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Strained Si/SiGe Heterostructures at Low Temperatures. A Monte Carlo Study

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Abstract. Monte Carlo simulations are used to study the transport properties of electrons in strained silicon inversion layers in Si/SiGe MOSFETs at low temperature. The strain produces an enhancement of electron mobility due to the reduction of intervalley scattering and a lower effective conduction mass as a consequence of the valley splitting. In this work, mobility curves for different Ge concentrations are obtained by Monte Carlo simulation at both low and room temperatures. It has been observed that at room temperature mobility enhancement saturates at a Ge concentration close to x=0.3, while the mole fraction of Ge at which the electron mobility curves saturate is much lower at low temperature. In addition, the relative enhancement at low temperatures is much less than at room temperature. Finally, mobility curves show a tendency to coincide at high transverse electric fields, regardless of the Ge concentration, as a consequence of the greater concentration of electrons in the ground subband.

1. INTRODUCTION

The expansion of the performance limits of existing MOS technology requires enhancement of the carrier mobility in MOSFET channels. Many efforts have been dedicated in recent years to the improvement of mobility, such as the use of specific doping substrates [1]. It has very recently been shown that another way of increasing electron mobility lies in employing strained silicon to build the MOSFET channel. Recently both theoretical and experimental works have shown spectacular electron mobility enhancement when silicon is grown pseudomorphically on relaxed $Si_{1-x}Ge_x$ [2,3]. At the same time, several research groups have reported very high experimental mobilities in modulation-doped layers with channel regions formed by pseudomorphic growth of strained Si at different temperatures [4,5]. The strain causes the six-fold degenerate valleys of the silicon conduction band minimum to split into two groups: two lowered valleys with the longitudinal mass axis perpendicular to the interface, and four raised valleys with the longitudinal mass axis parallel to the interface. This splitting is enough to suppress the intervalley phonon scattering of electrons from lower valleys to upper valleys, thus reducing the intervalley phonon scattering rate compared with that of unstrained silicon. In addition, in the lowered valleys, which are more populated in the strained case, electrons have a smaller mass (transverse mass) in transport parallel to the interface. The combination of the light effective mass and reduced intervalley scattering gives rise to higher electron mobility [6]. Moreover, the lower intervalley-scattering rates makes the energy relaxation times higher, originating spectacular electron velocity overshoot.

These advantages can be used to enhance the performance of $Si_{1-x}Ge_x$ MOSFETs. Welser et al. [7,8] have lately shown that using standard MOS fabrication techniques it is possible to make NMOS and PMOS transistors with strained silicon carrier channels. These researchers found that compared to unstrained silicon devices, the strained-Si NMOS devices studied exhibit significant enhancements in mobility at 300 K along the entire range of transverse effective field [9].

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In this paper, Monte Carlo simulations are used to study the transport properties of electrons in strained silicon inversion layers in Si/SiGe MOSFETs at low temperatures.

2.MONTE CARLO SIMULATION

We have adopted a one-electron Monte Carlo simulation to study the transport properties of the electrons and in particular to evaluate the stationary drift velocity, the low-field mobility, and the electron velocity overshoot. Electron quantization in the inversion layer has been properly taken into account. To do so, the Poisson and Schroedinger equations have been self-consistently solved. A detailed description of this simulator can be found elsewhere [10-12]. In addition, non-parabolicity effects have been included in this work [13-14]. The effect of strain is included only in the band structure as the valley splitting energy ΔE, assuming that the strain does not modify the shape of the valleys. The separation between the conduction band minima induced by the strain has been assumed to be $\Delta E = 0.67x$, x being the Germanium mole fraction. Changes in non-parabolicity with strain have been neglected as second-order effects. The effective masses of electrons and the semiconductor bandgap, E_g, are assumed to be unchanged. The coupling constants for phonon scattering are also assumed to be the same than in unstrained silicon. Electrons in the strained $Si/Si_{1-x}Ge_x$ MOSFET channel have been treated as a quasi-two-dimensional electron gas contained in energy subbands. The position of the subband minima and the electron concentration in each of them were obtained by the self-consistent solution of the Poisson and Schroedinger equations for each value of the effective transverse electric field [15,16], which is the mean transverse electric field in the channel. To do so, we have taken into account the actual doping profile. The simulation begins with an electron in a given subband and a wave vector $\mathbf{k_0}$. The applied longitudinal electric field modifies the electron wave vector according to the semiclassical model. The history of the electron is divided into different subhistories, and each subhistory is continued until the effective scattering events exceed 25000 to obtain good convergence for the electron-drift velocity. The number of subhistories considered is that necessary for the standard deviation of the velocity data to fall below 5% of the final mean value. The average drift velocity is calculated in this way for several values of the longitudinal electric field, and the low-field effective mobility is obtained by extrapolating to zero electric field. The upper limit of the longitudinal field is chosen sufficiently high to allow calculations without an excessive number of subhistories, but low enough to avoid electron heating.

