Substrate Orientation-Dependence of Electron Mobility in Strained SiGe Layers

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***Abstract*— The behavior of the low field electron mobility in strained active SiGe layers on SiGe substrates with arbitrary orientation and Ge mole fraction is investigated using Monte Carlo simulation. Euler's angles are introduced to determine the substrate orientation and direction for the in-plane component of the mobility. The strain tensor is transformed to a general form and the splitting of X and L valleys is then calculated using linear deformation potential theory. Additionally the hydrostatic shift is taken into account. For doped materials the ionized impurity scattering rate is modified to take into consideration all valleys and orientations. The Pauli exclusion principle is considered for high doping level and its interplay with the strain effects is discussed.**

I. Introduction

In advanced semiconductor devices strain can be used as an additional degree of freedom to enhance transport properties due to band structure changes. A dominant change is the degeneracy reduction of the conduction band extrema which are degenerate in a relaxed material because of the symmetry of the crystal. The conduction band minima splitting depends on the projections of the valleys' $\vec{k}$ vectors onto the stress direction. In this work we investigate homogeneously strained SiGe active layers on SiGe relaxed substrates. The stress direction is thus perpendicular to the substrate orientation. To describe the degeneracy reduction effect together with the hydrostatic pressure component which shifts the mean energy of valleys, the deformation-potential theory is applied to many-valley cubic semiconductors [1]-[3]. Within this theory the strain tensor is introduced and used to calculate the energy shifts. The form of the strain tensor strongly depends on the orientation of the interface. While the strain tensor has diagonal form for $[001]$ substrate orientation, it is non-diagonal for a general substrate orientation which can cause the splitting both of X and L valleys. As shown below the in-plane mobility depends on the in-plane angle for a general substrate orientation.

Other strain effects such as the splitting of degenerate orbital bands with $\vec{k}$ vectors which are not parallel to the stress and different stress-induced couplings between neighboring bands are neglected here. The shear distortion of the crystal lattice is also neglected. We employ an analytical description of the conduction bands to investigate the low-field mobility and use the zero-field Monte Carlo algorithm.

II. Strain Tensor and Energy Splitting

For a general substrate orientation the strain tensor assumes a non-diagonal form. In order to obtain a new form of the tensor a transformation of the coordinate system is performed. This conserves the symmetry of the strain tensor. The coordinate system transformation represents two successive rotations which can be specified by two Euler's angles. The third Euler's angle is superfluous for the strain tensor but is used to fix the in-plane direction for the calculation of the in-plane component of the mobility.

If the first and the second Euler's angels are denoted as α and β ($0 \leq \alpha \leq 2\pi$, $0 \leq \beta \leq \pi$), the transformed strain tensor can be written as follows:

$$\epsilon^{'} = U^T(\alpha,\beta) \cdot \epsilon \cdot U(\alpha,\beta), \tag{1}$$

where the unitary matrix $U(\alpha,\beta)$ is a product of the two rotation operators and has the form:

$$U(\alpha,\beta) = \begin{bmatrix} \cos\alpha\cos\beta & \sin\alpha\cos\beta & -\sin\beta \\ -\sin\alpha & \cos\alpha & 0 \\ \cos\alpha\sin\beta & \sin\alpha\sin\beta & \cos\beta \end{bmatrix}. \tag{2}$$

The strain tensor with respect to the interface coordinate system has diagonal form due to the absence of in-plane shear. We also neglect the shear distortion as an effect of the second order. Due to biaxial dilatation (or contraction) two diagonal components of the strain tensor are equal to each other. The condition of zero stress along the substrate orientation is imposed. To calculate the strain tensor elements Hooke's law is applied. As a result the strain tensor takes the following form in particular for $[110]$ substrate orientation:

$$\epsilon^{'}_{110} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & 0 \\ \epsilon_{yx} & \epsilon_{yy} & 0 \\ 0 & 0 & \epsilon_{zz} \end{bmatrix}, \tag{3}$$

$$\begin{aligned} \epsilon_{xx} &= \epsilon_{yy} = \frac{2\cdot c_{44} - c_{12}}{c_{11} + c_{12} + 2\cdot c_{44}} \cdot \epsilon_{\parallel} \\ \epsilon_{xy} &= \epsilon_{yx} = -\frac{c_{11} + 2\cdot c_{12}}{c_{11} + c_{12} + 2\cdot c_{44}} \cdot \epsilon_{\parallel} \\ \epsilon_{zz} &= \epsilon_{\parallel}, \end{aligned} \tag{4}$$

and for $[111]$ substrate orientation:

