Extended Abstracts of the 20th (1988 International) Conference on Solid State Devices and Materials, Tokyo, 1988, pp. 235-238 **C-4-1**

Formation and Properties of $Si_{1-x}Ge_x$/Si Structures by Solid Phase Heteroepitaxy

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Heteroepitaxal regrowth of a-$Si_{1-X}Ge_X$ films deposited on Si(100) substrate in the U.H.V. was accomplished in the solid phase by annealing at 500-850°C. The crystalline quality of SPE-$Si_{1-X}Ge_X$ films depends on the composition, and there are some of defects nearby $Si_{1-X}Ge_X$/Si interface. RBS measurement and observation of optical reflectivity of the samples shows that the value of $Si_{1-X}Ge_X$'s SPE rate at 600°C is almost close to that of Si's, but enhanced by existence of Ge. The diode characteristics of SPE-$Si_{1-X}Ge_X$/Si junction was measured at 70-300K. The improvement of the rectification was observed by following annealing process at 850°C.

§1. Introduction

With progress of high speed ICs, $Si_{1-X}Ge_X$ is expected to be one of good base materials for Si HBT (Heterojunction bipolar transistors) since the band gap is easily variable by changing Ge fraction.

So far, epitaxial growth of $Si_{1-X}Ge_X$ on Si has been done only by molecular beam epitaxy (MBE)[1]. Standing on the point of view such as low temperature fabrication process and high throughput process which might need no use of ultra-high-vacuum (U.H.V.) system, we propose the superiority of solid phase epitaxial (SPE) growth for fabrication of $Si_{1-X}Ge_X$/Si structure. This technique is potentially capable heavily to dope the base region by using plasma chemical vapor deposition (P-CVD) and so on. Basic study on SPE growth of $Si_{1-X}Ge_X$/Si is also important, because regrowth process of $Si_{1-X}Ge_X$ amorphized by implanted ions will be expected necessary in the future IC fabrication which would need ion implantation for self-align techniques.

§2. Experimental

After chemical cleaning, Si(100) substrate is thermally cleaned at 800°C for 30min in a U.H.V. chamber with a base pressure lower than $2x10^{-7}$Pa. The (100) orientation of the substrate was selected, taking into account superiority in SPE growth. Then, amorphous $Si_{1-X}Ge_X$ films having 50-480nm thicknesses were deposited on the substrate kept at room temperature by evaporation with use of two e-guns for Si and Ge respectively. And then, the samples were heated in the chamber at 250°C for 1h in order to densify a-$Si_{1-X}Ge_X$ films before they were exposed to the air. The samples were finally annealed in an N_2 atmosphere at 500-850°C for SPE.

§3. Results

3.1 Crystalline properties of SPE-$Si_{1-X}Ge_X$/Si films

Fig.1 shows Rutherford backscattering (RBS) spectra of SPE-$Si_{0.59}Ge_{0.41}$/Si(100) annealed at 600°C for 1hr. It shows that the $Si_{0.59}Ge_{0.41}$ has been grown epitaxially on Si(100) in solid phase. The channeling yields of the film estimated from Ge spectrum and Si spectrum respectively are almost same, so we can say that the Ge and the Si atoms of the film are located in the correct sites of diamond cubic structure without any segregation of Ge or Si. The channeling yield is about 9% at the surface and it increases gradually to reach about 45% at the $Si_{1-X}Ge_X/Si$ interface.

The crystalline quality of the SPE-$Si_{1-X}Ge_X$ films was dependent on the composition. When Ge fraction is above 50%, the SPE growth of a-$Si_{1-X}Ge_X$ films in single crystalline phase has not be observed and the surface morphologies of the samples become rough by 600°C annealing.

