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Transport Properties of Strained Si on $Si_{1-x}Ge_x$ Substrate by Monte Carlo Simulation

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Transport properties in strained Si grown on relaxed $Si_{1-x}Ge_x$ substrate were studied by an ensemble Monte Carlo technique. Electron drift velocities in strained Si were higher than that in unstrained Si at low fields, and the mobility was 3000 cm^2/Vs at 300 K and 23000 cm^2/Vs at 77 K, independently of Ge fraction in $Si_{1-x}Ge_x$ substrate over 17 %. Though there was not a significant improvement in the saturated velocity in strained Si, the overshoot of the drift velocity which was observed just after applying an electric field became larger with the Ge fraction in $Si_{1-x}Ge_x$ substrate. For the Ge fraction of 66 %, the peak velocity reached to 4.1 x 10^7 cm/s at 300 K and 5.2 x 10^7 cm/s at 77 K at the field of 50 kV/cm.

1. INTRODUCTION

Recent developments in epitaxial growth technique have realized heterostructures with no defect, even if there are several percent's differences between the lattice constants. In Si materials, $Si/Si_{1-x}Ge_x$ heterostructures attract much attention, which allow a bandgap engineering. In a modulation doped strained Si grown on $Si_{1-x}Ge_x$, substrate, two-dimensional electron gas (2DEG) appears in a strained Si layer, and the mobility is comparable to that of intrinsic Si. For example, it is 1600 cm^2/Vs at 300 K and 9600 cm^2/Vs at 77 K [1]. Also, high electron mobility transistors (HEMT) using strained Si channel grown on $Si_{1-x}Ge_x$ have been reported, whose transconductance is as high as 600 mS/mm at 77 K [2].

Here we show a high potential in electron transport in strained Si grown on $Si_{1-x}Ge_x$ substrate using Monte Carlo technique.

2. SIMULATION MODEL

Si grown epitaxially on a relaxed $Si_{1-x}Ge_x$ (100) substrate receives tensile stress that releases sixfold degenerate Δ-valleys in Si. The conduction band of twofold Δ-valleys whose (100) axis's are normal to the substrate (normal Δ-valleys) lowers and that of fourfold Δ-valleys whose (100) axis's are parallel to the substrate (parallel Δ-valleys) raises. The splitting of the conduction bands (ΔE) is given approximately by $0.6x$ eV, where x is Ge fraction in $Si_{1-x}Ge_x$ substrate [3]. In the scattering processes, ΔE affects the intervalley scatterings between normal and parallel Δ-valleys.

The transverse and the longitudinal mass were used as the electron effective masses, which were assumed to be the same independently of strain [4]. The effect of strain in the conductivity effective mass was automatically included to use the transverse and the longitudinal mass with the Herring-Vogt transformation [5] at each valley. Since the electrons are redistributed among the Δ-valleys due to strain, a ratio of the electrons that have the transverse mass and the longitudinal mass along the electric field changes. Therefore, the conductivity effective mass also changes corresponding to strain.

In the scattering processes, the intravalley scattering by acoustic phonon, the intervalley scattering by zeroth order f- and g- phonons and first order f- and g- phonons [6] and the impact ionization were included with the nonparabolicity. The velocity-field

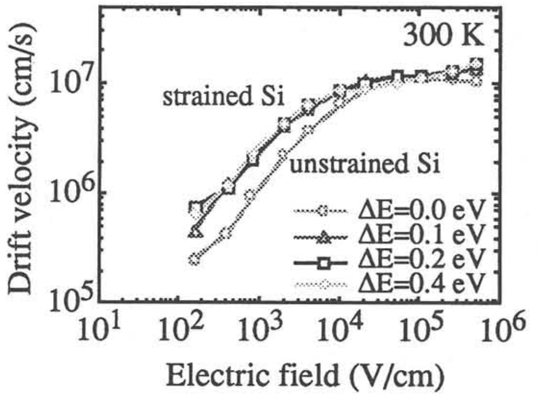

Fig. 1. Drift velocities in strained Si as a function of electric field.

characteristics for unstrained Si that calculated by our simulator could recover the measured results reported in [7].

The quantum effect of the 2DEG in strained Si was neglected in the scattering processes, because our simulations were done at high electric fields and high temperature.

3. RESULTS AND DISCUSSIONS

Electron drift velocities and average energies in strained Si were calculated at both 300 K and 77 K, which had different splittings of the conduction bands from 0 to 0.4 eV. Electric fields were applied parallel to the $Si/Si_{1-x}Ge_x$ heterointerface. In Fig.1, there are not significant differences in drift velocities among strained Si's. Electron drift velocities of strained Si are higher than those of unstrained Si at low fields. At 300 K, the mobility is 3000 cm^2/Vs in strained Si and 1400 cm^2/Vs in unstrained Si respectively. Both velocities, however, become close at high fields.

