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Influence of Strain on the Electrical Properties of Ge Channel in Modulation-Doped p-$Si_{0.5}Ge_{0.5}$/Ge/$Si_{1-x}Ge_x$ Heterostructure

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The influence of strain on the electrical properties of Ge channel in modulation-doped p-$Si_{0.5}Ge_{0.5}$/Ge/$Si_{1-X}Ge_X$ heterostructure is studied in relation to the Si mole fraction (1-X) and thickness in $Si_{1-X}Ge_X$ buffer layer. In the range of 1-X ≤ 0.25, hole concentration and mobility increase with strain in the Ge channel. However, in the range of 1-X > 0.25, hole concentration and mobility decrease with strain due to the large number of threading dislocations. Hole concentration and mobility increase with buffer layer thickness. As a result, a very high mobility of 7600 $cm^2/V\cdot s$ at 77 K is obtained at a Si mole fraction of 0.25 and buffer layer thickness of 1 μm.

1. Introduction

Much attention has been paid to Si-Ge heterostructures for introducing a new concept of band engineering into Si technology[1]. In particular, two dimensional (2-D) electron and hole gas systems in modulation-doped Si-Ge heterostructures have been investigated to realize high speed Si devices[2)-6)]. Recently, People proposed a p-$Si_{1-X}Ge_X$/Ge heterostructure using Ge as a channel[3]. In addition, Wagner et al. fabricated a p-$Si_{0.5}Ge_{0.5}$/Ge heterostructure; however, the valence band discontinuity (ΔE_v) at the interface was not large enough to confine the hole gas, and high hole mobility was not achieved[4].

To solve this problem, we have proposed a new heterostructure (p-$Si_{0.5}Ge_{0.5}$/Ge/$Si_{1-X}Ge_X$), where the strain in p-$Si_{0.5}Ge_{0.5}$/Ge hetero-interface was controlled by the Si fraction in the $Si_{1-X}Ge_X$ buffer layer. That strain caused a large band discontinuity (ΔE_v) at the p-$Si_{0.5}Ge_{0.5}$/Ge interface. Consequently, a two-dimensional hole gas with a high hole mobility (2400 $cm^2/V\cdot s$) was obtained at 77 K[7]. However, this mobility value was still lower than the theoretical one (> 20000 $cm^2/V\cdot s$)[8].

In this paper, the influence of strain on the electrical and crystal properties of the new heterostructure is quantitatively studied. In addition, an extremely high hole mobility (7600 $cm^2/V\cdot s$, 77 K) is obtained by optimizing the Si mole fraction and thickness in the buffer layer.

2. Experiments

A sample structure fabricated in the experiments is schematically shown in Fig.1. The growth of each layer was performed with VG-366 molecular beam epitaxy (MBE) equipment. Si and Ge were evaporated with E-gun and K-cell, respectively. Prior to growth, (100) Sb doped (10 Ω·cm) Ge substrate was chemically etched in solution (HNO_3:CH_3COOH:HF = 18:8:5) for 1-2 minutes and heated at 650 °C for 20 minutes in MBE chamber for surface cleaning. First, a thick $Si_{1-X}Ge_X$ buffer layer (0.2 ≤ 1-X ≤ 0.35, 0.2 - 1.0 μm thickness) was grown incommensurately on Ge substrate at 520 °C. Next, a thin Ge channel (20 nm) and a thin $Si_{0.5}Ge_{0.5}$ spacer layer (15 nm) were grown commensurately at 400 °C. Doping was performed by adsorption of Ga atoms from the

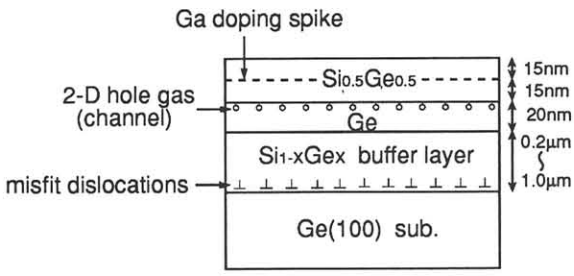

Fig.1 Schematic cross section of the p-$Si_{0.5}Ge_{0.5}$/Ge/$Si_{1-X}Ge_X$ heterostructure

K-cell at a substrate temperature below 100 °C. Finally, an amorphous $Si_{0.5}Ge_{0.5}$ film (15 nm) was deposited and crystallized by annealing at 450 °C for 1 hour.

Strain and crystal quality of the epitaxial layers were characterized using Raman spectroscopy and transmission electron microscopy (TEM), respectively. Electrical properties of the modulation-doped heterostructures were evaluated by Hall measurement at 77 K, using the van der Pauw pattern with alloyed AuGa contacts.

