IEICE TRANS. ELECTRON., VOL.E86–C, NO.3 MARCH 2003

PAPER *Special Issue on the IEEE International Conference on SISPAD '02*

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

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SUMMARY Monte Carlo simulation of the low field electron mobility of strained Si and SiGe active layers on Si and SiGe substrates 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 uniaxial strain along [001]. The energy shifts and the effective masses are assumed to be functions of the Ge mole fraction. It is shown that in spite of the fact that the *L*-valleys remain degenerate under strain conditions considered here, they play an important role at very high Ge compositions especially when SiGe as substrate is used. We found that in this case the repopulation effects of the *X*-valleys affect electron mobility much stronger than the alloy scattering. We also generalize the ionized impurity scattering rate to include strain effects for doped materials and show that some of the important parameters such as effective density of states, inverse screening length, and the screening function are split due to strain and must be properly modified. Finally, we perform several simulations for undoped and doped materials using Si and SiGe substrates.

key words: *Monte Carlo simulation, strained SiGe, low field electron mobility, doping and strain effects*

1. 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. On the one side strain is inevitable, but on the other side it can be considered to modify the band structure in a useful way as was pointed out by Osbourn [1], [2]. Semiconductor devices which make use of strain and bandgap engineering are heterojunction bipolar transistors [3] and modulation-doped FETs [4]. To obtain the proper electrical characteristics of SiGe devices it is necessary to have a proper mobility model including strain dependence. An analytical derivation of such models is an impossible task due to the complexity of physical phenomena which become even more complicated in strained semiconductors. 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.

The paper is organized as follows. In Sect. 2 the model of strained undoped SiGe layers is described. In Sect. 3 the ionized impurity scattering rate is introduced for the doped case and modifications accounting for strain effects are presented. Results are discussed in Sect. 4 and conclusions are finally given in Sect. 5.

2. Strain Effects in 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 both X and 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 [5]. 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

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

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 [6] was adopted for the effective masses in strained SiGe. This model gives

Manuscript received September 4, 2002.
Manuscript revised November 8, 2002.

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*This paper was presented at SISPAD 2002.

the effective masses versus Ge mole composition in the active layer and the substrate:

$$m_i^*(x,y) = \left(1,(x-y),(x-y)^2\right)\mathbf{W}_i\left(1,(x+y)\right) \quad (2)$$

where $\mathbf{W}$ contains parameterized transverse and longitudinal effective masses for the perpendicular and parallel X-valleys. In the case of the transverse effective masses index i also runs over the perpendicular and in-plane directions and x and y denote the Ge mole fractions of the active layer and the substrate, respectively.

The linear deformation potential theory [7] was used to calculate the splitting of the valleys. The shift of the i-th valley is expressed as

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

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 dilatation 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 it holds: $\Xi_u = \Xi_l - \Xi_t$, $\Xi_d = \Xi_t$. 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 the strained active layer $a_\parallel$, $a_\perp$ and of the relaxed substrate a_0. The strain components are $\epsilon_\parallel = (a_\parallel - a_0)/a_0$, $\epsilon_\perp = (a_\perp - a_0)/a_0$. 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 minimum for this valley type. The first component is given by expression (4), the second one can be obtained from (3):

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

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

This means that under 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 of modifying 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 [9] is applied. This algorithm is very efficient and allows the whole mobility tensor to be evaluated. For our simulation we consider phonon scattering of both types, intravalley and intervalley. Alloy scattering is taken into account as proposed in [10].

3. Inclusion of Ionized Impurity Scattering Rate

We adopted the model of ionized impurity scattering which was developed for majority electrons in Si [11], [12]. This model takes into account several effects such as momentum dependent screening, multipotential scattering and the second Born correction:

$$\lambda(k) = C(k)\int_0^{2k}\frac{1}{(q^2+\beta_s^2 G(\xi,\eta))^2}\cdot\left(1+\frac{\sin(qR)}{qR}\right)qdq \quad (8)$$

where k stands for the absolute value of the electron wave vector, q means the momentum transfer, β_s denotes the screening length, $G(\xi,\eta)$ is the screening function calculated by rational approximation, η is the reduced Fermi energy, and R is the average distance between impurity centers. The Pauli exclusion principle is also taken into account since it plays a very important role at high doping levels. Plasmon scattering is included as an additional mechanism with the following scattering rate [11]:

$$\lambda(k) = \frac{e^2\hbar}{16\pi\epsilon_0\epsilon_s m^{*2}\omega_p v_g(k)}\left(N(\omega_p)+\frac{1}{2}\mp\frac{1}{2}\right)\cdot(k^2-k_f^2)^2\cdot\ln\frac{q_c}{q_{min}} \quad (9)$$

$$q_{min} = |k-k_f|, \quad q_{max} = k+k_f,$$

$$q_c = \min(q_{max},\beta_s), \quad (10)$$

$$N(\omega_p) = \left(\exp\left(\frac{\hbar\omega_p}{k_B T_n}\right)-1\right)^{-1} \quad (11)$$

where $\omega_p = \left(\frac{e^2 n}{\epsilon_0\epsilon_s m^*}\right)^{\frac{1}{2}}$ is the plasmon frequency, $N(\omega_p)$ is the plasmon average number calculated from the

equilibrium Bose-Einstein distribution (11), k_f is the final wave vector, q_c and q_{min} are the cut-off wave vector and minimum momentum transfer defined by expression (10), T_n stands for the electron temperature. As in this work we investigate the low-field transport, the electron temperature is constant and equal to the lattice temperature. A method which reduces the number of small-angle scattering events [13] 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 [14], [15].

The presence of strain requires the proper calculation of the Fermi energy in strained SiGe active layers. It can be seen from (8) that the Fermi energy enters the expression for the ionized impurity scattering rate and hence will affect it. As opposed to the undoped material, the Fermi energy in the strained doped layer is now defined by the following nonlinear equation:

$$n = N_{c_\perp} \cdot \mathcal{F}_{1/2}\left(\frac{E_f - E_c - \Delta E_\perp}{k_B T}\right) + N_{c_\parallel} \cdot \mathcal{F}_{1/2}\left(\frac{E_f - E_c - \Delta E_\parallel}{k_B T}\right) \tag{12}$$

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.

After the Fermi energy has been found as described above, it becomes possible to calculate the inverse screening length which is also split due to splitting of the electron density. The inverse screening length enters the ionized impurity scattering rate (8) and the plasmon scattering rate (9) through expression (10) and thus the strain will affect these scattering processes. The expression for the inverse screening length changes in the presence of strain and takes the following form:

$$\beta_s^2 = \frac{e^2}{\varepsilon_s \varepsilon_0 k_B T}\left(N_{c_\perp}\mathcal{F}_{-1/2}(\eta_\perp) + N_{c_\parallel}\mathcal{F}_{-1/2}(\eta_\parallel)\right) \tag{13}$$

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, one has to take into account the splitting of the product of the inverse screening length and the screening function and not only the screening length. This product enters the denominator of (8) and must be modified properly. The necessary modification for this effect follows from the formula for the dielectric function which under the strain considered here takes the following form:

$$\varepsilon(q) = \varepsilon(0)\left(1 + \frac{1}{q^2}(\beta_{s_\perp}^2 G(\xi, \eta_\perp) + \beta_{s_\parallel}^2 G(\xi, \eta_\parallel))\right) \tag{14}$$

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

4. Results

In Fig. 1 the behavior of electron mobility in unstrained SiGe and in strained SiGe on Si substrate is shown. The experimental data are taken from [16]. As can be seen from this figure, the electron mobility in the strained case has Si like character over the whole range of Ge mole fraction. The mobility in the strained layer is higher than that in the unstrained one up to $x = 0.8$. It follows from the fact that the two X-valleys along the direction of the strain move up and have only little contribution to the mobility. Thus only four in-plane valleys with transverse effective masses determine the mobility. This gives an increase in comparison to unstrained SiGe. At very high Ge mole fractions the mobility in the unstrained case increases rapidly while for the strained SiGe it has lower values. This is related to the increase of the biaxial compressive strain which at high x makes the four in-plane valleys move strongly down setting them equal or even lower than the L-valleys. Figure 2 demonstrates the parallel component of the electron mobility. As can be seen from this plot the mobility in the strained layer is lower compared to