In our Monte Carlo procedure we have allowed the electron to travel in six subbands and to move between them [10]. In addition, we have considered phonon [17,18] and surface-roughness [19,20] scattering. Phonon scattering mainly causes one of two types of electron transitions: (a) intravalley acoustic transitions and (b) intervalley transitions (strongly weakened by the strain), both of which have been adapted from their treatment in silicon bulk for use in Si(100) inversion layers. The phonon-scattering rates have been deduced by using Price's formulation [21]. The intervalley transitions are described according to Jacoboni's bulk phonon model [17]. Surface-roughness scattering has been considered in Ando's approach with a Gaussian model dependent on the spectral distribution of roughness at the interface. The Gaussian model has been widely used in the literature [19], although it has been proved [22] that other models, having perhaps more physical basis, such as the exponential one, provide the same results as the Gaussian model. To take into account Coulomb scattering, a comprehensive model has been developed (see Refs.10 and 11). We have chosen a Monte Carlo method because its flexibility allows us to easily include a comprehensive Coulomb scattering model, that could hardly have been incorporated in any other sort of simulator. Such a model simultaneously takes into consideration the effects of i) screening by mobile carriers, ii) space correlation of the external charged centres (which may be important at high concentrations), iii) distribution of the charged centres in the oxide and semiconductor bulk, iv) distributions of the electrons in the inversion layer, and v) image effects caused by the difference in the dielectric constants of Si and SiO_2.

3.RESULTS AND DISCUSSION

Simulated mobility curves, neglecting Coulomb scattering, both at room temperature and at 77 K are shown in Figure 1. Observe that, at room temperature, the mobility enhancement saturates at a Ge concentration close to x=0.3, as was expected [3]. This is due to the fact that the energy splitting between the two lowered valleys and the four raised valleys becomes greater than the intervalley optical phonon energy, thus avoiding intervalley scattering between them. However, the mole fraction of Ge at which the electron mobility curves saturate is much lower at 77 K. This can be seen in Figure 1-b, where the electron mobility at 77 K is shown versus the effective field. Note that in this case mobility is saturated even for a Germanium mole fraction of x=0.1. This behaviour is a consequence of the fact that at low temperatures, and for the same transverse effective field, the separation between the electric subbands ($E_{0'}$-E_0) is higher than at room temperature. In addition, at low temperatures most of the electrons are in the ground subband (in which the electrons have a light effective conduction mass). Therefore, a lower valley splitting due to the strain will greatly reduce intervalley scattering, thus producing the same effect as higher splitting at room temperature.

