

High Hole Mobility in Modulation-Doped p-Si_{0.5}Ge_{0.5}/Ge/Si_{1-x}Ge_x Heterostructures fabricated Using Molecular Beam Epitaxy

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New heterostructures of modulation-doped p-Si_{0.5}Ge_{0.5}/Ge/Si_{1-x}Ge_x are fabricated using molecular beam epitaxy. The strain in the Ge channel layer can be precisely controlled by changing the composition of the Si_{1-x}Ge_x buffer layer. As a result, a large energy discontinuity of valence band (0.17eV) is expected. This leads to the high hole mobility of 2400 cm²/Vs at 77 K.

1. Introduction

Si-Ge hetero-epitaxy has attracted attention as the key technology for introducing the concept of band engineering into Si devices. Several studies on the fabrication of heterostructure devices have been reported,¹⁻³ where Si-rich SiGe alloys/Si structures are mainly used. However, from the standpoint of high speed device operation, the very high hole mobility of pure Ge are desired. People has already proposed p-Si_{1-x}Ge_x/Ge structures,⁴ and Wagner et al. have reported the observation of 2DHG (two-dimensional hole gas) in p-Si_{0.5}Ge_{0.5}/Ge structure.⁵ However, in these structures, sufficient confinement of holes is difficult.

Under such background, we propose new structures of p-Si_{0.5}Ge_{0.5}/Ge/Si_{1-x}Ge_x, where strain in p-Si_{0.5}Ge_{0.5}/Ge structure is controlled by a Si_{1-x}Ge_x buffer layer. Consequently, sufficient confinement of holes are considered to become possible.

2. Proposal of p-Si_{0.5}Ge_{0.5}/Ge/Si_{1-x}Ge_x heterostructures

Most important material parameters for hetero-devices are energy discontinuities at the edges of conduction and valence bands (ΔE_v and ΔE_c). People et al. have proposed an equation to estimate ΔE_v and ΔE_c in Si-Ge heterostructures.⁶ Using this rule, ΔE_v of p-Si_{0.5}Ge_{0.5}/Ge structure is calculated as 0.1 eV, which is insufficient for the hole confinement.

The main idea for solving this problem is the utilization of new heterostructures of p-Si_{0.5}Ge_{0.5}/Ge/Si_{1-x}Ge_x, where

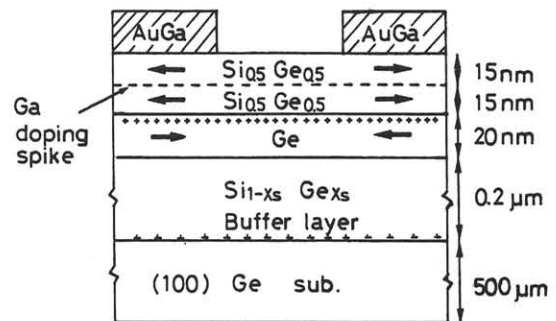


Fig. 1 Cross-sectional view of p-Si_{0.5}Ge_{0.5}/Ge/Si_{1-x}Ge_x heterostructures

compressive strain in the Ge channel can be controlled by changing the composition of the $\text{Si}_{1-X_s}\text{Ge}_{X_s}$ buffer layer. This compressive strain is expected to result in the large valence-band discontinuity ΔE_v . To estimate the ΔE_v values of the proposed structure, the natural modification of People's equation,

$$\Delta E_v = (0.74 - 0.58X_s)(1 - 0.5) \text{ (eV)}$$

is used. This indicates that ΔE_v increases as X_s value decreases. For example, large ΔE_v value of 0.17 eV is obtained at a typical X_s value of 0.75.

This increased ΔE_v leads to a large hole concentration⁷, which means the increase of hole velocity in degenerate hole gas. Thus high hole mobility is expected due to reduction of Coulomb scattering.⁸

In addition, the compressive strain is expected to cause valence band splitting, which realizes light hole conduction.⁹

3. Experiments

A sample structure fabricated in the present experiments is shown in Fig. 1. The epitaxial growth of each layer was performed with VG366 MBE (Molecular Beam Epitaxy) equipment. Base pressure of the UHV (Ultra High Vacuum) chamber was about 10^{-8} Pa. Si and Ge were evaporated with E-gun and K-cell, respectively. (100) Sb-doped ($10 \text{ } \Omega \text{ cm}$) Ge substrate was chemically etched¹⁰ and heated at 650°C for 20 min in UHV for surface cleaning. Ge buffer layer of 20 nm thick and $\text{Si}_{1-X_s}\text{Ge}_{X_s}$ buffer layer of 200 nm thick were successively grown at 400°C and 520°C , respectively. Then, Ge channel layer of 20 nm thick and $\text{Si}_{0.5}\text{Ge}_{0.5}$ layer of 15 nm thick were grown at 400°C . Ga doping was performed by adsorption of Ga atoms from K-cell at the substrate temperature below 100°C . Finally, amorphous $\text{Si}_{0.5}\text{Ge}_{0.5}$ film of 15 nm thick was deposited, and crystallization was followed through 450°C

1hr annealing in UHV (Solid Phase Epitaxy).