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$$\epsilon'_{111} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix}, \tag{5}$$

$$\begin{aligned} \epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz} = \frac{4 \cdot c_{44}}{c_{11} + 2 \cdot c_{12} + 4 \cdot c_{44}} \cdot \epsilon_{\parallel} \\ \epsilon_{xy} = \epsilon_{yx} = \epsilon_{xz} = \\ = \epsilon_{zx} = \epsilon_{yz} = \epsilon_{zy} = -\frac{c_{11} + 2 \cdot c_{12}}{c_{11} + 2 \cdot c_{12} + 4 \cdot c_{44}} \cdot \epsilon_{\parallel}, \end{aligned} \tag{6}$$

where c_{11}, c_{12} and c_{44} are the elasticity constants, $\epsilon_{\parallel} = (a_{\parallel} - a_0)/a_0$ is the relative lattice mismatch, a_0 is the substrate lattice constant and $a_{\parallel}$ denotes the active layer lattice constant.

Using linear deformation-potential theory we obtain for the conduction band minima splitting of the X valleys:

$$\begin{aligned} \Delta E_c^{[100]} &= \frac{2}{3} \cdot \Xi_u^{\Delta} \cdot \epsilon_{xx} - \frac{1}{3} \cdot \Xi_u^{\Delta} \cdot (\epsilon_{yy} + \epsilon_{zz}) \\ \Delta E_c^{[010]} &= \frac{2}{3} \cdot \Xi_u^{\Delta} \cdot \epsilon_{yy} - \frac{1}{3} \cdot \Xi_u^{\Delta} \cdot (\epsilon_{xx} + \epsilon_{zz}) \\ \Delta E_c^{[001]} &= \frac{2}{3} \cdot \Xi_u^{\Delta} \cdot \epsilon_{zz} - \frac{1}{3} \cdot \Xi_u^{\Delta} \cdot (\epsilon_{xx} + \epsilon_{yy}), \end{aligned} \tag{7}$$

and the L valleys:

$$\begin{aligned} \Delta E_c^{[111]} &= \frac{2}{3} \cdot \Xi_u^{L} \cdot (\epsilon_{xy} + \epsilon_{xz} + \epsilon_{yz}) \\ \Delta E_c^{[\bar{1}11]} &= \frac{2}{3} \cdot \Xi_u^{L} \cdot (-\epsilon_{xy} - \epsilon_{xz} + \epsilon_{yz}) \\ \Delta E_c^{[1\bar{1}1]} &= \frac{2}{3} \cdot \Xi_u^{L} \cdot (\epsilon_{xy} - \epsilon_{xz} - \epsilon_{yz}) \\ \Delta E_c^{[11\bar{1}]} &= \frac{2}{3} \cdot \Xi_u^{L} \cdot (-\epsilon_{xy} + \epsilon_{xz} - \epsilon_{yz}). \end{aligned} \tag{8}$$

The hydrostatic pressure component for the X and L valley shifts plays an important role because of $\Xi^{\Delta} \neq \Xi^{L}$. The hydrostatic shift is given as:

$$\Delta E_c^{\Delta,L} = \left(\Xi_d^{\Delta,L} + \frac{\Xi_u^{\Delta,L}}{3} \right) (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}). \tag{9}$$

From (7) it follows that in the case when all diagonal elements of the strain tensor are equal, the X conduction band minima are not split. This happens for example in case of $[111]$ substrate (see (6)). L conduction band minima are split for $[111]$ substrate orientation as it is seen from (8). For a general substrate orientation both X and L valleys are split and the strength and symmetry of the splitting depend on the values of Euler's angles. In particular, as shown below there are combinations of Ge compositions of the active layer and substrate orientations where the L valley splitting is so strong that some L valley may become dominant even in pure Si.

The influence of strain on the effective masses is taken into account for $[001]$ substrate orientation using the Rieger-Vogl model [5]. For general substrate orientation the unstrained effective masses for Si and Ge are used and a linear interpolation is adopted for the SiGe alloy.

III. Strain Effects and Ionized Impurity Scattering

In this work we consider the influence of strain on the Fermi level and the screening parameters of the ionized impurity scattering model taken from [6]. The effects of strain on impurity centers [4] in doped layers are not considered here.