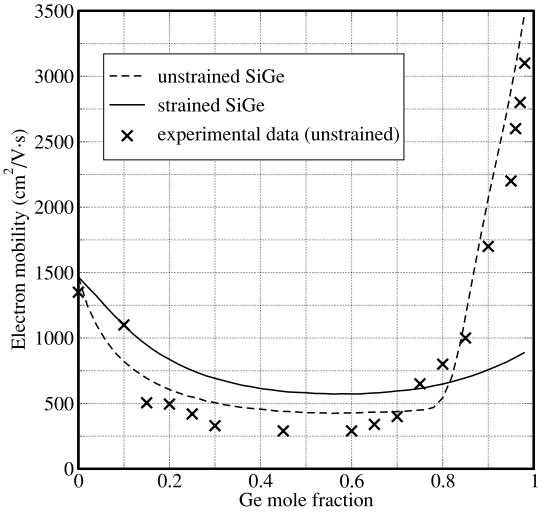

Fig. 1 Electron mobility perpendicular to the interface in $Si_{1-x}Ge_x$ on a Si substrate at 300 K.

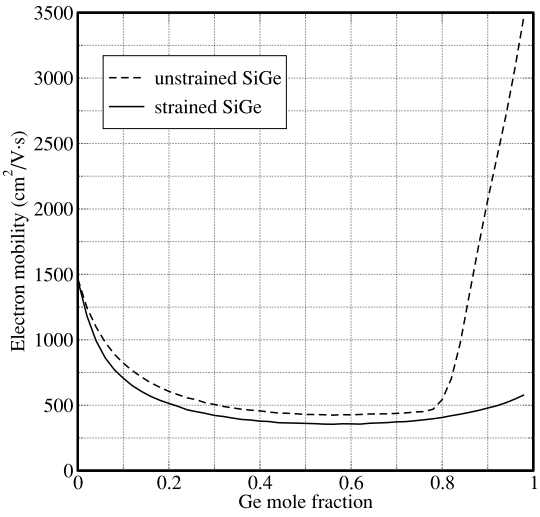

Fig. 2 Electron mobility parallel to the interface in $Si_{1-x}Ge_x$ on a Si substrate at 300 K.

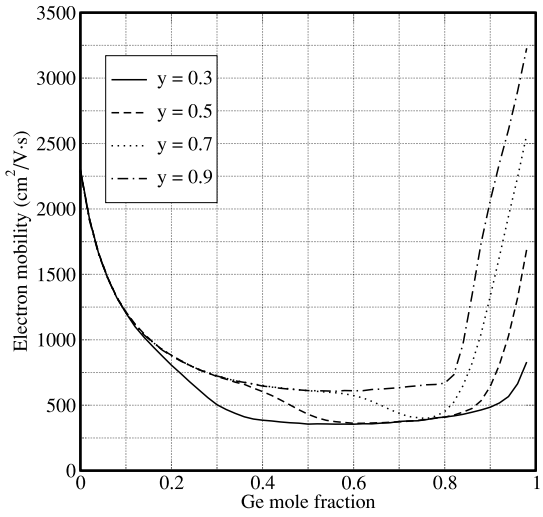

Fig. 4 Electron mobility parallel to the interface in $Si_{1-x}Ge_x$ on a $Si_{1-y}Ge_y$ substrate at 300 K.

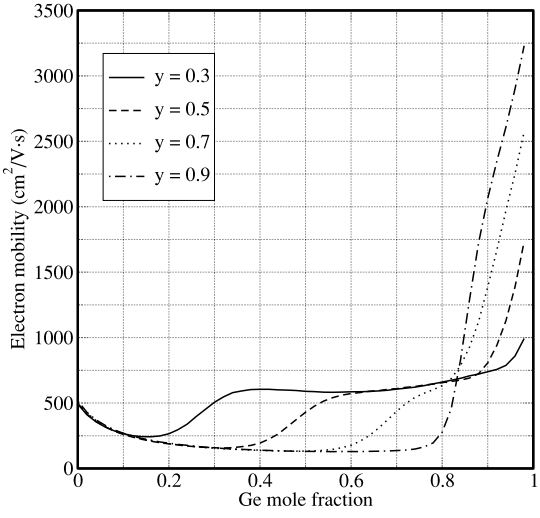

Fig. 3 Electron mobility perpendicular to the interface in $Si_{1-x}Ge_x$ on a $Si_{1-y}Ge_y$ substrate at 300 K.

that in unstrained SiGe. This is explained by the fact that unlike the relaxed material where four transverse effective masses determine the electron mobility only two transverse effective masses are left in the strained SiGe that leads to a decrease of the in-plane component.