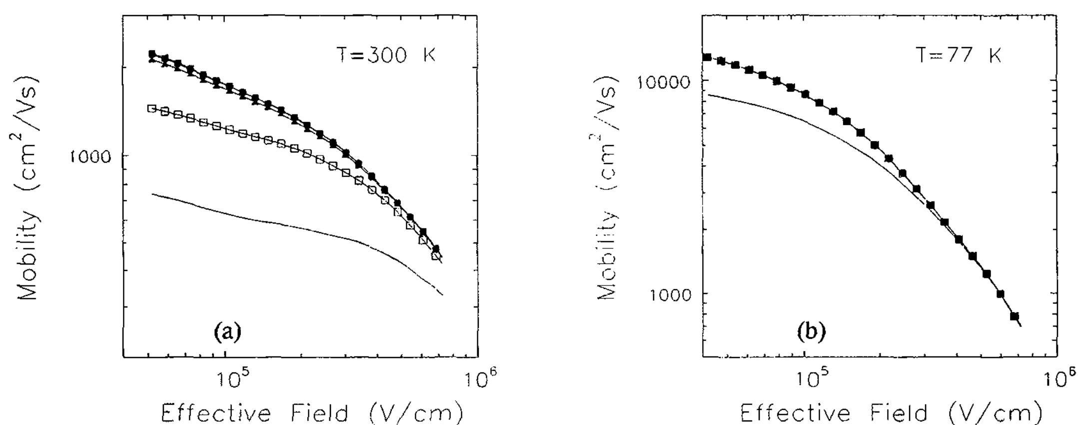

Figure 1: Electron mobility versus transverse electric field at room temperature and at 77 K in strained silicon inversion layers pseudomorphically grown on $Si_{1-x}Ge_x$. (solid line: x=0; □: x=0.1; ▴:x=0.2; ●: x=0.3; ■:x=0.4)

Figure 2 shows the ratio between the mobility enhancement for a fixed value of the inversion charge ($N_{inv}=1x10^{12}cm^{-2}$) as a function of the Germanium mole fraction both at room temperature and at 77 K. Two conclusions can be drawn from this figure:

i) mobility enhancement saturates at low temperatures for a much lower germanium mole fraction than at room temperature.

ii) mobility enhancement is much higher at room temperature than at 77 K.

The greater mobility enhancement at room temperature can be explained as follows: Intervalley scattering is much more important at room than at lower temperatures, since the number of phonons is greater and the separation of the subband energy levels smaller. In addition, at low temperatures most of the electrons are already occupying the ground subband in the unstrained silicon inversion layer, and therefore the strain does not significantly contribute to decrease the effective conduction mass.

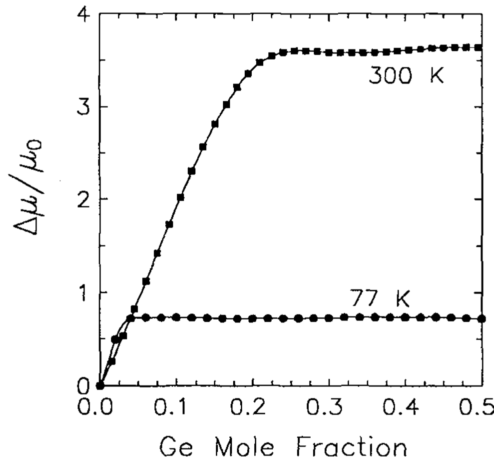

Figure 2: Ratio between the mobility enhancement for a strained silicon inversion layer in a $Si/Si_{1-x}Ge_x$ heterostructure and the mobility in an unstrained silicon inversion layer, at both 300 K and 77 K as a function of the Ge mole fraction for a fixed value of the inversion charge ($N_{inv}=1x10^{12}cm^{-2}$).

Figure 1 also shows that mobility curves tend to coincide at high transverse electric fields, regardless of the Ge mole fraction. In this region, even in unstrained silicon, the separation between the electric subbands is very high [19], higher than the intervalley phonon energy, and therefore intervalley scattering hardly influences electron mobility, which will now be controlled now by surface roughness scattering.

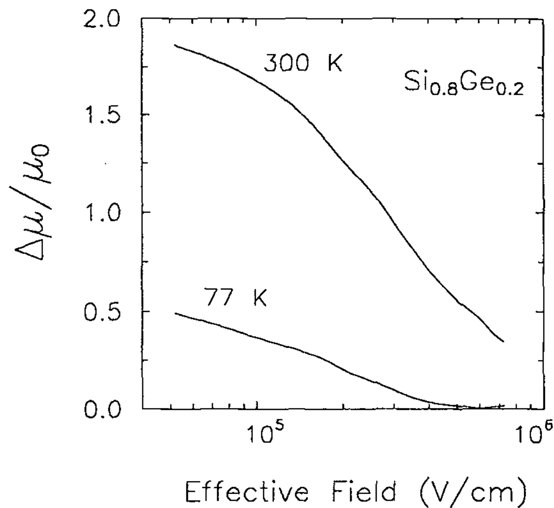

Figure 3: Ratio between the mobility enhancement for a strained silicon inversion layer in an $Si/Si_{0.8}Ge_{0.2}$ heterostructure and the mobility in an unstrained silicon inversion layer, at both 300 K and 77 K.