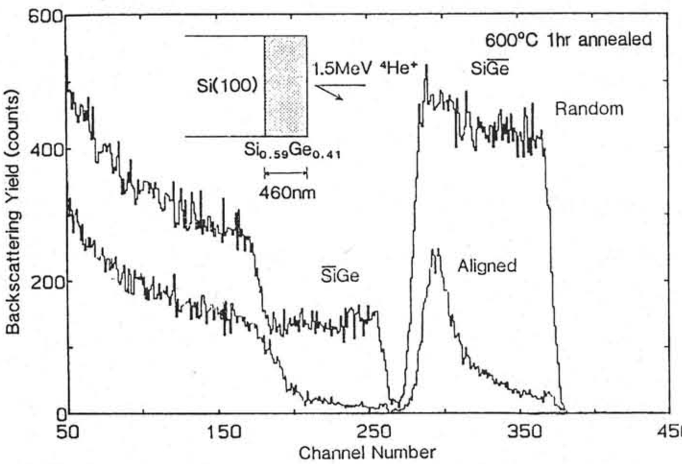

Fig.1 Backscattering spectra of the SPE $Si_{0.59}Ge_{0.41}/Si$ structure. The thickness of the film is 460nm. The sample was annealed at 600°C for 1h.

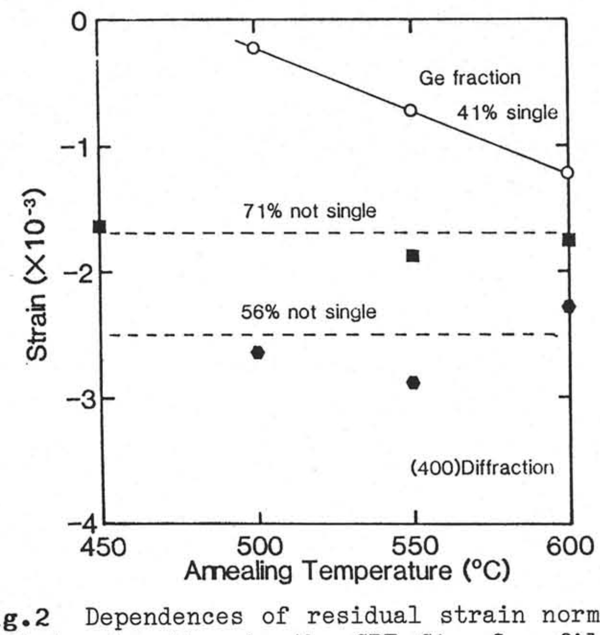

Fig.2 Dependences of residual strain normal to heterojunction in the SPE $Si_{1-X}Ge_X$ films on SPE annealing temperature for several compositions.

Fig.2 shows the residual strains which is normal to heterojunction in the SPE-$Si_{1-X}Ge_X$ film annealed at 450-600°C measured by 2 crystal X-ray diffraction analysis. It is normalized on the values of bulk $Si_{1-X}Ge_X$[2]. Every values have negative sign, so we can say that the tensile strain remains in the SPE films after annealing. Since the thermal expansion coefficients of $Si_{1-X}Ge_X$ is larger than that of Si, it is reasonable that the residual tensile strain is observed in such $Si_{1-X}Ge_X/Si$ system.

People et al.[3] have calculated the critical layer thickness for coherent growth of $Si_{1-X}Ge_X$ strained layers on Si by MBE. Fig.3 shows cross-sectional TEM photograph of SPE-Si(200nm)/$Si_{0.89}Ge_{0.11}$(260nm)/Si structure annealed at 600°C for 1h. Although the critical thickness of $Si_{0.89}Ge_{0.11}$ is about 800nm from People's theory, misfit dislocations are generated in the $Si_{0.89}Ge_{0.11}$ layer and they have propagated into Si upper layer. Taking attention more precisely to observe this photograph, we can see that the defects free layer of $Si_{0.89}Ge_{0.11}$ has grown from the $Si_{1-X}Ge_X/Si$ interface for about 25nm. From this observation, we estimate that the critical thickness of $Si_{1-X}Ge_X$ by SPE will be smaller than that by MBE.