Within this work we consider an analytical band structure taking into account nonparabolicity and anisotropy. In this case the density of states is given by the following expression:

$$g(\epsilon) = \frac{\sqrt{2} m_d^{\frac{3}{2}} \sqrt{\epsilon}}{\pi^2 \hbar^3} \sqrt{1 + \alpha\epsilon} \cdot (1 + 2\alpha\epsilon) \tag{10}$$

In order to find the Fermi energy in strained material we keep only terms up to the second order in the nonparabolicity coefficient and obtain a nonlinear equation for the Fermi energy:

$$\begin{aligned} n = \sum_i N_{c_i}^{(or)} \sum_j \Bigg[\mathcal{F}_{1/2}\left(\frac{E_f - E_{c_i} - \Delta E_{c_{ij}}}{k_B T_0} \right) + \\ + \frac{15}{4} \alpha k_B T_0 \mathcal{F}_{3/2}\left(\frac{E_f - E_{c_i} - \Delta E_{c_{ij}}}{k_B T_0} \right) + \\ + \frac{105}{32} \alpha^2 k_B^2 T_0^2 \mathcal{F}_{5/2}\left(\frac{E_f - E_{c_i} - \Delta E_{c_{ij}}}{k_B T_0} \right) \Bigg] \end{aligned} \tag{11}$$

$N_{c_i}^{(or)}$ stands for the effective density of states of the conduction band for one orientation of Valley i, index j denotes a number of orientations available for Valley i, $\Delta E_{c_{ij}}$ is the energy splitting of the conduction band minima of Valley i with orientation j in strained material, and T_0 is the lattice temperature. The linear and quadratic terms in (11) play an important role if the Pauli exclusion principle is taken into consideration as carriers can populate higher energy levels in highly degenerate semiconductors. (11) is solved by Newton iterations using as an initial guess the solution obtained for non-degenerate statistics and parabolic conduction band structure.

Under strain conditions with arbitrary substrate orientation the expression for the inverse screening length including nonparabolicity up to the second order takes the following form:

$$\begin{aligned} \beta_{s_{ij}}^2 = \frac{e^2}{\varepsilon_s \varepsilon_0 k_B T_0} N_{c_i}^{(or)} \cdot [\mathcal{F}_{-1/2}(\eta_{ij}) + \\ + \frac{15}{4} \alpha K_B T_0 \cdot \mathcal{F}_{1/2}(\eta_{ij}) + \frac{105}{32} \alpha^2 K_B^2 T_0^2 \cdot \mathcal{F}_{3/2}(\eta_{ij})], \end{aligned} \tag{12}$$

where $\eta_{ij} = (E_f - E_{c_i} - \Delta E_{c_{ij}})/k_B T_0$. It should be noted that in semiconductors with non-parabolic bands the inverse screening length increases which may weaken the ionized impurity scattering rate in particular for a high doping level when due to the Pauli exclusion principle the population of higher energies increases significantly. Thus there are two opposite factors which determine the strength of ionized impurity scattering. Another interesting effect occurs in strained doped materials. Due to the energy band minima splitting some

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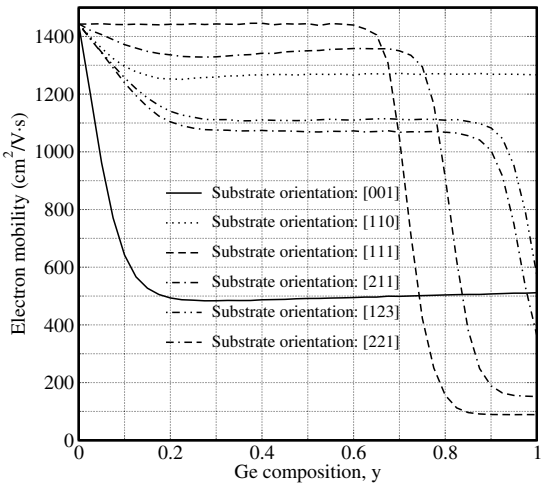

Fig. 1. Electron mobility perpendicular to the interface in strained Si on a $Si_{1-y}Ge_y$ substrate with several different substrate orientations at 300K.