Nevertheless, at room temperature the unstrained mobility curve deviates strongly from the strained ones even for high electric fields. This behaviour can not be observed at low temperatures, where all the curves coincide at high electric fields. At high electric fields, intervalley scattering significantly decreases, and the mobility enhancement in strained samples is mainly due to the reduction of the effective conduction mass as a consequence of a greater population of valleys with the longitudinal

effective mass perpendicular to the interface. However, at low temperatures, and even for unstrained silicon inversion layers, most of the electrons are occupying the ground subband, and therefore the strain does not improve the conduction mass. Figure 3 shows the ratio between the mobility enhancement for a strained silicon inversion layer in an $Si/Si_{0.8}Ge_{0.2}$ heterostructure and the mobility in an unstrained silicon inversion layer, at both 300 K and 77 K.

Unlike modulation doped structures, where scattering by ionized impurities is dramatically reduced due to the spatial separation of charge carriers from their donor atoms, Coulomb scattering can play a very important role when the MOSFET channel is scaled down, since bulk doping has to be increased in order to avoid short-channel effects. It would be interesting to study the effect of Coulomb scattering on the transport properties of electrons in strained silicon inversion layers. Nevertheless, the introduction of Coulomb scattering does not significantly modify the above picture. Figure 4 shows simulated mobility curves including Coulomb scattering for strained silicon inversion layers for different germanium mole fractions. It has been assumed that a two-dimensional charged centre distribution of $N_{it}=1\times10^{11}cm^{-2}$ is located right at the interface. The bulk doping concentration was assumed to be $N_A=9\times10^{14}cm^{-3}$.

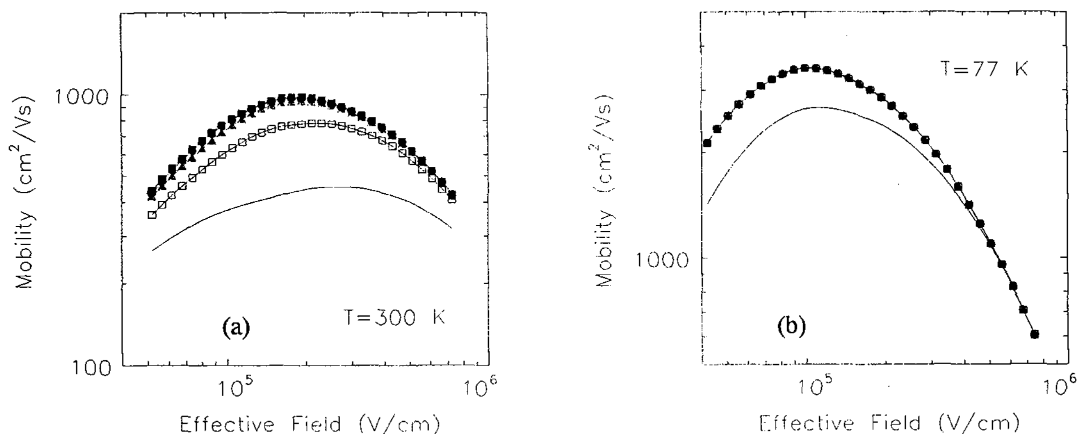

Figure 4: Electron mobility including Coulomb scattering versus transverse electric field at room temperature and at 77 K in strained silicon inversion layers pseudomorphically grown on $Si_{1-x}Ge_x$. (solid line: x=0; □: x=0.1; ▲:x=0.2; ●: x=0.3; ■:x=0.4)

4. CONCLUSIONS

Monte Carlo simulations have been used to study the transport properties of electrons in strained silicon inversion layers in Si/SiGe MOSFETs at low temperatures. The strain has been shown to produce an enhancement of electron mobility due to the reduction of intervalley scattering and a lower effective conduction mass as a consequence of the valley splitting. It has been observed that, at room temperature, the mobility enhancement saturates at a Ge concentration close to x=0.3, while the mole fraction of Ge at which the electron mobility curves saturate is much lower at 77 K. In addition, the relative enhancement at low temperatures is much less than at room temperature. Mobility curves tend to coincide at high transverse electric fields, regardless of the Ge mole fraction, although this coincidence is more marked at low temperatures. Finally, it has been shown that, from the mobility viewpoint, the advantages obtained by using strained silicon inversion layers are significantly reduced as temperature decreases.

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