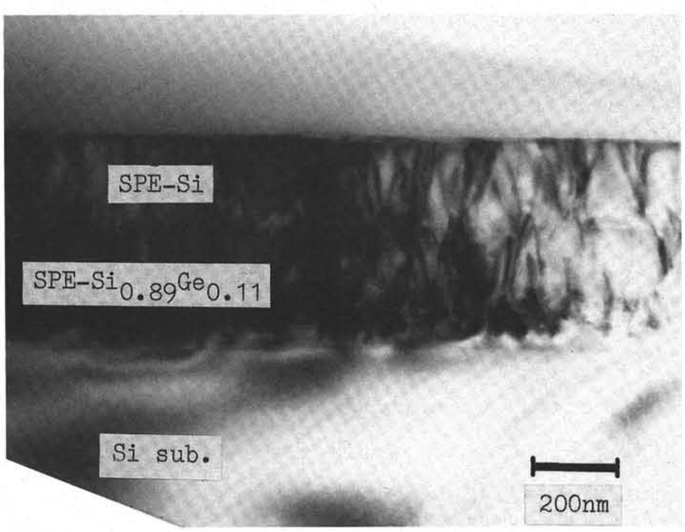

Fig.3 Cross-sectional TEM photograph of SPE $Si/Si_{0.89}Ge_{0.11}/Si$ structure annealed at 600°C for 1h.

3.2 SPE process of $Si_{1-X}Ge_X$ alloy

The process of the SPE growth has been studied by sequential RBS measurements. Fig.4 shows the variation of the thickness of regrowth region of $Si_{0.76}Ge_{0.24}$(250nm)/Si as a function of annealing time. From this figure, the maximum SPE rate was estimated to be 5.7×10^{-8}cm/s, which is almost close to that of pure Si ($3\text{-}5\times10^{-8}$cm/s, 600°C, (100))[4]. It is also shown that there is a incubation time before occurring of SPE. This incubation time of SPE may be due to the contamination at the $Si_{1-X}Ge_X$/Si interface.

The SPE growth rate of $Si_{1-X}Ge_X$ was also measured by the observation of optical reflectivity changes during annealing process. The results show that the SPE growth rate of $Si_{1-X}Ge_X$ is enhanced by the Ge fraction increase as shown in Fig.5. This dependences of the SPE rate on the Ge fraction can be explained by the difference of the activation energies of Ge and Si's SPE rates.

It is reported that the activation energy of the SPE rate of a-Ge is 2.0eV as compared with 2.7eV of a-Si and pre-exponential factor of the Arrhenius' equations on Si and Ge are both almost 3×10^{8}cm/s [5,6]. So, supposing that the SPE rate of $Si_{1-X}Ge_X$ would depend on only the activation energy which varies lineally as the composition, the SPE rate of $Si_{1-X}Ge_X$ can be expressed as follows,

$$V_{SPE}=3\times10^{8}*\exp[-(2.7*(1-X)+2.0*X)/kT],$$

where X is Ge fraction. Solid curves in Fig.5 shows the SPE rate of $Si_{1-X}Ge_X$ for Ge fraction taking annealing temperature as parameter, calculated by this equation.

3.3 I-V characteristics of SPE-$Si_{1-X}Ge_X$/Si junction

The forward and the reverse I-V characteristics of SPE-$Si_{0.84}Ge_{0.16}$/n-Si diodes which were grown by SPE at 600°C for 1h are shown in Fig.6. The SPE-$Si_{0.84}Ge_{0.16}$ layer which was not doped at the amorphous layer deposition shows p-type. The rectification characteristics was poor for

