Investigation of the Electron Mobility in Strained $Si_{1-x}Ge_x$ at High Ge Composition

S. Smirnov, H. Kosina, and S. Selberherr

Institute for Microelectronics, TU Vienna
Gusshausstrasse 27–29, A-1040 Vienna, Austria
Email: Smirnov@iue.tuwien.ac.at

***Abstract* – Monte Carlo simulation of the low field electron mobility of strained Si and SiGe active layers on SiGe substrate is considered. The Ge mole fractions of both the active layer and the substrate are varied in a wide range. The linear deformation potential theory is used to calculate the shifts of the conduction band minima due to the uniaxial strain along [001]. The energy shifts and the effective masses are assumed to be functions of the Ge mole fraction. Finally, the ionized impurity scattering rate is generalized to include strain effects for doped materials.**

I. INTRODUCTION

Materials which are compatible with the established Si technology are of particular interest if they allow to improve the transport properties of advanced devices. One such material is the alloy of Si and Ge parameterized by the Ge mole fraction x, which can be used both for $Si_{1-x}Ge_x$ active layers and $Si_{1-y}Ge_y$ substrates separately or together. If the Ge mole fraction in an active layer is different from that of the substrate, the resulting strain will cause changes in the band structure of the alloy and thus affects the kinetic properties of the material, in particular, the carrier mobility. To obtain the proper electrical characteristics of SiGe devices it is necessary to have a correct mobility model including strain dependence. A rather good description of physics in semiconductors is possible by solving the Boltzmann transport equation using the Monte Carlo technique which allows semiclassical transport to be analyzed in a relatively complete form. It requires, however, accurate models for scattering rates which are in general functions of strain.

II. STRAIN EFFECTS. UNDOPED MATERIAL

In this work we study the behavior of electron mobility in $Si_{1-x}Ge_x$ strained active layers grown on relaxed (001) $Si_{1-y}Ge_y$ substrate and the influence of scattering processes involving L valleys on electron mobility at high Ge mole fraction. The electron mobility at high Ge mole fraction strongly depends on the L-X scattering processes in strained SiGe alloys and may even have Si-like character in pure strained Ge, that is Ge with Si-like band structure.

Our analysis was performed by Monte Carlo simulations using the band structure reported in [1]. It consists of one conduction band and takes into account nonparabolicity and anisotropicity. Within this model the energy dependence on wave-vector is given by the following relation

$$E(\vec{k})(1+\alpha E(\vec{k})) = \frac{\hbar^2}{2}\left(\frac{k_1^2}{m_1}+\frac{k_2^2}{m_2}+\frac{k_3^2}{m_3}\right) \tag{1}$$

where α is a nonparabolicity parameter equal 0.5 for X valleys in Si and 0.3 for L valleys in Ge $m_1 = m_2 = m_t$ are transverse components of the effective mass tensor and $m_3 = m_l$ is the longitudinal component. As we investigate the low-field electron mobility, the analytical description will be sufficient to describe the main characteristic features of strained SiGe active layers. To study high-field transport phenomena, one has to use the full-band representation of the band structure.

The model of Rieger and Vogl [2] was adopted for the effective masses in strained SiGe. This model gives the effective masses versus Ge mole composition in the active layer and the substrate:

$$m^*(x,y) = \begin{pmatrix} 1, & (x-y), & (x-y)^2 \end{pmatrix} \mathbf{W} \begin{pmatrix} 1 \\ (x+y) \end{pmatrix} \tag{2}$$

where $\mathbf{W}$ contains parameterized transverse and longitudinal effective masses for the perpendicular and parallel X-valleys, and x and y denote the Ge mole fractions of the active layer and the substrate, respectively.