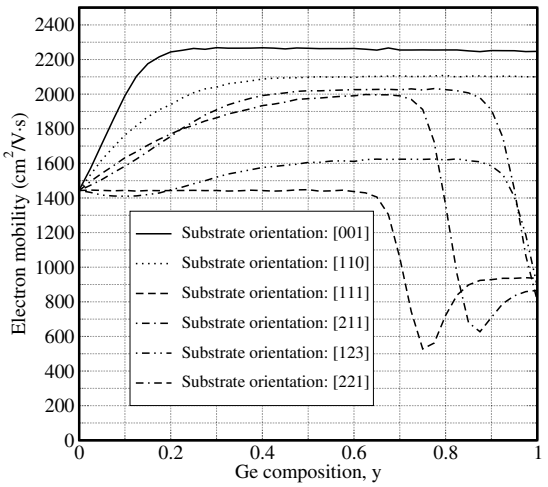

Fig. 2. Electron mobility parallel to the interface in strained Si on a $Si_{1-y}Ge_y$ substrate with several different substrate orientations at 300K.

valleys shift up and do not contribute to the kinetics. However this changes at high degeneracy when the Pauli principle causes a repopulation effect and upper split bands also give a contribution to the transport properties. The repopulation may be significant leading to a reduction of the conduction band minima splitting effect.

In case of momentum-dependent screening we modify the expression for the dielectric function to take into account the strain induced splitting of the conduction band minima for different valleys and orientations:

$$\varepsilon(q) = \varepsilon(0) \cdot \left(1 + \frac{1}{q^2} \sum_{ij} \beta_{s_{ij}}^2 G_{ij}(\xi, \eta_{ij})\right), \qquad (13)$$

where G_{ij} stands for the screening function in Valley i with orientation j. The momentum transfer $\vec{q} = \vec{p'} - \vec{p}$ and temperature dependence enters through ξ.

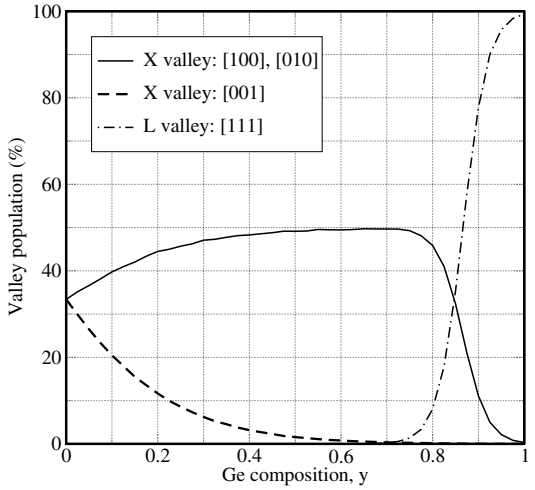

Fig. 3. Populations of different valleys and orientations in strained Si on [221] $Si_{1-y}Ge_y$ substrate at 300K.

IV. Results

Here some results for the low field electron mobility in a strained SiGe active layer grown on a SiGe substrate with various orientations are presented. All calculations have been performed using the zero-field Monte Carlo algorithms developed for non-degenerate and degenerate semiconductors in [7] and [8] respectively.

Fig.1 and Fig.2 show the low field perpendicular and in-plane electron mobility in strained Si on $Si_{1-y}Ge_y$ substrate for several orientations. The in-plane direction coincides with the x-direction of the coordinate system related to the interface (perpendicular to the node line). As it is seen from these figures there is a strong dependence on the substrate orientation. The behavior of the curves can be understood in terms of the valley populations presented in Fig.3 for $[221]$ orientation. It is clearly seen that there is a repopulation effect and the L valley comes into play which leads to a decrease of the mobility because of the heavier effective masses. Fig.4 demonstrates the in-plane component of the mobility as a function of Ge composition in the active layer on a $Si_{0.1}Ge_{0.9}$ substrate with several orientations. For general substrate orientation there exists a dependence of the in-plane component of the mobility on the in-plane angle that is the third Euler angle as shown for $[110]$ substrate orientation in Fig.5 using polar coordinates. The mobility in doped Si on a $Si_{0.1}Ge_{0.9}$ substrate is shown in Fig.6. The doping dependence of the perpendicular component shows an increase at high donor concentrations. As lower energy levels have already been occupied by electrons, due to the Pauli exclusion principle electrons cannot scatter to them and must scatter to higher energy levels which increases the probability of intervalley scattering and causes the repopulation effect from the lowest orientation of the split L valley to the higher X valleys as it is shown in Fig.7. The X valleys come into play which gives an increase of the perpendicular component of the mobility because of the lower values of

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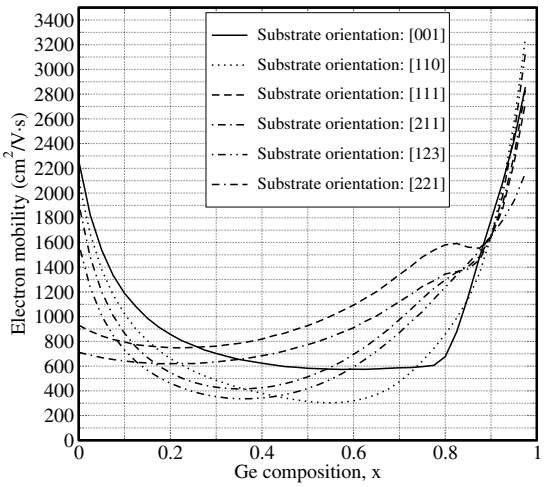

Fig. 4. Electron mobility parallel to the interface in strained $Si_{1-x}Ge_x$ on a $Si_{0.1}Ge_{0.9}$ substrate with several different substrate orientations at 300K.