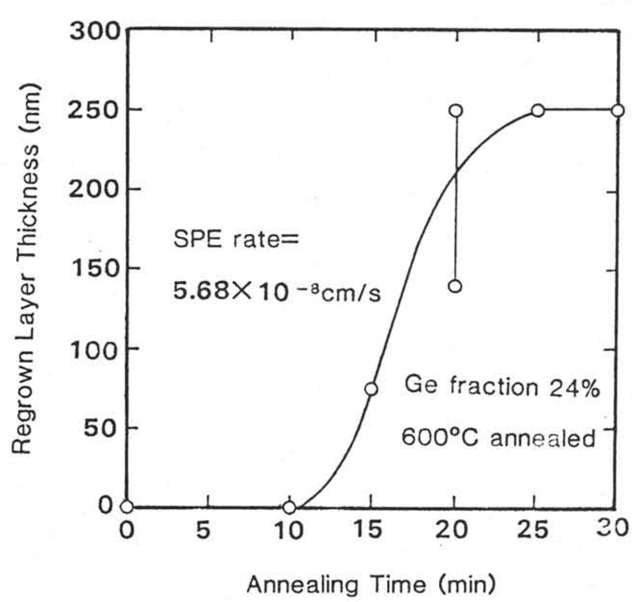

Fig.4 Changing of the thickness of regrowth region of a-$Si_{0.76}Ge_{0.24}$ film of 250nm thick by SPE annealing at 600°C as a function of annealing time.

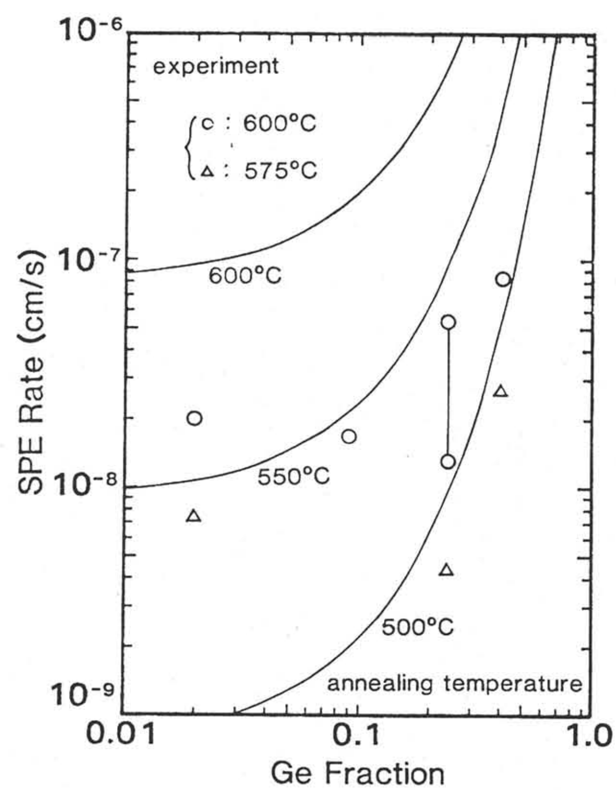

Fig.5 Dependence of SPE rate of $Si_{1-X}Ge_X$ on Ge fraction. The SPE rates at annealing temperature of 575°C - open triangles ;600°C - open circles were measured by observation of reflectivity against He-Ne laser. Solid curves are results of calculation.

as-grown sample. But yet, by following annealing process at 850°C for 30min, the both forward and the reverse currents have been improved remarkably. Values of the n factor (I=A*exp(qV/nkT)) is 2.3 at room temperature. Fig.7 shows temperature dependences of I-V characteristics of the diode. Although the values of the n factor become large with decreasing of the temperature, the improvement of the rectification characteristics is shown at low temperature.

§4. Conclusion

We have succeeded in formation of c-$Si_{1-X}Ge_X$/Si structure by SPE. The crystalline quality of SPE-$Si_{1-X}Ge_X$ films depends on the composition. It is found that the value of $Si_{1-X}Ge_X$'s SPE rate is almost close to that of Si's, but enhanced by existence of Ge. In the case when $Si_{1-X}Ge_X$ has not been doped at the deposition of amorphous film, the SPE-$Si_{1-X}Ge_X$ shows p-type and, the I-V characteristics of SPE-$Si_{1-X}Ge_X$/Si diode fabricated by such method is observed, at a moment, leaky.

Acknowledgments

The authors gratefully acknowledge the useful discussions with Assoc. Prof. H.Ishiwara.

