

## High Field Transport of Hot Electrons in Strained Si/SiGe Heterostructure

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Monte Carlo simulation of two-dimensional electron gas in strained Si/SiGe heterostructures has been carried out to investigate the high electric field transport phenomena. In the Monte Carlo simulation we take into account the intervalley scattering between twofold and fourfold valleys of Si well layer splitted by the tensile strain in addition to the g-phonon scattering. We obtained the electron drift velocity at room temperature as high as  $1 \times 10^7$  cm/s at 10KV/cm. Ohmic mobility calculated by using self-consistent wave functions is also demonstrated. Results are given for strained Si well width of 10nm. Obtained low field electron mobility at temperatures 10-100K shows a good agreement with the experimental results reported so far.

### 1. Introduction

There has been considerable interest recently in strained Si/SiGe heterostructures because of their extremely high electron mobility at low temperatures<sup>1-5)</sup>. This high electron mobility is achieved by employing modulation doping and introducing strain-control buffer layer. Both of those are realized by using MBE or UHV/CVD technique. The mechanism that the electrons confined in this system show high mobility is explained as follows. In the case of the layers grown on (100) Si substrate and the tensile in-plane strain induced on the Si layer surrounded by the SiGe layers, the sixfold valleys of Si split into four in-plane valleys and two perpendicular valleys<sup>1)</sup>. Since the twofold degenerate level becomes lower than the conduction band of SiGe layer, electrons supplied by the donors doped in the SiGe barrier layer are confined and form 2DEG in the Si layer. The 2DEG is mainly conformed by the electrons in the twofold valley which is characterized with the lighter effective mass and separated from the ionized donors in SiGe layers, thus the electron mobility becomes higher than that of bulk Si. As mentioned above, experimental results of low field mobility at temperatures 2-300K are reported by several groups, whereas, electron transport at high electric field has not yet studied.

In this paper, we report on high field transport of hot electrons in strained Si/SiGe heterostructures calculated by using Monte Carlo method as well as the low field mobility calculated by using the self-consistent wave functions. Obtained low field mobility at temperatures 10-100 K shows a good agreement with experimental results reported so far. High field drift velocity and mobility at room temperature is quite high compared to that of Si MOS inversion layer.

### 2. Ohmic Mobility

It is well known that the electron mobility in bulk Si is limited by acoustic phonon deformation potential scattering and intervalley phonon scatterings due to g- and f-type phonons. In the two-dimensional electron gas (2DEG) system the electron mobility is calculated by taking into account these scatterings and quantized wave functions using the method proposed by Price<sup>7)</sup>. We reported that the ohmic mobility in Si inversion layers is analytically calculated when the electrons are scattered by these phonons. In the present work we use the same method to obtain the ohmic mobility. First we solve Schrodinger equation and Poisson equation self-consistently, and then overlap integrals are calculated which determine the strength of the scattering probabilities. Since we are interested in ohmic mobility, we take into account electrons in thermal equilibrium which occupy several subbands. In the strained layer Si in Si/SiGe heterostructures the conduction band discontinuity between the lower twofold valleys in Si and the conduction band of SiGe is 180meV and the energy separation between the two- and four-fold valleys is estimated to be 150meV. Therefore, we take into account four subbands, and we neglect higher subbands and fourfold valleys. Under this assumption the calculation is straight forward, where we included acoustic deformation potential scattering and g-type phonon scatterings. The deformation potentials are 9eV for the acoustic phonon deformation potential. Parameters of f- and g-type intervalley scatterings of Si<sup>6)</sup> are summarized in Table 1. In the Monte Carlo simulation shown in the next section we are interested in the high field transport of electrons and thus we have to take into account intervalley scattering between the twofold and fourfold

In Figure 1 we present the calculated results of the ohmic mobility as a function of lattice temperature in the range 1 to 300K, along with the experimental data reported by Schaffler *et al.*<sup>5)</sup> (open circles), and Nelson *et al.*<sup>4)</sup> (crosses). We find in the figure that the calculated mobility agrees well with these experimental results in the higher temperature region, but the calculated mobility is much higher than the experimental results at lower temperatures. This discrepancy may be interpreted in terms of impurity scattering. In the present calculation we neglected the impurity scattering and thus the calculated mobility is the expected highest mobility. At low temperatures the electron scattering is dominated by impurity scattering and thus the mobility saturates.

