higher subbands. This situation is similar to the one in atoms, where spin-orbit interaction has greater influence on lower energy states. Dependence of splitting energy on polar angle φ when only Rashba ISOI is taken into account is presented on Fig. 1c and we can notice it is isotropic.

Fig. 2 presents the dependences of energy splitting on the wavenumber $k_p$ and the polar angle, when Rashba ISOI and SIOI are taken into account. Calculation shows that dependence on wave number is almost linear. Energy splitting is independent on polar angle, i.e., splitting is isotropic in described model. It is worth mentioning that splitting energy for some value of a wave number, let it be $4 \cdot 10^8\ \mathrm{m}^{-1}$, is about 2.5 times higher when Rasba SISOI is taken into account (compare Figs. 1b and 2a).

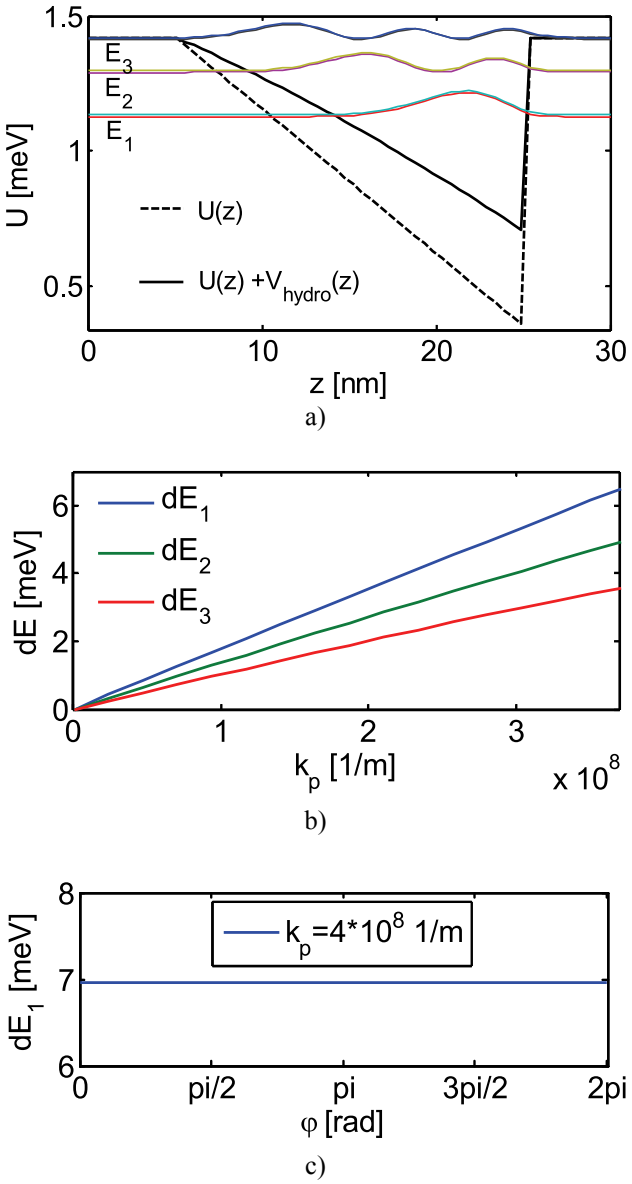
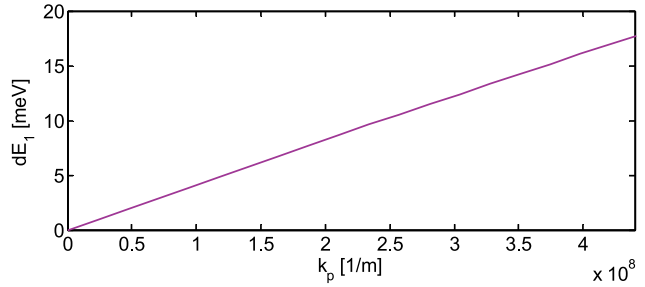
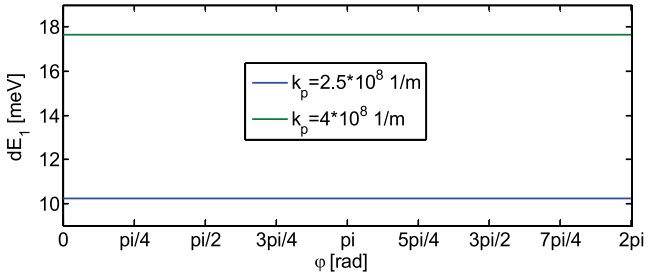



**Fig. 1** – a) *Conduction band edge in* (In, Ga)As/GaAs *qauntum well*; b) *Subband splitting versus transversal wavenumber when only intrinsic Rashba effect is taken into account*; c) *First subband splitting versus* $\varphi$ .




