Electron transport in Si/SiGe modulation-doped heterostructures using Monte Carlo simulation

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The electron transport in two-dimensional gas formed in tensile-strained Si1−xGe y/Si/Si1−xGe y heterostructures is investigated using Monte Carlo simulation. First the electron mobility is studied in ungated modulation-doped structures. Calculation matches the experimental results very well over a wide range of electron densities. The mobility typically varies between 1100 cm²/V s in highly-doped structures and 2800 cm²/V s at low electron density. The mobility is shown to be significantly influenced by the thickness of the spacer layer separating the strained Si channel from the pulse-doped supply layers. Then the electron transport is investigated in a gated modulation-doped structure in which the contribution of parasitic paths is negligible. The mobility is shown to be higher than in comparable ungated structures and dependent on the gate voltage as a result of the electron density dependence of remote impurity screening. © 2004 American Institute of Physics. [DOI: 10.1063/1.1650885]

I. INTRODUCTION

The use of strained-Si quantum wells pseudomorphically grown on a SiGe virtual substrate is becoming a key factor in channel engineering to improve the performance of Si-based field-effect transistors (FETs) for both microwave and logic application. This type of biaxial strain introduces splitting of degenerate bands, which results, for both electrons and holes, in smaller in-plane effective mass and reduced intervalley scattering thereby yielding improved transport properties. N-type Si/SiGe modulation-doped FETs (MODFETs) have demonstrated a low noise figure and high cut-off and maximum oscillation frequencies. The strain-induced enhancement of carrier transport properties is also shown to improve significantly the current in P-channel and N-channel metal–oxide–semiconductor FETs (MOSFETs) designed for complementary MOS (CMOS) application.

A starting point for these device concepts is the growth of high-quality Si/SiGe heterostructures that take advantage of the strain-induced enhancement in mobility. Understanding of their transport properties and of the underlying physics is then a key issue. The aim of this article is to investigate electron transport at room temperature in two-dimensional electron gas (2DEG) formed in Si1−xGe y/Si/Si1−xGe y heterostructures. The particle Monte Carlo method is used to do this. The model includes all relevant scattering mechanisms, i.e., phonon, impurity and alloy scattering. We first study the electron mobility in ungated modulation-doped structures in which the conducting electrons are provided by either single-side or double-side pulse-doped supply layers. The results calculated are carefully compared with measurements for a wide range of electron sheet densities. The mobility in such structures is proven to be very sensitive to the doping parameters that influence the impurity scattering rate, i.e., the doping dose and the position and the shape of the doping profile. These parameters influence the strength of electron–impurity interaction and the role of possible conducting parasitic paths. To make relevant the comparison with measurements it is thus necessary to overcome the uncertainty in the actual doping profile. An empirical methodology is used to adjust the doping profile in simulated structures which makes them as close as possible to the samples fabricated. Then the influence of the thickness of the spacer layer separating the strained-Si channel from the supply layers is analyzed. We finally study the effect of gate bias on the electron mobility in a gated stack designed for MODFET processing. In this case the pulse-doped layer between the gate and the strained-Si channel is fully depleted, which suppresses any parasitic path and modifies the overall transport properties. The mobility is found to increase as the gate voltage increases, which is essentially due to more effective screening of remote doping impurities.

II. THEORITICAL MODELS

Here in Sec. II we give details of the main features of the Monte Carlo simulator used to calculate the electron mobility in the 2DEG formed in Si1−xGe y/Si/Si1−xGe y modulation-doped heterostructures.

A. Conduction band structure

In this work, the conduction band structure used to model electron transport in Si and SiGe consists of six ellipsoidal nonparabolic Δ valleys located along the [100] directions at 85% of the Brillouin zone edge. The longitudinal effective mass, transverse effective mass and nonparabolicity coefficient are assumed to be $m_l = 0.9163 m_0$, $m_t = \ldots$
order intervalley processes in the following. The scattering models are described where

\[ D \]

and impurity scattering. The scattering models are described not to be modified by the strain.