The linear deformation potential theory [3] was used to calculate the splittings of the valleys. The shift of the i-th valley is expressed as

$$\Delta E_c^i = \Xi_d \cdot \mathbf{Tr}(\epsilon) + \Xi_u \cdot \mathbf{a}_i^T \cdot \epsilon \cdot \mathbf{a}_i \tag{3}$$

where ϵ is the strain tensor, $\mathbf{a}_i$ is a unit vector parallel to the $\vec{k}$ vector of the i-th valley, Ξ_d and Ξ_u are the dilata-

tion and shear deformation potentials. The deformation potential tensor which is diagonal along the Δ axis, has two independent components Ξ_l^Δ, Ξ_t^Δ and $\Xi_u = \Xi_l - \Xi_t$, $\Xi_d = \Xi_t$. For the shift of the mean energy of the conduction band minima one obtains from (3):

$$\Delta E_c = (\Xi_d + \frac{1}{3}\Xi_u) \cdot \mathbf{Tr}(\epsilon). \quad (4)$$

For the uniaxial strain along [001] the strain tensor has diagonal form in the principle coordinate system:

$$\epsilon = \begin{bmatrix} \epsilon_{xx} & 0 & 0 \\ 0 & \epsilon_{yy} & 0 \\ 0 & 0 & \epsilon_{zz} \end{bmatrix} \quad (5)$$

where $\epsilon_{xx} = \epsilon_{yy} = \epsilon_\parallel$ and $\epsilon_{zz} = \epsilon_\perp$ are expressed in terms of the lattice constants of strained active layer $a_\parallel$, $a_\perp$ and relaxed material a_0 by $\epsilon_\parallel = (a_\parallel - a_0)/a_0$, $\epsilon_\perp = (a_\perp - a_0)/a_0$. The energy splitting within a given valley is the difference of two components: the shift of the mean energy of the band minima and the shift of an individual direction minimum for this valley. The first component is given by expression (4), the second one can be obtained from (3). From these relations it follows:

$$\Delta E_c^{[001]} = \Delta E_c^{[00\bar{1}]} = \frac{2}{3} \cdot \Xi_u^\Delta \cdot (\epsilon_{zz} - \epsilon_{xx}) \quad (6)$$

$$\Delta E_c^{[100]} = \Delta E_c^{[\bar{1}00]} = \Delta E_c^{[010]} = \Delta E_c^{[0\bar{1}0]} = = -\frac{1}{3} \cdot \Xi_u^\Delta \cdot (\epsilon_{zz} - \epsilon_{xx}) \quad (7)$$

This means that under the uniaxial strain along [001] the minima of the conduction band at Δ near the X-points are shifted with respect to the mean energy. Two valleys along the strain direction are shifted in the opposite direction to the shift of the in-plane valleys. It is easy to see from the derivation given above that the L-valleys remain degenerate under [001] strain. However, these valleys are split under [111] strain making the Monte Carlo analysis more complex due to the necessity to modify all scattering processes which involve the L-valleys.

As the valleys on the Δ axes are not equivalent any longer, all scattering mechanisms which include the X-valleys as an initial or final valley have to be changed accordingly. This point is important for the L-X and *f-type* X-X scattering processes.

Since we study the low field electron mobility in undoped strained bulk SiGe, a Monte Carlo algorithm for zero field which was developed for the nondegenerate case [5] is applied. This algorithm is very efficient and allows to obtain the whole mobility tensor. For our simulation we consider phonon scattering of both types intravalley and intervalley. Alloy scattering is taken into account as proposed in [6].

III. INCLUSION OF IONIZED IMPURITY SCATTERING RATE

We adopted the model of ionized impurity scattering which was developed for majority electrons in Si [7]. This model takes into account several effects such as momentum dependent screening, multi-potential scattering, the second Born correction, and the Pauli exclusion principle. Plasmon scattering is included as an additional mechanism. A method which reduces the number of small-angle scattering events [8] is applied. It gives the same momentum relaxation time and represents an isotropic process.

In order to account for minority carrier transport the same model is used, but without momentum-dependent screening, Pauli exclusion principle and plasmon scattering. In addition, screening by holes is considered and modeling of the valence bands is taken into account as suggested in [9, 10]. The presence of strain requires the proper calculation of the Fermi energy in strained SiGe active layers. As opposed to the undoped material, the Fermi energy in the strained layer is now defined by the following nonlinear equation:

$$n = N_{c_\perp} \cdot \mathcal{F}_{1/2}\left(\frac{E_f - E_c - \Delta E_\perp}{k_B T}\right) + N_{c_\parallel} \cdot \mathcal{F}_{1/2}\left(\frac{E_f - E_c - \Delta E_\parallel}{k_B T}\right) \quad (8)$$

where n is the electron concentration, $N_{c_\perp}$, $N_{c_\parallel}$ are the effective density of states for the split set of valleys of expressions (6) and (7) respectively, $\Delta E_\perp$, $\Delta E_\parallel$ are the energy shifts for the same set of valleys, $\mathcal{F}_{1/2}$ is the Fermi integral of respective order, $\frac{E_f - E_c}{k_B T}$ is the reduced Fermi energy which has to be found. This equation is solved by a Newton nonlinear iteration, and Maxwell-Boltzmann statistics is used to define the initial guess.