Figure 3 shows the perpendicular component of the electron mobility for a strained SiGe active layer on a relaxed SiGe substrate. In this case at the beginning of all curves the four parallel valleys are already shifted up by the biaxial tensile strain and thus the perpendicular component of the electron mobility is only determined by the longitudinal effective masses and has a very low value. As the Ge mole fraction in the active layer increases, the alloy scattering increases yielding a decrease of the electron mobility. But in parallel with this effect the tensile strain decreases and the four in-plane valleys move down. The perpendicular component begins to be determined by transverse effective masses that gives the first increase of the mobility. It can be seen from the figure that this effect is much stronger than the decreasing factor of the alloy scattering. For example the curve for the substrate composition $y = 0.5$ increases even at the layer composition $x = 0.5$ where the alloy scattering has its maximum which means that in this case the alloy scattering cannot suppress the mobility enhancement due to the removal of the X-valley degeneracy. This can be explained as a repopulation effect of the same valley type (in this instance X-valley) but for different orientations available for this kind of valley. At very high Ge compositions the four in-plane X-valleys keep on moving down but now they are always higher than the L-valleys in such conditions and mobility is determined by L-valleys, which provides the last increase. The results for the corresponding in-plane mobility are presented in Fig. 4. This component has a very high value at the beginning of the curve, because only the transverse effective masses contribute and alloy scattering is absent at $x = 0.0$. However as the Ge composition grows, the four in-plane valleys move down and together with the alloy scattering this gives the first decrease of the in-plane component. At some point (near the strain-less one: $x = y$) the mobility is determined by two longitudinal and four transverse effective masses. After the Ge mole fraction grows further, the two transverse effective masses are only left. This leads to the second decrease of the parallel component of the electron mobility. The last increase is related to the dominance of the L-valleys at very high Ge compositions.

The doping dependence of the perpendicular and the in-plane components of the electron mobility in a strained SiGe active layer on a Si substrate is shown in Fig. 5 and Fig. 6. The increase of the perpendicular

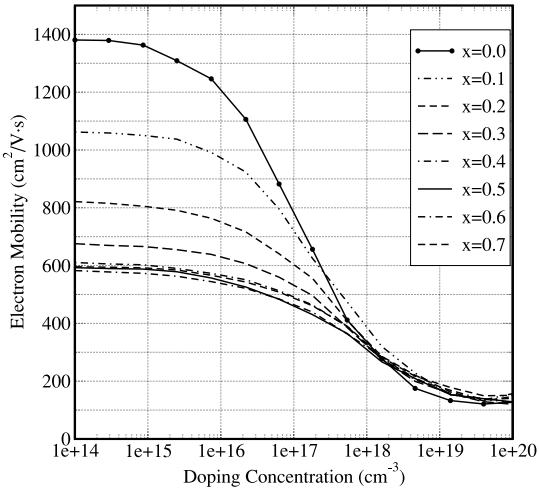

Fig. 5 Doping dependence of electron mobility perpendicular to the interface in $Si_{1-x}Ge_x$ on a Si substrate at 300 K.

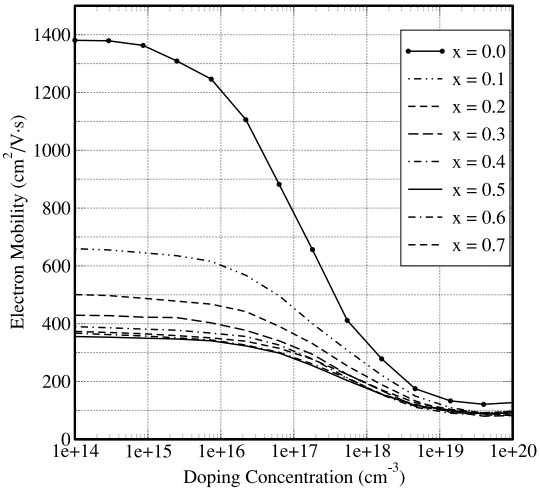

Fig. 6 Doping dependence of electron mobility parallel to the interface in $Si_{1-x}Ge_x$ on a Si substrate at 300 K.