Electrons in Δ-valleys redistribute in strained Si. Electron population becomes large in twofold normal Δ-valleys, because the conduction band lowers due to strain. On the other hand, the electron population in fourfold parallel Δ-valleys becomes small. Because the electrons in twofold normal Δ-valleys have the transverse mass along to the electric field, the conductivity effective mass of strained Si reduces to 0.19 m_0, which is smaller than that of unstrained Si of 0.26 m_0 as shown in Fig.2. In the scattering processes, the intervalley scattering rate by the f-phonons between the twofold normal Δ-valleys and the fourfold parallel Δ-valleys are suppressed by the splitting of the conduction bands. The splitting is larger than the electron energies at low fields even for 0.1 eV as shown in Fig.3. So the total scattering rates in strained Si's are same, in spite of the different splittings of the conduction bands between 0.1 and 0.4 eV. For the same reason, the mobilities of strained Si's become same. In strained Si, the small conductivity effective mass and low scattering rate enhance the mobility, and it is same over the splitting of 0.1eV that is obtained from strained Si grown on $Si_{0.83}Ge_{0.17}$.

Time dependence of electron drift velocities were also calculated at the electric field of 50 kV/cm. The overshoot of the drift velocities are observed in Fig.4. For the conduction band splitting of 0.4 eV, the peak velocity is $4.1x10^7$ cm/s that is about two times larger than that of unstrained Si. Because the electrons in strained Si can be

$$m_c = \frac{3m_t m_l}{2m_t + m_l} = 0.26\ m_0$$

(a) unstrained Si

$$m_c = m_t = 0.19\ m_0$$

(b) strained Si

Fig. 2. Equivalent valleys of conduction minima and conductivity effective mass in Si.

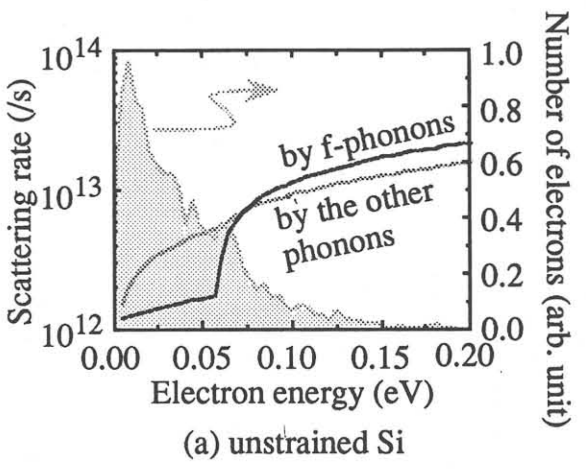

Fig. 3. Scattering rates by the phonons and electron distribution at the electric field of 400 V/cm as a function of electron energy.

accelerated with lower scattering rate before their energy reach to the steady state.

4. CONCLUSIONS

We showed that the electron transport properties in strained Si are superior to those in unstrained Si. At low fields, the conductivity effective mass of strained Si reduces to 0.19 m_0 by the electron redistribution among the Δ-valleys. The intervalley scatterings by the f-phonons are suppressed due to the splitting of the conduction bands. So the electron mobility of strained Si is expected to become 3000 cm^2/Vs at 300 K and 23000 cm^2/Vs at 77 K. At high fields, there is a significant improvement in the overshoot velocity in strained Si. For the splitting of 0.4 eV that is correspond to the Ge fraction of 66 % in $Si_{1-x}Ge_x$ substrate, the peak velocity reaches to $4.1x10^7$ cm/s at 300 K and $5.2x10^7$ cm/s at 77 K, which is ~2 times larger than that of unstrained Si.

Those excellent properties of strained Si will contribute to improvements in silicon based devices.

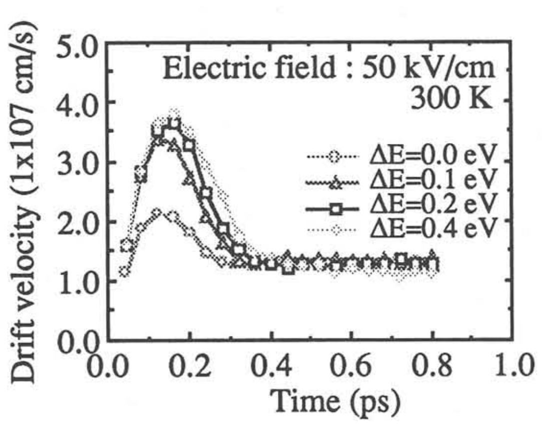

Fig. 4. Time dependence of the drift velocties in strained Si.

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