Also the expression for the inverse screening length changes in the presence of strain,

$$\beta_s^2 = \frac{e^2}{\varepsilon_s \varepsilon_0 k_B T}\left(N_{c_\perp}\mathcal{F}_{-1/2}(\eta_\perp) + N_{c_\parallel}\mathcal{F}_{-1/2}(\eta_\parallel)\right) \quad (9)$$

where ε_s is the relative dielectric permittivity of the semiconductor and $\eta_i = \frac{E_f - E_c - \Delta E_i}{k_B T}$.

Additionally, if the case of momentum-dependent screening is considered, the screening function has to be modified. The proper modification for this effect follows from the formula for the dielectric function which under the strain considered here takes the following form:

$$\varepsilon(q) = \varepsilon(0)\left(1 + \frac{1}{q^2}(\beta_{s_\perp}^2 G(\xi, \eta_\perp) + \beta_{s_\parallel}^2 G(\xi, \eta_\parallel))\right) \quad (10)$$

where q is the momentum transfer, G is the screening function, $\xi = \frac{\hbar^2 q^2}{8 m^* k_B T}$ and $\beta_{s_i}^2 = \frac{e^2}{\varepsilon_s \varepsilon_0 k_B T} N_{c_i} \cdot \mathcal{F}_{-1/2}(\eta_i)$.

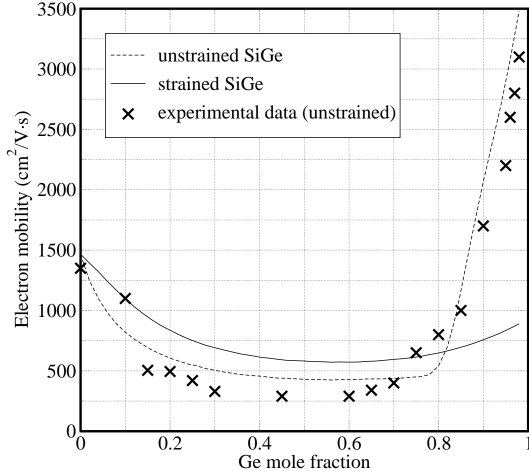

Figure 1: Electron mobility perpendicular to the interface in $Si_{1-x}Ge_x$ on a Si substrate at 300K.

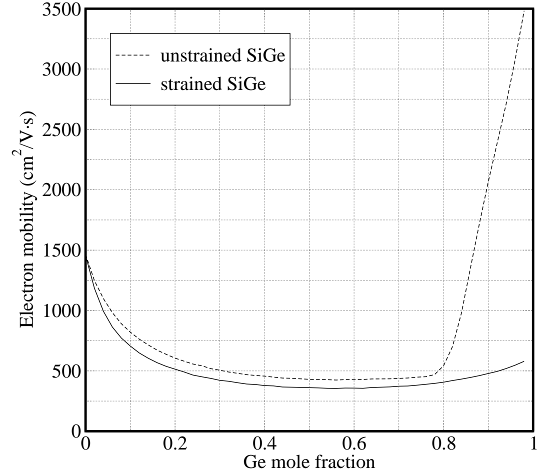

Figure 2: Electron mobility parallel to the interface in $Si_{1-x}Ge_x$ on a Si substrate at 300K.

IV. RESULTS

In Fig. 1 the behavior of electron mobility in an unstrained SiGe layer and a strained SiGe layer on Si is shown. The experimental data are taken from [11]. As can be seen from this figure, mobility in the strained case has Si like character over the whole range of Ge mole fraction. It is related to the increase of the biaxial compressive strain which at high x makes the four in-plane valleys move down getting equal or even lower than the L-valleys. Figure 3 shows the mobility for strained SiGe on relaxed SiGe substrate. In this case at the beginning of the curves the four parallel valleys are shifted up. As the Ge mole fraction in the layer increases, the tensile strain decreases and turns at the point $x = y$ (unstrained point) into compressive strain. In this case the four in-plane X-valleys move down but they are always higher than the L-valleys in such conditions. The results for the corresponding in-plane mobility are presented in Fig. 4. The doping dependence of the perpendicular and the in-plane components is shown in Fig. 5 and 6. The increase of the perpendicular component at high doping concentrations is explained by the dominance of ionized impurity scattering over alloy scattering. This is also clearly seen in Fig. 7 while the in-plane component Fig. 8 does not have this increase as it follows from the energy splitting.