Strain in the epitaxial layers were characterized by Raman spectroscopy. In addition, hole mobility and concentration were evaluated with Hall measurement using van der Paw pattern with alloyed AuGa contact.

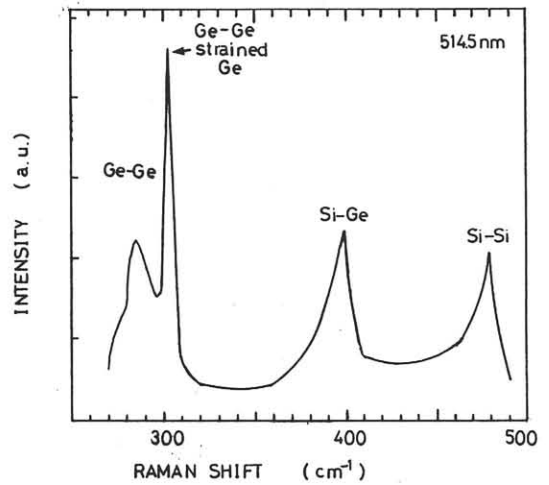


Fig. 2 A Raman spectrum of the $\text{p-Si}_{0.5}\text{Ge}_{0.5}/\text{Ge}/\text{Si}_{0.25}\text{Ge}_{0.75}$ heterostructure. The wavelength of incident light is 514.5 nm. Optical phonon modes from $\text{Si}_{0.5}\text{Ge}_{0.5}$ and Ge layers are observed.

4. Results and Discussion

4.1 Strain control in the Ge channel layer

A Raman spectrum from a typical sample ($X_s=0.75$ in Fig. 1) is shown in Fig. 2. Four peaks originating from optical phonon modes were observed, i.e. Ge-Ge mode of Ge layer and Ge-Ge, Si-Ge, and Si-Si modes of $\text{Si}_{0.5}\text{Ge}_{0.5}$ layer, respectively. The strain (ϵ) in the Ge layer can be evaluated using the wave number shift $\Delta\omega$ from the bulk value using the relationship of $\Delta\omega = -413.2 \epsilon^{11,12}$. The experimental values of ϵ are summarized in Fig. 3 as a function of $1-X_s$ of the buffer layer.

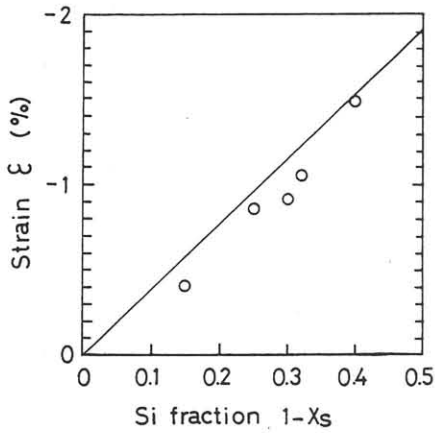


Fig. 3 Strain in the Ge layer from the Raman shift of the Ge-Ge mode vs. the Si content of the buffer layer ($1-X_s$). The solid line shows the theoretical relationship.

In the figure, theoretical values are shown for comparison, where the relation of $\epsilon = 0.0381(X_s - 1)$ is used by assuming Vegard's law for the lattice constant of $\text{Si}_{1-X_s}\text{Ge}_{X_s}$. Experimental results agreed with the theoretical values. In this way, it was demonstrated that strain in the Ge channel can be precisely controlled by changing the composition of the buffer layer.

4.2 Hole conduction in the Ge channel layer

Current-Voltage characteristics of a typical sample are shown in Fig. 4. Measurement temperature was varied from 77 K to 300 K. Around room temperature, a large leakage current was observed, which was also observed in Ge substrate and Ga δ -doped Ge (Fig. 5). These large leakage currents are due to small band gap of Ge substrate. Below 250 K the leakage currents were disappeared. In the modulation-doped sample, holes were not completely trapped by Ga ions (freeze-out) even at 77 K in contrast to the case of Ga δ -doped Ge sample. These results suggested that two-dimensional hole gas was formed at the $\text{p-Si}_{0.5}\text{Ge}_{0.5}/\text{Ge}$ interface.