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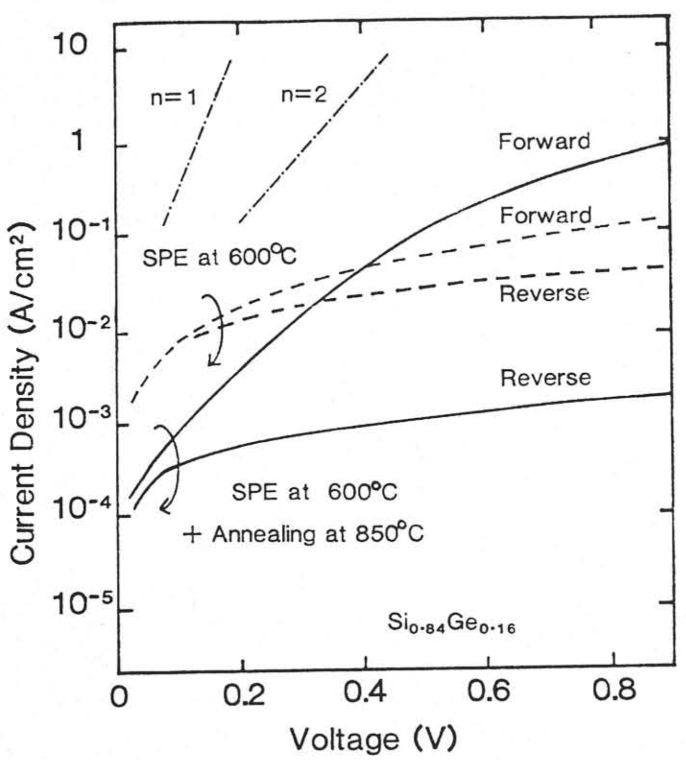

Fig.6 I-V characteristics of SPE $Si_{0.84}Ge_{0.16}$/Si diode grown at 600°C with and without following annealing at 850°C for 30min.

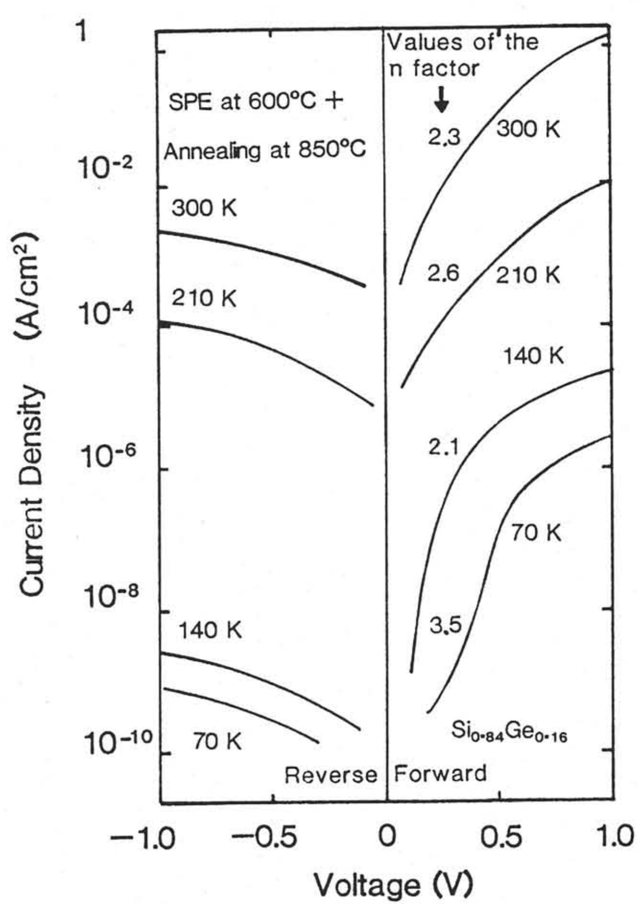

Fig.7 Dependences of I-V characteristics of SPE $Si_{0.84}Ge_{0.16}$/Si diode grown at 600°C with following annealing at 850°C on temperature.