3. Results and discussion

The strain in the Ge channel commensurately grown on the $Si_{1-X}Ge_X$ buffer layer was evaluated using Raman spectroscopy. In the Raman spectrum, four peaks caused by optical phonon modes were observed : the Ge-Ge vibration in the Ge channel, and the Ge-Ge, Ge-Si, Si-Si vibrations in the $Si_{0.5}Ge_{0.5}$ layer, respectively. From the frequency difference between the two Raman peaks, i.e., the Ge-Ge vibrations in a strained Ge channel and in an unstrained bulk Ge, the relationship between the strain (ε) in the Ge channel and the (1-X) value in the buffer layer was determined to be $\varepsilon(\%) = -4.0(1-X)$. This relationship agreed well with the theoretical calculation of the strain in the Ge channel which is commensurately grown on the fully relaxed $Si_{1-X}Ge_X$ buffer layer[7]. In this way, accurate control of strain in the Ge channel becomes possible by changing the (1-X) value in the buffer layer.

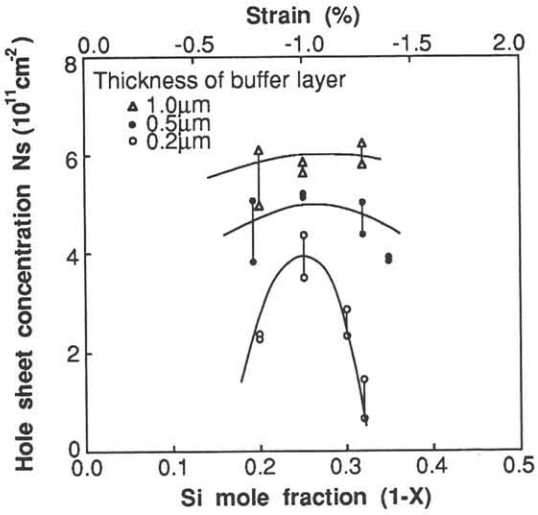

Fig.2 Hole concentration of p-$Si_{0.5}Ge_{0.5}$/Ge/$Si_{1-X}Ge_X$ heterostructure at 77 K vs. Si mole fraction (1-X) in the buffer layer and strain in the Ge channel.

The hole concentrations of p-$Si_{0.5}Ge_{0.5}$/Ge/$Si_{1-X}Ge_X$ heterostructures measured at 77 K are shown as a function of the (1-X) value in Fig.2. In the figure, strains in the Ge channel are also shown. In the low strain region ($\varepsilon \leq 1.0$ %), hole concentration increases with strain for all buffer layer thicknesses. However, in the high strain region ($\varepsilon > 1.0$ %), hole concentration decreases with strain. People suggested that the band discontinuity (ΔE_v) at the p-$Si_{0.5}Ge_{0.5}$/Ge hetero-interface grown on unstrained $Si_{1-X}Ge_X$ buffer layer commensurately changed by the strain. Using People's equation[5], the relationship between the ΔE_v value and Si mole fraction (1-X) in the buffer layer is estimated to be $\Delta E_v = 0.5[0.31 + 0.53(1-X)]$[7]. This indicates that the ΔE_v value at the p-$Si_{0.5}Ge_{0.5}$/Ge hetero-interface increases with the (1-X) value and reaches ~0.22 eV at ε = 1.0 % (1-X = 0.25). In the low strain region, the increase in hole concentration with the (1-X) value is due to the increase in the ΔE_v value with the strain. The decrease in concentration with Si mole fraction in the high strain region will be discussed later.

The hole mobilities of the heterostructures measured at 77 K are shown as

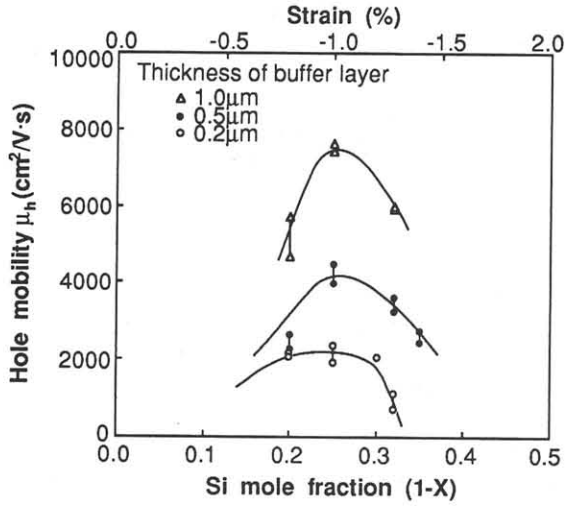

Fig.3 Hole mobility of p-$Si_{0.5}Ge_{0.5}$/Ge/ $Si_{1-X}Ge_X$ heterostructure at 77 K vs. Si mole fraction (1-X) in the buffer layer and strain in the Ge channel.