component at high doping concentrations can be explained as followings. If we consider the undoped material then there are two factors which depend on the Ge mole fraction: the splitting of the X-valleys and the alloy scattering. The first factor increases the perpendicular component of the electron mobility and the second one decreases it. In the doped SiGe at high doping levels the ionized impurity scattering rate dominates the alloy scattering rate and thus suppresses the second factor leaving the first one that leads to an increase. This increase is also clearly seen in Fig. 7 while the in-plane component Fig. 8 does not have this increase as it follows from the fact that both the energy splitting and the alloy scattering decrease the in-plane component. Thus after removing the second factor there still exists the second one which decreases the parallel component. Figure 9 shows the doping dependence of the perpendicular component of the electron mobility in a

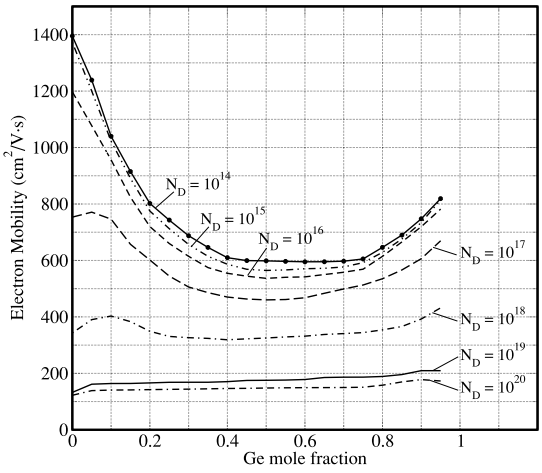

Fig. 7 Ge composition dependence of electron mobility perpendicular to the interface in $Si_{1-x}Ge_x$ on a Si substrate for different doping levels at 300 K.

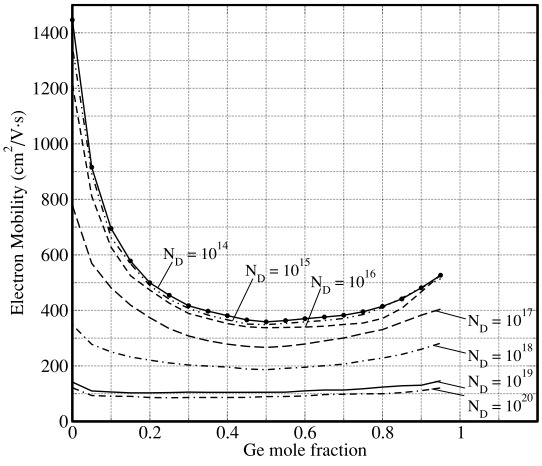

Fig. 8 Ge composition dependence of electron mobility parallel to the interface in $Si_{1-x}Ge_x$ on a Si substrate for different doping levels at 300 K.

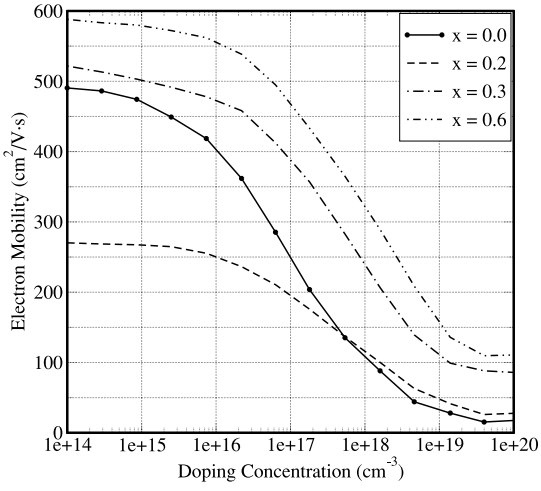

Fig. 9 Doping dependence of electron mobility perpendicular to the interface in $Si_{1-x}Ge_x$ on a $Si_{0.7}Ge_{0.3}$ substrate at 300 K.