### 3. Monte Carlo Simulation

To investigate the high electric field transport of hot electrons in the system, we carried out Monte Carlo simulation of 2DEG. In the simulation, we take into account the intervalley scattering between the twofold and fourfold valleys. This scattering process is characteristic of the strained Si well in terms of the change of the kinetic energy of the motion in the plane parallel to the layers. To calculate the probability of this scattering, we use the parameters corresponding to the three types of f-scattering of bulk Si<sup>6)</sup>. The splitting of the conduction bands of the twofold valleys and fourfold valleys of the strained Si well is taken to be 150meV<sup>1)</sup>. Acoustic phonon scattering and intervalley scattering within the twofold valleys or fourfold valleys are also taken into account. To calculate each scattering probability, it is needed to obtain the overlap integral of the wave functions quantized in the direction perpendicular to the layers<sup>7)</sup>. For simplicity, we assume the wave function of the quantized electronic states in the Si layer are given by sinusoidal forms. The number of subbands are set to be 6 for twofold valleys and 3 for fourfold valleys in the case of 10nm Si well. This is determined by the consideration that the subband energies should not exceed the barrier height, which is chosen to be 180meV<sup>8)</sup>.

Figure 1 shows the calculated drift velocity as a function of the electric field at 4.2, 77 and 300K. We can see the drift velocity shows a remarkable saturation, especially at low temperatures. At room temperature the drift velocity is as high as  $1 \times 10^7$  cm/s at the electric field of 10KV/cm. This value is as about 5 times greater than that of Si MOS inversion layer<sup>9)</sup>. The high electron drift velocity reflects two factors, low electron effective mass in the twofold valleys and the weakened intervalley scattering of f-type phonons between the twofold and fourfold valleys. The latter factor arises from the splitting of the sixfold valleys in the strained Si.

Figure 2 represents the obtained temperature dependence of the electron mobility at electric field of 0.01, 0.1, 1 and 10KV/cm. Low field mobility at low temperatures is found to be in a good agreement with the experimental result reported so far. The low field mobility at room temperature is estimated to be higher than 2000cm<sup>2</sup>/Vs, which agrees well with the calculations shown in section 2.

### 4. Conclusion

Analysis of high field transport of hot electrons in strained Si/SiGe heterostructures by using Monte Carlo method is presented as well as the low field mobility calculated using the self-consistent wave functions. Obtained low field electron mobility at temperatures 10-100K is found to be in a good agreement with the experimental result reported so far. At room temperature the high field drift velocity is high as  $1 \times 10^7$  cm/s at 10KV/cm, and the low field mobility is found to be higher than 2000cm<sup>2</sup>/Vs. These results indicate that devices utilizing the strained Si/SiGe heterostructures will provide a superior performance compared to the conventional Si MOSFETs.

### 5. References

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Table 1. Intervalley scattering parameters of Si<sup>(6)</sup>.

| Type of Intervalley Scattering | T[K] | Dj<br>[10 <sup>8</sup> eV/cm] |
|--------------------------------|------|-------------------------------|
| f1                             | 220  | 0.3                           |
| f2                             | 550  | 2.0                           |
| f3                             | 685  | 2.0                           |
| g1                             | 140  | 0.50                          |
| g2                             | 215  | 0.80                          |
| g3                             | 720  | 11.0                          |