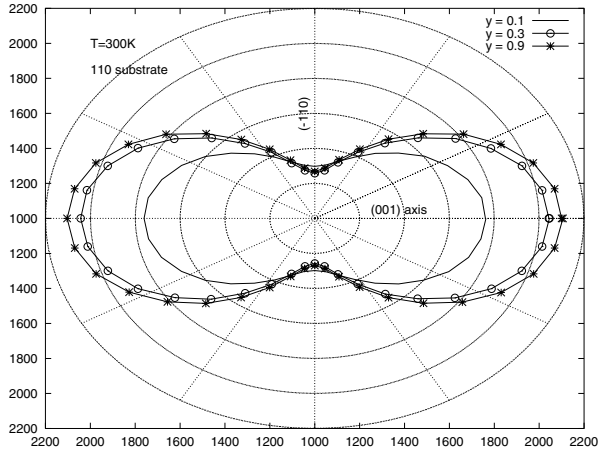

Fig. 5. In-plane mobility ($cm^2/V \cdot s$) in strained Si on [110] $Si_{1-y}Ge_y$ substrate versus the third Euler's angle at 300K.

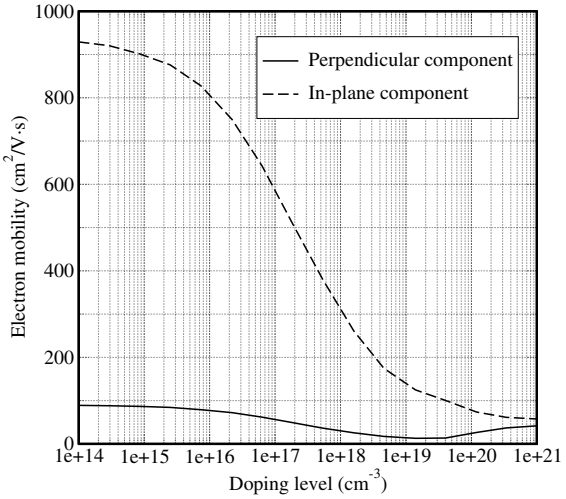

Fig. 6. Doping dependence of the electron mobility in Si on [111] $Si_{0.1}Ge_{0.9}$ substrate at 300K.

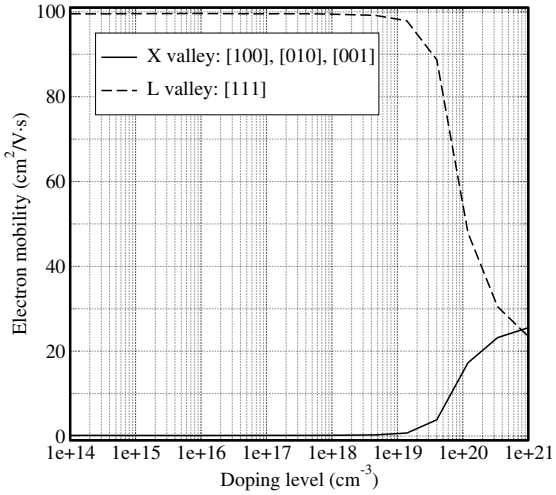

Fig. 7. Doping dependence of the valley population in Si on [111] $Si_{0.1}Ge_{0.9}$ substrate at 300K.

effective masses in this valley.

V. Conclusion

Strain effects on the electron mobility in an active SiGe layer grown on a SiGe substrate with the arbitrary orientation have been analyzed using Monte Carlo simulations. It has been shown that the splitting of different valleys strongly depends on the substrate orientation and causes different behavior of the low field electron mobility. In particular the dependence of the in-plane mobility on the in-plane angle has been analyzed. The mobility in doped strained SiGe has been investigated for different substrate orientations and the influence of the Pauli exclusion principle has been shown to have a significant impact on the repopulation caused by strain induced splitting of the conduction band minima.

Acknowledgment

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