The subband energies in normal and parallel valleys are given by 13 and three valley transitions. All phonon energies and deformation potentials are assumed to be found in Ref. 11. The acoustic intravalley phonon scattering is treated as an elastic process with a scattering rate given by

\[ \Gamma_{iv}(E) = \frac{k_B T D_{ac}^2}{2h^3 \rho v^2} \sqrt{m_x m_y} (1 + 2 \alpha E) \int \xi_m^2(z) \xi_m^2(z) dz, \]

where \( D_{ac} \) is the deformation potential, \( \rho \) is the crystal density, \( v \) is the sound velocity, \( k_B \) is the Boltzmann constant, \( T \) is the temperature, \( m_x \) and \( m_y \) are effective masses in the \( x \) and \( y \) directions, respectively, and \( \xi_m \) and \( \xi_n \) are envelope functions of the initial and final subbands with energies \( E_m \) and \( E_n \). The final energy is \( E' = E + E_m - E_n \).

Intervalley transitions are treated by considering three \( f \) and three \( g \) phonons via either a zeroth-order or first-order process in agreement with selection rules. 11, 12 For zeroth-order intervalley processes (i.e., for high energy phonons \( f_2 \), \( f_3 \) and \( g_3 \)), we use the common model of the scattering rate given by

\[ \Gamma_{iv0}(E) = \frac{Z_{iv} D_{iv0}^2}{2 \rho h^2 \omega_{iv}} \left[ N_q + \frac{1}{2} + \frac{\sigma}{2} \right] \sqrt{m_x m_y} (1 + 2 \alpha E') \times \int \xi_m^2(z) \xi_n^2(z) dz, \]

where \( N_q \) is the average number of phonons at temperature \( T \), \( D_{iv0} \) is the deformation potential for the zeroth-order intervalley process, \( Z_{iv0} \) is the number of possible final valleys and \( h \omega_{iv} \) is the phonon energy. \( \sigma \) is equal to \(-1\) in the case of phonon absorption and to \( +1 \) in the case of emission. Note that superscript primes refer to the final valley. The final energy is \( E' = E + E_m - E_n - \sigma h \omega_{iv} \).

For first-order intervalley phonon scattering (i.e., for low energy phonons \( f_1 \), \( g_1 \) and \( g_2 \)), we use the scattering rate derived in Ref. 14 including the nonparabolicity of the conduction band,

\[ \Gamma_{iv}(E) = \frac{D_{iv}^2}{\rho h^2 \omega} (1 + 2 \alpha E') \sqrt{m_x m_y} \left[ N_q + \frac{1}{2} + \frac{\sigma}{2} \right] \times \left( \frac{e}{h^2} \left[ \gamma(E) \sqrt{m_x m_y} + \gamma(E') \sqrt{m_x m_y} \right] F_{mn} \right) \]

\[ - \frac{1}{2} G_{mn} \]
\[ \frac{1}{\tau_{\text{all}}} = \frac{3^{2/3} \pi^2}{2^{1/3} \sqrt{\pi}} \frac{E_{\text{all}}}{h^3} (1 - x) \frac{m_p m}{m_e} (1 + 2aE) I_p, \]

where \( I_p \) is the partial overlap integral defined as
\[ I_p = \int_{z_{p-1/2}}^{z_{p+1/2}} \xi_m(z) \xi_n(z) dz. \]

By adding the contribution of all planes the total relaxation time is finally given by
\[ \frac{1}{\tau_{\text{all}}} = \frac{3^{2/3} \pi^2}{2^{1/3} \sqrt{\pi}} \frac{E_{\text{all}}}{h^3} (1 - x) \frac{m_p m}{m_e} (1 + 2aE) \sum_p I_p^2. \]

Each overlap integral \( I_p \) is numerically evaluated.