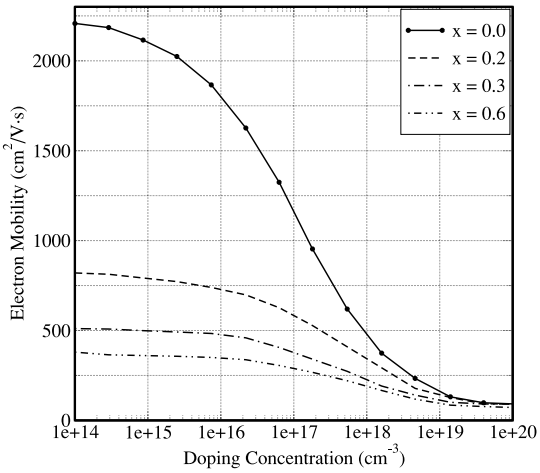

Fig. 10 Doping dependence of electron mobility parallel to the interface in $Si_{1-x}Ge_x$ on a $Si_{0.7}Ge_{0.3}$ substrate at 300 K.

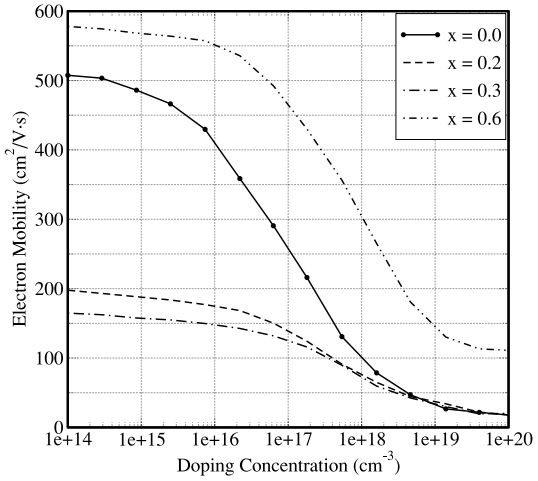

Fig. 11 Doping dependence of electron mobility perpendicular to the interface in $Si_{1-x}Ge_x$ on a $Si_{0.5}Ge_{0.5}$ substrate at 300 K.

strained SiGe on a $Si_{0.7}Ge_{0.3}$ substrate while Fig. 10 demonstrates the doping dependence of the in-plane component for the same substrate. The doping dependence of the the perpendicular and the in-plane components of the electron mobility in a strained SiGe active layer on a $Si_{0.5}Ge_{0.5}$ substrate is shown in Fig. 11 and Fig. 12, respectively.

5. Conclusion

We presented a Monte Carlo study of electron mobility in strained SiGe active layers grown on a 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. The low-field electron mobility of strained SiGe layers for the whole range of Ge mole fraction has been calculated. Good agreement of the

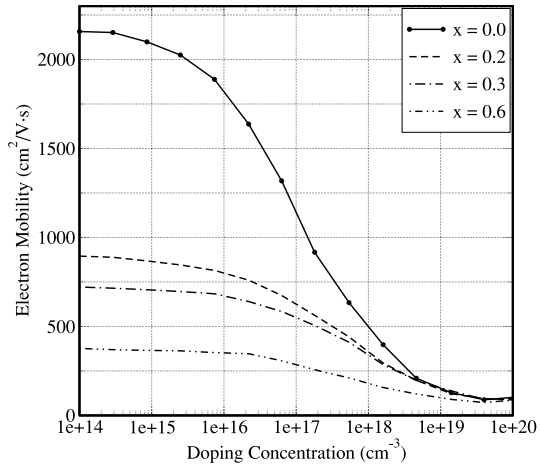

Fig. 12 Doping dependence of electron mobility parallel to the interface in $Si_{1-x}Ge_x$ on a $Si_{0.5}Ge_{0.5}$ substrate at 300 K.

obtained results with experimental data is achieved. It has been shown that for SiGe on a Si substrate, there is no such steep increase at very high Ge mole fractions as it is observed in unstrained SiGe. In this case even the pure Ge strained layer has a Si like band structure. On the other side the use of SiGe substrates gives a steep increase of the electron mobility at very high Ge compositions as in this case *L*-valleys are more populated than the *X*-valleys. The importance of the repopulation effects has been demonstrated and their dominance over alloy scattering has been found. For doped layers the increase of the perpendicular component of the electron mobility has been obtained while for the in-plane component no such increase is observed.

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