In-Situ Impurity Doping in Si_{1-x-y}Ge_xC_y Epitaxial Growth Using Ultraclean LPCVD

D. Lee, T. Noda, H. Shim, M. Sakuraba, T. Matsuura and J. Murota

Laboratory for Electronic Intelligent Systems Research Institute of Electrical Communication, Tohoku University 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan *Phone: +81-22-217-5550 Fax: +81-22-217-5565 E-mail: murota@ riec.tohoku.ac.jp

1. Introduction

The $Si_{1-x-y}Ge_xC_y$ alloys have significant potential for the fabrication of novel Si-based devices [1]. By introduction of C into SiGe alloy, new Si-based band gap engineering [2], compensation of strain, and blocking the diffusion of dopant such as B [3] can be considered. For the fabrication of novel device structures, low-pressure chemical vapor deposition (LPCVD) at low temperatures, which is compatible to the conventional Si-base technology, allows us to control the film thickness and the doping concentration. However, in-situ impurity doping in Si1-x-yGexCy heteroepitaxy on Si and electrical characteristics of impurity-doped Si_{1-x-v}Ge_xC_v epitaxial films have not been completely understood.

In this work, in-situ B or P doping in Si_{1-x-v}Ge_xC_v epitaxial growth with the ultraclean LPCVD technique and the fundamental electrical characteristics of impurity-doped $Si_{1-x-y}Ge_xC_y$ have been investigated.

2. Experimental Procedure

The epitaxial growth of impurity-doped Si_{1-x-v}Ge_xC_v films was carried out at 550°C in a SiH₄-GeH₄-CH₃SiH₃-H₂ and B₂H₆ or PH₃ gas mixture using an ultraclean hot-wall LPCVD system, the details of which is described elsewhere [4]. The substrates used were n- or p-type Si (100) with mirror polished surfaces. The wafers were cleaned several cycles in a 4:1 solution of H₂SO₄ and H₂O₂, a high-purity DI water, and 1-2 % HF with a final rinse in DI water, and then the wafers, placed on a quartz boat, were transported into the reactor through a N₂ purged transfer chamber below 100°C. The wafers were heated up to 750°C under H₂ atmosphere to prevent any contamination from the exhaust line of the equipment as well as to lower the contamination level on the Si surface. Then the wafers were cooled down to 550°C and deposition was carried out (thickness: 100-300 nm). The partial pressures of SiH₄, GeH₄, CH₃SiH₃, and B₂H₆ or PH₃ are in the range of 6, 0.2-1.2, 0.016-0.09, and 6.5×10^{-5} - 8.125×10^{-3} Pa, respectively. With H₂ as a carrier gas, total pressure during deposition is fixed as about 30 Pa.

RHEED was used to evaluate the surface structure. Ge, C fraction, and B or P concentration were evaluated by SIMS results. The carrier concentration was determined by the van der Pauw method at room temperature.

3. Results and Discussion

In this experimental range, i.e., x = 0.16-0.6, y = 0-0.02, and $C_B \leq 2.44 \times 10^{21}$ or $C_P \leq 2.7 \times 10^{20}$ cm⁻³, the electron diffraction pattern showed all of the impurity-doped $Si_{1-x-y}Ge_xC_y$ films were epitaxially grown on Si (100).

For B-doped Si_{1-x-y}Ge_xC_y, reduction of the deposition rate occurs only at the higher P_{GeH4} (Fig. 1-a). The Ge fraction was not changed with the B2H6 and CH3SiH3 addition and it was determined by PSiH4 and PGeH4. The C



Fig.1 The deposition rate of in-situ (a) B- or (b) P-doped Si_{1-x-y}Ge_xC_y



Fig.1 The carrier concentration of in-situ (a) B- or (b) P-doped Si_{1-x-y}Ge_xC_y

fraction linearly increased with $P_{CH3SiH3}$ and with the B_2H_6 addition, no significant changes in the C fraction were observed except a small decrease at higher P_{B2H6} . C_B had a linear relationship with P_{B2H6} up to 2.4×10^{21} cm⁻³. In the case of P-doped Si_{1-x-y}Ge_xC_y, the deposition rate becomes abruptly reduced at higher P_{PH3} and the reduction is shift to higher P_{PH3} with increasing P_{GeH4} (Fig. 1-b). Ge fraction increased at higher P_{PH3} , and the tendency seemed severe at higher $P_{CH3SiH3}$. C fraction became slightly lower at higher P_{PH3} . C_P increased linearly with increasing P_{PH3} up to about 2 $\times 10^{20}$ cm⁻³ and tended to saturate at about 2.5×10^{20} cm⁻³.