### D. Impurity scattering

From a modeling point of view, the electron-impurity scattering in a 2DEG has given rise to much work, but at the cost of a complicated and computational demand. Therefore, we neglect intersubband transitions, as most authors do.\(^{19,22}\)

Within these approximations the impurity momentum relaxation time \( \tau_{\text{imp}} \) for electrons in the \( m \)th subband may be written as\(^{24}\)
\[ \frac{1}{\tau_{\text{imp}}} = \frac{e^4 \sqrt{m_p m_r}}{4 \pi \hbar^3 e_0^2 e_r^2} (1 + 2aE') \times \left( \int N_i(z_0) \int \left| \frac{\xi_m(z)}{Q(\theta) + Q_{\text{scr}}(\theta)} \right|^2 dz \right) \times (1 - \cos \theta) d\theta dz_0, \]

where \( N_i(z_0) \) is the ionized impurity concentration at the \( z_0 \) position, \( Q = |k - k'| \) is the scattering wave vector, \( \theta \) is the scattering angle, \( e_0 \epsilon_r \) is the dielectric permittivity and \( Q_{\text{scr}} \) is the screening function. It has been shown that the approach that introduces the relaxation time in the Monte Carlo algorithm is equivalent to the use of the actual scattering rate in terms of computed mobility.\(^{25}\)

By considering a single-subband in the screening effect and including the temperature dependence given by Fetter\(^{13,26}\) the screening function \( Q_{\text{scr}} \) is given as a function of \( Q \) by
\[ Q_{\text{scr}}(Q) = \frac{e^2 n_1}{2 \epsilon_0 \epsilon_r k_B T} g_1(Q\lambda) \times \left( \int d'z \int dz \frac{\xi_m(z)\xi_n(z')}{e^{-Q|z-z'|}} \right), \]

where \( n_1 \) is the electron density of the screening subband and \( g_1(x) \) is defined as
\[ g_1(x) = \frac{2 \sqrt{\pi}}{x} \Phi \left( \frac{x}{4 \sqrt{\pi}} \right), \]

and \( \Phi \) is the dispersion plasma function, defined as
\[ \Phi(y) = 2e^{-x^2} \int_0^y e^{-t^2} dt. \]

For each simulated electron, the subband to be considered in the screening effects must be chosen carefully according to the electron subband and the relative population of the main and parasitic paths. In Si/SiGe modulation-doped structures a subband may be bound to either the strained Si layer (main channel) or a SiGe supply layer (parasitic path).

For an electron bound to the supply layer, the subband to be considered in the screening function is clearly the lowest subband of the corresponding parasitic path. For an electron bound to the main channel, the subband chosen is the lowest of the main channel in most cases. In the unfortunate case where the electron concentration in a supply layer would approach the impurity concentration, which is not suitable for getting high mobility, the lowest subband of the corresponding parasitic path is certainly the most effective in the screening mechanism and must be considered for evaluation of the screening function defined by Eq. (9).

### III. MODULATION DOPED STRUCTURES: MEASUREMENTS AND CALCULATIONS

Here in Sec. III, we carefully compare transport calculations with mobility measurement in Si/SiGe modulation-doped structures. We consider a wide range of layer stacks and doping profiles. We then analyze the influence of the thickness of the spacer layer that separates the strained Si channel from \( \delta \)-doped SiGe layers. We then study electron transport in a gated structure.

#### A. Structures studied

The \( N \)-type modulation-doped structures realized for mobility measurements consist of a strained-Si channel embedded in unstrained \( \text{Si}_{1-x} \text{Ge}_x \) layers. Single-side doping (SSD) or double-side doping (DSD) layers are introduced in the epilayer stack (Sb doping) to supply the 2DEG with conducting electrons.\(^{8}\) A cross section of SSD and DSD struc-
tures is shown in Fig. 1. The thickness of the Si channel is always \( W_{ch} = 9 \) nm, whereas the spacer thicknesses \( (W_{sp1} \) and \( W_{sp2} ) \), nominal doping doses \( (W_{d1}, W_{d2}, N_{d1}, N_{d2} ) \) may vary from one structure to another. The main nominal parameters of the structures considered for both measurement and calculation are summarized in Table I. All samples are grown on top of a high-resistivity \( p \)-type Si substrate by molecular beam epitaxy. The virtual substrate consists of a graded buffer with a slope of 20\% Ge/\( \mu \)m. Hall mobility measurements were performed using either a standard van der Pauw or differential Hall technique.\(^8\)

The gated structure simulated to study in Sec. III E the gate effect on electron transport is not compared with experiments.