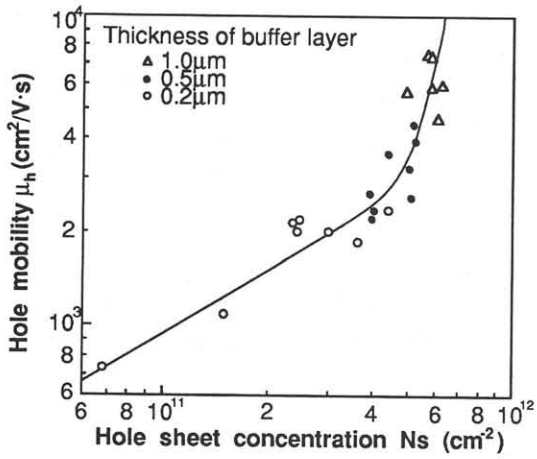

Fig.4 Hole mobility vs. concentration of p-$Si_{0.5}Ge_{0.5}$/Ge/$Si_{1-X}Ge_X$ heterostructure at 77 K.

functions of the (1-X) value and strain in Fig.3. The dependence of the mobility on the strain is similar to the dependence of the concentration on the strain. In fact, hole mobilities increase with strain in the low strain region ($\varepsilon \leq 1.0$ %), although they decrease with strain in the high strain region ($\varepsilon > 1.0$ %). Maximum hole mobilities are obtained at $\varepsilon = 1.0$ %. These values increase with the buffer layer thickness (h), i.e. μ = 2400, 4500, and 7600 $cm^2/V{\cdot}s$ for h = 0.2, 0.5, and 1 μm, respectively. These mobility values are about 4-12 times higher than those of a conventional modulation-doped p-Si/$Si_{0.8}Ge_{0.2}$

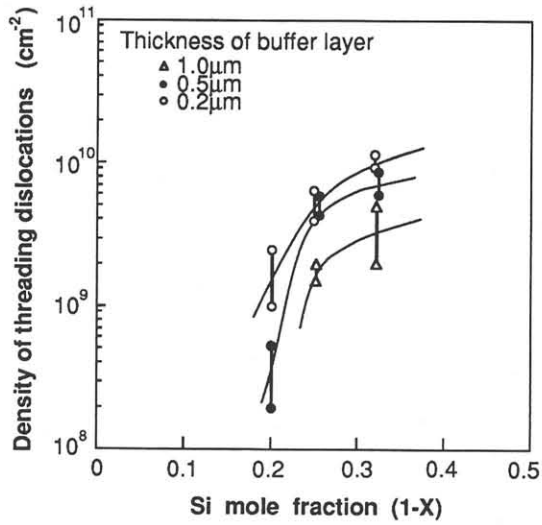

Fig.5 Density of threading dislocations vs. Si mole fraction (1-X) in the buffer layer.

heterostructure (600 $cm^2/V{\cdot}s$)[2].

The relationship between hole concentration and mobility is summarized in Fig.4. The figure shows that hole mobility increases with concentration. This property is different from that of bulk Ge where mobility decreases as concentration increases. This property also indicates that 2-D hole gas is confined at the p-$Si_{0.5}Ge_{0.5}$/Ge hetero-interface. To examine 2-D hole gas behavior, the angular (θ) dependence of the magneto-resistance of the heterostructure ($\varepsilon = 1.0$ %) was measured at 77 K and indicated a clear $\sin^2\theta$ dependence, thus confirming the 2-D behavior of hole gas[9].

To understand the phenomena shown in the high strain region, the influences of the Si mole fraction and thickness in buffer layer on the crystallinity were evaluated using TEM. The density of the threading dislocations at the p-$Si_{0.5}Ge_{0.5}$/Ge layers is shown as a function of the Si mole fraction (1-X) in Fig.5. Dislocation density increases with the (1-X) value. In particular, in the range of $0.2 \leq 1\text{-}X \leq 0.25$, dislocation density drastically increases (10^8 to 10^{10} cm^{-2}) with the Si mole fraction. Threading dislocations are considered to act as trapping centers, which result in the decrease of hole

concentration and mobility.

In addition, the density of threading dislocations decreases with the buffer layer thickness. As discussed in a previous report, in a GaAs/Si system[10], density of threading dislocation at p-$Si_{0.5}Ge_{0.5}$/Ge interface is considered to decrease due to the dislocation-dislocation coalescence and/or dislocation annihilation reaction when the buffer layer becomes thick. This decrease of dislocation density provides an ample explanation as to the increases in hole concentration and mobility with buffer layer thickness.

4. Summary

In summary, the influence of the strain field on the electrical and crystal properties of modulation-doped p-$Si_{0.5}Ge_{0.5}$/Ge/$Si_{1-x}Ge_x$ heterostructures was clarified. In the low strain region ($\varepsilon \leq 1.0$ %), hole concentration and mobility increase with strain, due to an increase in the band discontinuity at the p-$Si_{0.5}Ge_{0.5}$/Ge hetero-interface. However, in the high strain region ($\varepsilon > 1.0$ %), they decrease due to an increase in the density of threading dislocations. In addition, hole concentration and mobility increase with buffer layer thickness, due to a reduction in the density of threading dislocations. As a result, an extremely high hole mobility (7600 $cm^2/V \cdot s$) was obtained by optimizing the strain ($\varepsilon = 1.0$ %) and the buffer layer thickness ($h = 1$ μm).

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