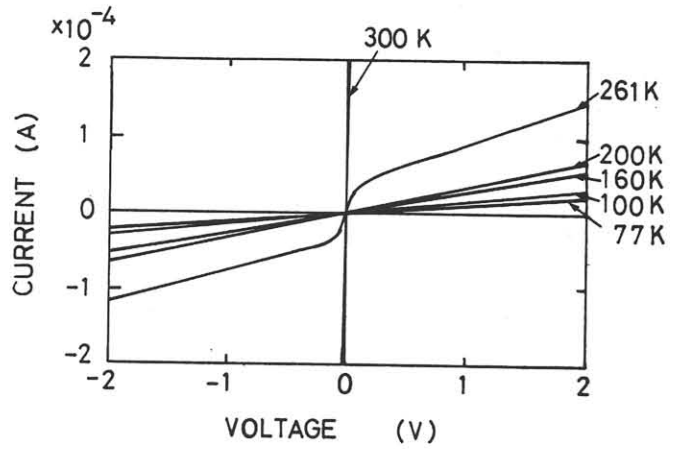


Fig. 4 Current-Voltage characteristics of the $\text{p-Si}_{0.5}\text{Ge}_{0.5}/\text{Ge}/\text{Si}_{0.25}\text{Ge}_{0.75}$ heterostructure. Temperature is varied from 77 K to 300 K.

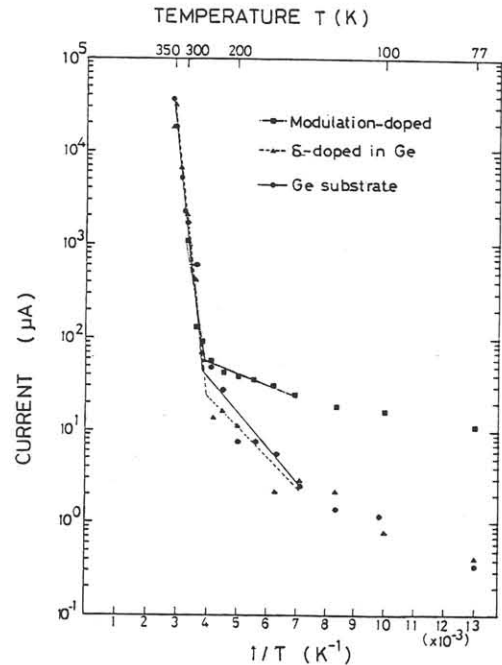


Fig. 5 Temperature dependence of the currents at 1 V for various samples.

Hole mobilities (μ_h) and hole concentration (N_h) were estimated by measuring the Hall effect (77 K), and results are shown in Fig. 5 as a function of $1-X_s$. In the low strain region ($0 < 1-X_s < 0.25$), hole mobility and concentration increase as the strain increases. This suggested that some change in the band structure increase the ΔE_v value, and/or change the hole population in light and heavy hole bands.

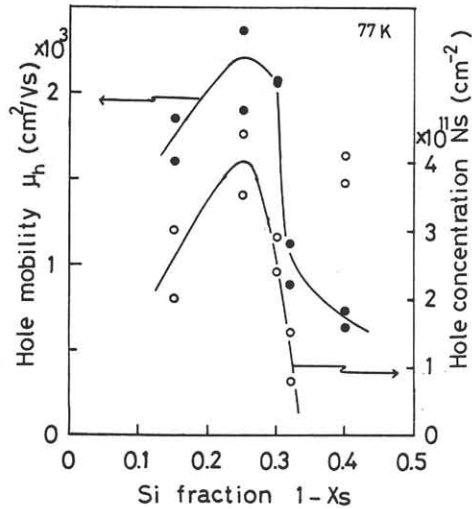


Fig. 6 Hole mobility and concentration of the $p\text{-Si}_{0.5}\text{Ge}_{0.5}/\text{Ge}/\text{Si}_{1-X_s}\text{Ge}_{X_s}$ heterostructures at 77 K vs. the Si content of the buffer layer ($1-X_s$). Magnetic field strength is 8 kG.

However, for $1-X_s > 0.25$, hole mobility and concentration suddenly decreases with an increase in the strain. A possible reason for this phenomenon is the propagation of dislocations from the buffer layer to the $p\text{-Si}_{0.5}\text{Ge}_{0.5}/\text{Ge}$ interface.

At present, the highest value of μ_h is $2400 \text{ cm}^2/\text{Vs}$ for $1-X_s = 0.25$, in which surface carrier density N_s is $4.4 \times 10^{11} \text{ cm}^{-2}$. This μ_h is larger than the bulk value of p-Ge doped more than 10^{17} cm^{-3} ,¹⁸ and is about four times greater than that reported for $p\text{-Si}/\text{Si}_{0.8}\text{Ge}_{0.2}$ structure.¹⁴

4. Conclusions

The usefulness of modulation-doped $p\text{-Si}_{0.5}\text{Ge}_{0.5}/\text{Ge}/\text{Si}_{1-X_s}\text{Ge}_{X_s}$ structure was demonstrated. Compressive strain in the Ge films was found to be controlled by the composition of the buffer layer. As a result, high hole mobility ($2400 \text{ cm}^2/\text{Vs}$) originating from 2DHG at $p\text{-Si}_{0.5}\text{Ge}_{0.5}/\text{Ge}$ interface was obtained.

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