**B. Nominal and effective doping profiles**

One of the aims of the study is to validate our modeling approach by comparing the calculations with experimental data. To make the comparison relevant we must ensure that the simulated doping profiles are close to actual ones. Each sample includes pulse-doped layers characterized by the nominal width and doping level (see Table I). In practice, a quite important difference may occur between actual activated dopant concentrations and nominal values which, in addition, do not consider any effect of dopant diffusion. In other words, a structure may have a doping profile very different from that expected. It has been estimated that in some cases the uncertainty in the doping levels can reach a factor of 2. Such uncertainty is not acceptable if we consider that the impurity scattering rate is proportional to doping density, as stated in Eq. (8). Correction of the effective profile is then required in most cases for a useful comparison with measurements.

In the ungated structures considered here in Sec. III, the carrier density is directly correlated to the impurity concentration. As an initial guess, the nominal density can be roughly estimated from the width and nominal doping levels of the supply layers. The first step in the correction procedure consists of comparing nominal and measured densities. A strong discrepancy is a clear sign that correction is required. The measured density is then compared with the density calculated by solving self-consistently the Poisson and Schrödinger equations for a nominal doping profile.

The procedure starts at low temperature (\( T = 77 \) K), i.e., when most free carriers reside in the main channel, as shown in Fig. 2. The width, the doping level and profile of supply layers are then empirically adjusted to get a simulated electron density equal to the measured one. We proceed in the same way at 300 K to refine the doping profile. As shown in Fig. 2, for a given doping profile the carrier density in the strained channel is almost the same at 300 and 77 K. The temperature only influences the carrier density in the supply layers and their surroundings. Thus adjustment of the doping profile at room temperature must be made to fit the measured density.

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**TABLE I. Nominal technological parameters of Si\(_{1-x}\)Ge\(_x\)/Si/Si\(_{1-x}\)Ge\(_x\) modulation-doped structures investigated both experimentally and theoretically. The thickness symbols are defined in Fig. 1. \( N_{d1} \) and \( N_{d2} \) are the doping levels in the top and bottom supply layers, respectively.**

<table>
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<tr>
<th>Sample No.</th>
<th>( x )</th>
<th>( W_{cap} ) (nm)</th>
<th>( W_1 ) (nm)</th>
<th>( W_{ch} ) (nm)</th>
<th>( W_{sp1} ) (nm)</th>
<th>( W_{sp2} ) (nm)</th>
<th>( N_{d1} ) (cm(^{-3}))</th>
<th>( W_{d1} ) (nm)</th>
<th>( W_{d2} ) (nm)</th>
<th>( N_{d2} ) (cm(^{-3}))</th>
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<tr>
<td>C2311</td>
<td>35</td>
<td>4 20 9 15 10</td>
<td>5 \times 10(^{18})</td>
<td>3 4 4 \times 10(^{18})</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>C2014</td>
<td>45</td>
<td>4 7 9 6 4</td>
<td>1.5 \times 10(^{19})</td>
<td>4 6 4 \times 10(^{18})</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>C2309</td>
<td>45</td>
<td>3 7 9 3.1 3.6</td>
<td>1.5 \times 10(^{19})</td>
<td>4 3.1 4 \times 10(^{18})</td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>C2589</td>
<td>40</td>
<td>4 8 9 3</td>
<td>1.5 \times 10(^{19})</td>
<td>4 5 2.4 \times 10(^{18})</td>
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<tr>
<td>C1898</td>
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<td>4 8 9 3</td>
<td>1.5 \times 10(^{19})</td>
<td>4 3 4 \times 10(^{18})</td>
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<tr>
<td>C2766</td>
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<td>3 8 9 4.5 5</td>
<td>1.5 \times 10(^{19})</td>
<td>4 3 4 \times 10(^{18})</td>
<td></td>
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<tr>
<td>C2720</td>
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<td>1.5 \times 10(^{19})</td>
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<td></td>
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</tbody>
</table>

FIG. 1. Schematic of the cross section of \( n \)-type modulation-doped structures with either a single-side pulse-doped layer or a double-side pulse-doped layer.

FIG. 2. Electron concentration in sample C2766 calculated with a nominal doping profile at 77 and 300 K.
total density without changing the density in the strained-Si channel.