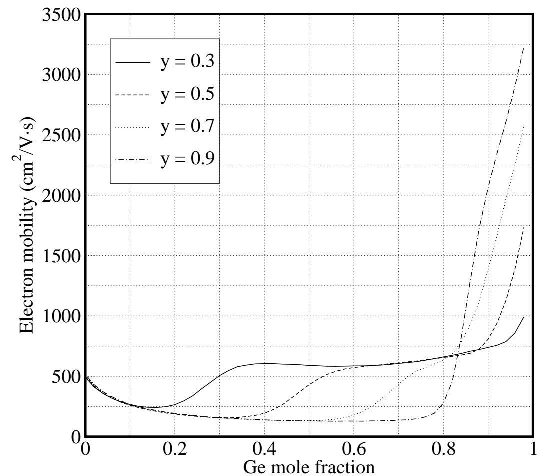

Figure 3: Electron mobility perpendicular to the interface in $Si_{1-x}Ge_x$ on a $Si_{1-y}Ge_y$ substrate at 300K.

V. CONCLUSION

We presented the Monte Carlo simulations of strained SiGe active layers grown on relaxed (001) SiGe substrate. The physical model based on the analytical representation of the band structure includes strain effects for undoped and doped cases and allows important effects in highly doped semiconductors to be taken into account.

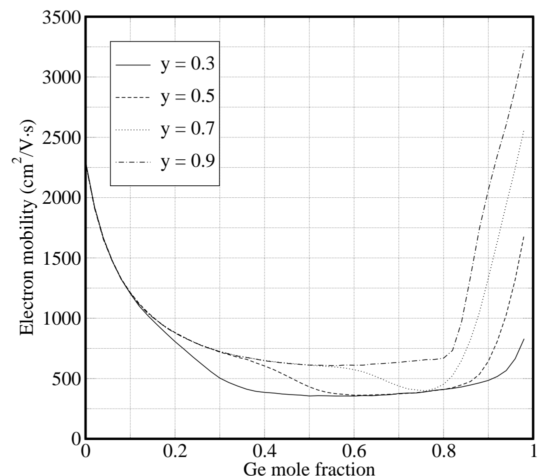

Figure 4: Electron mobility parallel to the interface in $Si_{1-x}Ge_x$ on a $Si_{1-y}Ge_y$ substrate at 300K.

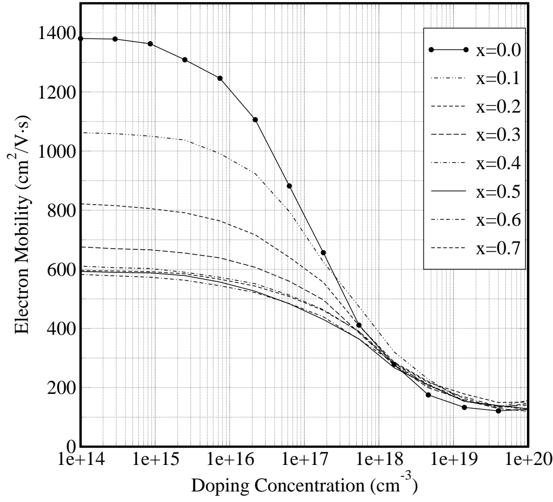

Figure 5: Doping dependence of electron mobility perpendicular to the interface in $Si_{1-x}Ge_x$ on a Si substrate at 300K.