a)

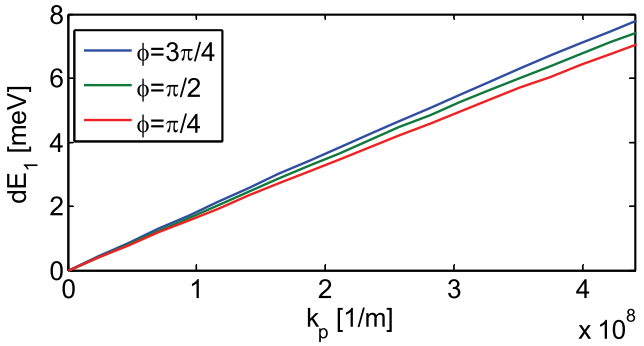



b)

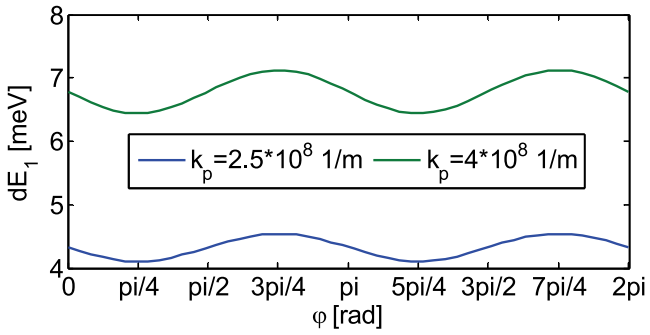
**Fig. 2** – *Splitting energy of first subband for* R+R SOI *case*: a) *versus* $k_p$; b) *versus* $\varphi$.

In Fig. 3 we presented splitting energy dependence on wavenumber $k_p$ and polar angle for both Rashba ISOI and Dresselhaus SISOI. Energy splitting for $R+D$ is almost equal to energy splitting when only intrinsic Rashba effect is taken into account. It means that strain induced Dresselhaus effect is very small. In other words, splitting energy is about 2.5 times less then for R+R combination. On the other hand, electronic structure for $R+D$ combination is very anisotropic in $(k_x, k_y)$ plain. This anisotropy is a result of interference of different spin-orbit coupling types.

At the end, we will mention that electronic structure for $D+D$ combination gives 10 times less values of splitting energies, and 2 times less for $D+R$ combination for same value of wave number comparing to $R+R$ case.




a)




b)

**Fig. 3 –** *Splitting energy of the first energy state in* (In,Ga)As/GaAs *well for* $R + D$ *case*: (a) *versus* $k_p$; (b) *versus* $\varphi$.

## 4 Conclusion

We analyzed influence of mechanical strain on SOI and subband splitting in asymmetric <110> oriented quantum well. Intrinsic Rashba SOI is assumed. After numerical calculations we can say that strain-induced Rashba SOI induces the increase of splitting energies, while strain-induced Dresselhaus SOI does not affect value of splitting energies but brings anisotropy of splitting energies in transversal plain. Interference of different types of SOI depends on parameters which describe them: $\alpha_{BR}$, $y_D$, $C_3$ and $D$. If corresponding parameters in nanostructure are small enough, the results of used model shows that strain can significantly increase subband splitting energies and that way cause characteristics enhancement of strained nanostuctures.

## 5 References

[1] I. Zutic, J. Fabian, S. Das Sarma: Spintronics: Fundamentals and Applications, Reviews of Modern Physics, Vol. 76, No. 2, Apr. 2004, pp. 323 – 410.

[2] Y.K. Kato, R.C. Myers, A.C. Gossard, D.D. Awschalom: Observation of the Spin Hall Effect in Semiconductors, Science, Vol. 306, No. 5703, Dec. 2004, pp. 1910 – 1913.

[3] Y. Li, Y.Q. Li: Strain-assisted Spin Manipulation in a Quantum Well, The European Physical Journal B – Condensed Matter, Vol. 63, No. 4, June 2008, pp. 493 – 500.

[4] B.A. Bernevig, S.C. Zhang: Spin Splitting and Spin Current in Strained Bulk Semiconductors, Physical Review B, Vol. 72, No. 11, Sept. 2005, pp. 115204 – 115210.

[5] G.L. Bir, G.E. Pikus: Symmetry and Strain-induced Effects in Semiconductors, Wiley, New York, 1974.

[6] I. Vurgftman, R. Meyer: Band Parameters for III–V Compound Semiconductors and their Alloys, Journal of Applied Physics, Vol. 89, No. 11, June 2001, pp. 5815 – 5875.