C. Mobility results: Comparison with measurements

The drift mobility is computed under uniform in-plane electric field of 0.5 kV/cm at room temperature. Measured and calculated mobilities are displayed in Fig. 3 as a function of the total electron density. Three values of germanium content $x$ are considered: $x = 45\%$ (circles), 40\% (triangles), and 35\% (diamonds).

FIG. 3. Experimental (open symbols) and calculated (closed symbols) mobility for various samples as a function of the total electron density. Three values of germanium content $x$ are considered: $x = 45\%$ (circles), 40\% (triangles), and 35\% (diamonds).

As shown in Fig. 3, for each simulated structure fairly good agreement is found with measurements over a wide range of electron densities. At very low density, the maximum calculated mobility reaches 2800 cm$^2$/V s. In this structure the supply doping is small and remote enough to make the impurity scattering negligible. The electrons are confined in the strained-Si channel and the predominant scattering mechanisms are electron–phonon interactions. This calculated mobility matches very well the value measured by the differential Hall technique (2700 cm$^2$/V s, open square in Fig. 3) and the other best values reported at low electron density.\(^7\) This agreement validates our approach for phonon scattering modeling. The increase of quantum well (QW) thickness reduces the level spacing and affects the phonon scattering rates but it results in a limited effect on the peak mobility. For QWs larger than 9 nm the phonon-limited mobility does not exceed 3000 cm$^2$/V s. It should be noted that by using the same phonon coupling parameters the mobility calculated in a 2DEG is slightly lower than that calculated by neglecting quantization effects (3250 cm$^2$/V s).\(^1\) This is consistent with the calculated phonon scattering rates: in the energy range of 0–50 meV, for each electron–phonon process the scattering rate is smaller in a three-dimensional (3D) EG than in a 2DEG.\(^13\,14\) With a different set of phonon parameters Yamada et al. calculated a phonon-limited mobility of 4000 cm$^2$/V s for a 3DEG formed in strained Si.\(^28\) Bufler and Fichtner obtained a mobility of 2250 cm$^2$/V s using full-band Monte Carlo simulation.\(^29\) Better agreement with experimental results is found using our model.

The Hall scattering factor for electrons in a 2DEG was shown to be very close to unity for a large range of temperatures.\(^27\) Assuming this result is unchanged for strained material makes possible a direct comparison of our calculated density and the drift mobility with Hall measurements. This assumption, however, may fail for electrons in SiGe, which can be a possible source of error in the case of a structure with a strong parasitic path.

D. Influence of the spacer thickness

The influence of remote impurities is partially controlled by the width of the spacer layers that strongly influences the exponential term in Eq. (8). At a given supply doping, increasing the spacer thickness reduces the impurity scattering rate for electrons in the main channel but also reduces electron transfer from the supply layers to the channel. The current in the structure results from a balance between these two effects.

This balance is illustrated in Fig. 4 which shows the electron density and mobility as a function of the top spacer width $W_{sp1}$ with all other things equal. $W_{sp1} = 4.5$ nm corresponds to sample C2766.
from 1 to 5 nm causes a small reduction in the total electron density (from $5.6 \times 10^{12}$ to $5.3 \times 10^{12}$ cm$^{-2}$) but also yields a significant increase in mobility (from 1180 to 1540 cm$^2$/V s).

This clearly confirms that the mobility in this type of structure is not a unique function of the carrier density.

It should be noted that this increase in mobility is obtained in spite of detrimental enhancement of the fraction of electron density in the parasitic paths in which the transport properties are poor. As shown in Fig. 5, the fraction of electrons in the main strained-Si channel decreases from 93% to 63% as $w_{\text{sp}}$ increases to 5 nm.

The strong effect of impurity scattering on electron transport in this structure is clearly shown in Fig. 6 where we plot the mobility calculated as a function of $w_{\text{sp}}$ depending on whether the impurity scattering mechanism is included (solid line) or not (dashed line). If impurity scattering is not taken into account the mobility tends to decrease as $w_{\text{sp}}$ increases. This only results from an increase of the overlap integral in the phonon scattering rates given in Eqs. (1)–(3). The introduction of remote impurity scattering into the algorithm significantly reduces the mobility but as $w_{\text{sp}}$ increases the reduction in impurity scattering rate dominates the increase in phonon scattering rate, which results in higher overall mobility.