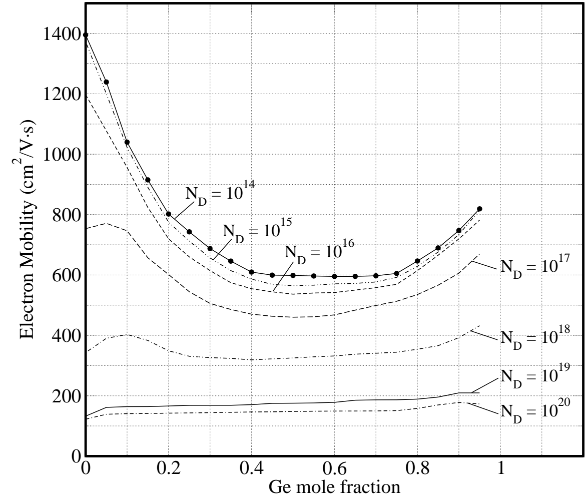

Figure 7: Ge composition dependence of electron mobility perpendicular to the interface in $Si_{1-x}Ge_x$ on a Si substrate for different doping levels at 300K.

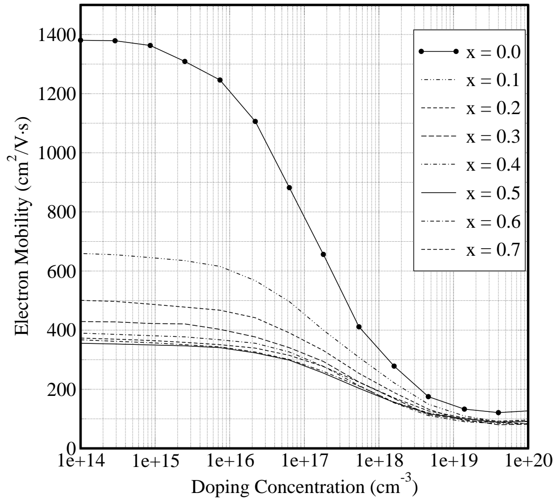

Figure 6: Doping dependence of electron mobility parallel to the interface in $Si_{1-x}Ge_x$ on a Si substrate at 300K.

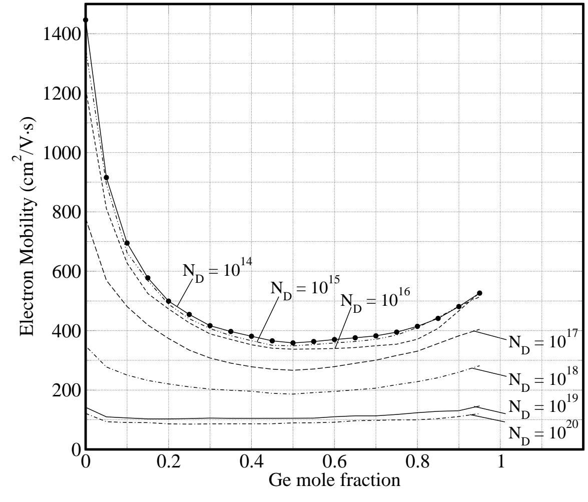

Figure 8: Ge composition dependence of electron mobility prallel to the interface in $Si_{1-x}Ge_x$ on a Si substrate for different doping levels at 300K.

The low-field electron mobility of strained SiGe layers including high Ge mole fraction was calculated. A good agreement of the obtained results with the experiment is achieved.

REFERENCES

[1] C. Jacoboni and L. Reggiani, Rev. Mod. Phys., **55**, p.645(1983)

[2] M. M. Rieger and P. Vogl, Phys. Rev. B, **48**, p.14276(1993)

[3] C. Herring and E. Vogt, Phys. Rev.,**101**, p.944(1956)

[4] C. G. Van de Walle, R. M. Martin, Phys. Rev. B, **34**, p.5621(1986)

[5] H. Kosina, M. Nedjalkov, and S. Selberherr, in Proc. 3rd Intl. Conf. on Large-Scale Scientific Computations, (Sozopol), p.A-23(2001)

[6] J. W. Harrison and J. R. Hauser, Phys. Rev. B, **13**, p.5347(1976)

[7] H. Kosina, and G. Kaiblinger-Grujin, Solid-State Electron., **42**, p.331(1998)

[8] H. Kosina, IEEE Trans. Electron Devices, **46**, p.1196(1999)

[9] M. V. Fischetti, Phys. Rev. B, **44**, p.5527(1991)

[10] T. Kaneto, K. W. Kim, M. A. Littlejohn, Phys. Rev. B, **47**, p.16257(1993)

[11] M. Glicksman, Phys. Rev., **111**, p.125(1958)