It has been reported that the doping characteristics of Si_{1-x}Ge_x or the CH₃SiH₃-introduced impurity-doped deposition characteristics can be explained according to the Langmuir-type adsorption/reaction scheme [4, 5]. Assuming that one CH3SiH3 or dopant molecule (B-hydride or P-hydride) occupies one free surface site according to Langmuir's adsorption isotherm and that such an occupancy is different at the Si-Si, Si-Ge and Ge-Ge pair sites, the characteristics in this study can be explained. From the present experimental results, it is suggested that the B-, P-hydride and CH₃SiH₃ are adsorbed easily at the Si-Ge pair site compared with SiH4 and GeH4, and that the adsorption rate constant of CH₃SiH₃ on the Si-Ge pair site is larger than that of B-hydride and is smaller than that of P-hydride, leading the decrease in the density of free surface adsorption sites.

Carrier concentration of impurity-doped $Si_{1-x-y}Ge_xC_y$ is shown in Fig. 2. In B-doped $Si_{1-x-y}Ge_xC_y$ with y = 0.0054 or below, carrier concentration is nearly equal to C_B up to about 2×10^{20} cm⁻³ and saturates at about 5×10^{20} cm⁻³ regardless the Ge fraction (Fig. 2-a), and the B-doped $Si_{1-x-y}Ge_xC_y$ with y = 0.02 seems to have some electrically inactive B even at the lower C_B region. Concerning the P-doped films, it has been reported that P-doped $Si_{1-x}Ge_x$ with x = 0.5 or higher has electrically inactive P atoms independent to C_P due to its lower solid solubility of P [4]. With incorporation of C into P-doped $Si_{1-x}Ge_x$, inactive P atoms independently to C_P can be observed for the sample with lower Ge fraction than 0.5 and shown in Fig. 2-b. It can be considered that the films with 0.01 or higher atomic fraction of C should contain some interstitial C and the discrepancy of lattice constant from Vegard's law can support it [5].

4. Conclusions

In-situ B-or P-doped Si_{1-x-y}Ge_xC_y was epitaxially grown on Si (100) by using ultraclean hot-wall LPCVD system, and the doping characteristics of impurity-doped Si_{1-x-y}Ge_xC_y can be explained according to the Langmuir-type adsorption/ reaction scheme. C fraction in in-situ impurity-doped Si_{1-x-y}Ge_xC_y can affect carrier concentration even at the lower level of dopant concentration, especially for Si_{1-x-y}Ge_xC_y containing 1-2 % of C, which may contain some interstitial C.

Acknowledgement

This study was partially supported by Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports, and Culture of Japan, the Telecommunications Advancement Organization of Japan, and JSPS Research for the Future Program (No. JSPS-RFTF96R13101).

References

[1] Z. Atmon, A.E. Bair, E. J. Jaquez, I. W. Mayer, D. Chandrasekhar, D. J. Smith, R. L. Hervig and McD. Robinson, Appl. Phys. Lett. **65**, 2559 (1994).

[2] R. A. Soref, J. Appl. Phys. 70, 2470 (1991).

[3] H. J. Osten, B. Heinemann. D. Knoll, G. Lippert and H. Rücker,J. Vac. Sci. Technol., B16(3), 1750 (1998).

[4] J. Murota, M. Sakuraba and T. Matsuura, in *Defects in Silicon* Ⅲ (Electrochemical Society, Pennington, 1999), **PV99-1**, p 189.

[5] A. Ichikawa, Y. Hirose, T. Ikeda, T. Noda, M. Fujiu, T. Takatsuka, A. Moriya, M. Sakuraba, T. Matsuura and J. Murota, Thin Solid Films, in press.