E. Influence of the bias in a MODFET structure

We now consider a gated device whose vertical architecture is of the same type as the DSD structure shown schematically in Fig. 1, with a Schottky gate on top. The technological parameters are very similar to those of sample C2309 but are optimized for MODFET operation: $W_{\text{ch}} = 9$ nm, $W_{\text{SiCap}} = 4$ nm, $W_{1} = 3.6$ nm, $W_{\text{sp}} = 3.6$ nm, $W_{\text{sp}} = 3$ nm, $W_{\delta_1} = 3.4$ nm, $W_{\delta_2} = 4$ nm, $N_{\delta_1} = 1.5 \times 10^{19}$ cm$^{-3}$, and $N_{\delta_2} = 4 \times 10^{18}$ cm$^{-3}$. In this gated structure the conducting electron density is no longer controlled by the doping density in the supply layers but by the gate field effect, which modifies the influence of remote impurity scattering.

With a Schottky gate in normal operation the top $\delta$-doped layer is fully depleted and most carriers stand in the strained channel. Hence, within the framework of our impurity screening model, the first subband of the normal valleys is obviously the subband that should be taken into account in evaluation of the screening function from Eq. (9). The influence of gate voltage $V_{\text{GS}}$ on the calculated electron mobility is shown in Fig. 7. As the gate voltage increases, the mobility tends to increase and then to saturate near 2140 cm$^2$/V s for positive gate bias. The rise in this curve can be easily explained: it is due to gate-induced enhancement of density $n_1$ on the lowest subband, which increases the screening function $Q_{\text{scr}}$ [Eq. (9)] and reduces the impurity scattering rate [Eq. (8)]. Mobility saturation at high gate bias, however, is somewhat unexpected. Consistently, the intrasubband impurity scattering rate for the first level of the normal valleys exhibits a similar plateau in Fig. 8. To understand this behavior, we also plot in Fig. 8 the density of this level as a function of $V_{\text{GS}}$. A significant increase in the slope of $n_1$ is observed for voltages larger than 0 V, which is a sign of a significant change in charge-control operation, resulting in higher gate capacitance. This observation is confirmed in Fig. 9 where the electron concentration profile in the channel is shown for different gate voltages. The maximum electron concentration is shown on the right side (bottom) of the channel at low gate bias, for $V_{\text{GS}}$ greater than 0.1 V this maximum concentration shifts toward the left side of the channel. This reduces the distance between the electron charge and the gate, hence increasing charge-control capacitance. This space change of the maximum electron concen-
tration with the bias increases the numerator of the integrand in the impurity scattering rate given by Eq. (8), which tends to compensate for the increase of screening function $Q_{sc}$ in the denominator. It is the origin of the plateau in the scattering rate observed in Fig. 8, which is directly reflected in the mobility in Fig. 7.

It should be noted that whatever the bias voltage, the fraction of carriers that contributes to parasitic conduction remains low and reaches only 4% of the total electron density at $V_{GS}=0.4$ V. This explains why the mobility is always greater than in the ungated modulation-doped structure with a similar layer stack (sample C2309; see Fig. 3).

IV. CONCLUSION

We have computed the electron mobility in 2DEG formed in tensile-strained Si/Ge modulation-doped structures by Monte Carlo simulation. To make the direct comparison with experimental data relevant, we have empirically modified the nominal doping profile in simulated structures. In ungated structures, good agreement is found with Hall measurements for a wide range of doping conditions and carrier densities, which demonstrates the correctness of the scattering models used. The mobility typically varies between 1100 and 2800 cm$^2$/V·s. It is shown to be significantly influenced by the thickness of the spacer layer that separates the strained-Si channel from the pulse-doped supply layers.

In a gated structure designed for MODFET operation, the contribution of conducting parasitic paths becomes negligible and the mobility is higher than in comparable ungated samples. Additionally, the variation of gate bias $V_{GS}$ modulates screening of remote impurities by free carriers. The most important consequence is in an increase in mobility as $V_{GS}$ increases.

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