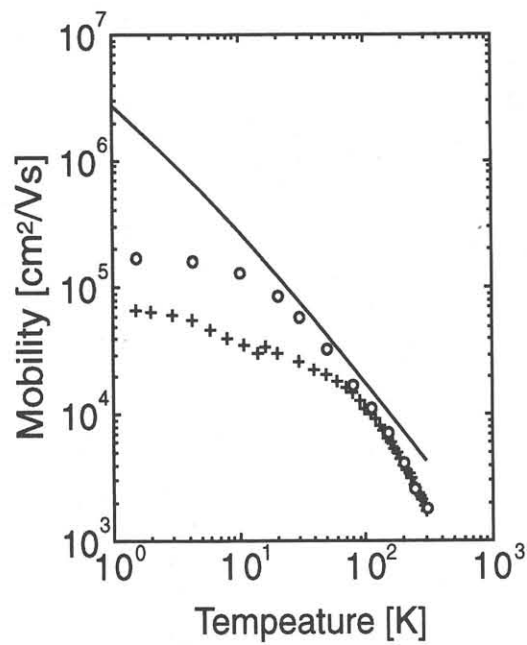


Figure 1. Temperature dependence of the ohmic mobility in strained Si/SiGe heterostructure. The solid line is the calculated result. The open circles are experimental results by Schaffler *et al.*<sup>5</sup>, and the crosses are by Nelson *et al.*<sup>4</sup>

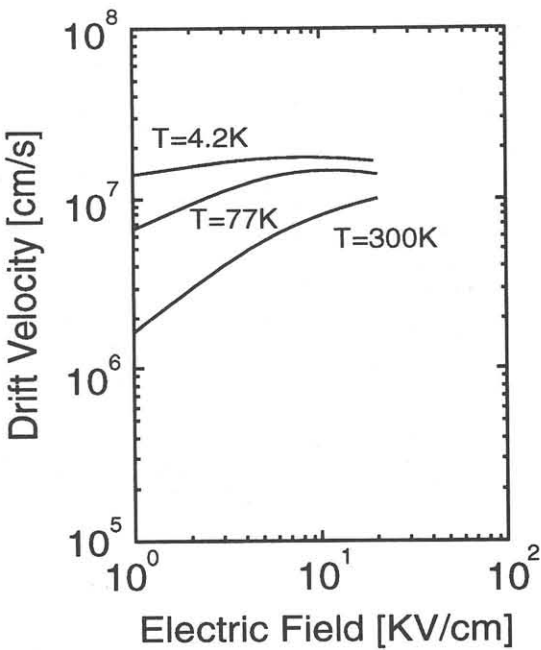


Figure 2. Drift velocity as a function of electric field in strained Si/SiGe heterostructure, at 4.2, 77 and 300K.

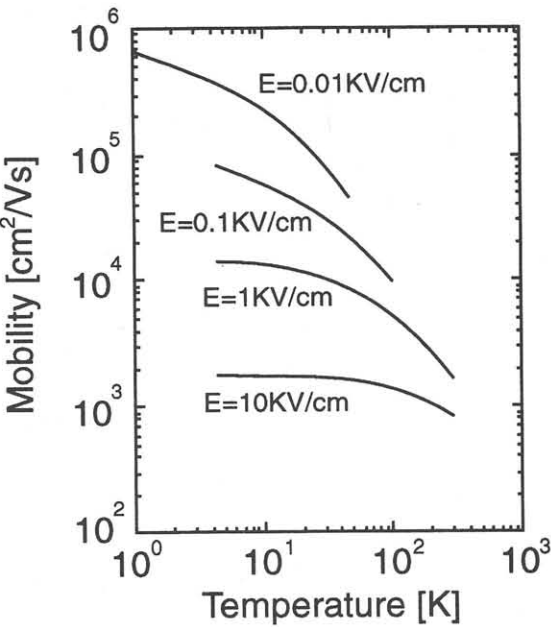


Figure 3. Temperature dependence of the electron mobility in strained Si/SiGe heterostructure, at electric fields 0.01, 0.1, 1, and 10KV/cm.

