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HIGH QUALITY HETEROEPITAXIAL Ge GROWTH ON (100) Si BY MBE

Yukio FUKUDA and Yoshitaka KOHAMA

NTT Electrical Communications Laboratories, 3-9-11 Midori-Cho, Musashino-Shi, Tokyo 180, Japan

An approach to high quality heteroepitaxial Ge growth on Si substrates by MBE has been studied. In the growth method studied here, the Ge layers were grown by a two-step procedure involving a thermal annealing process between the first and second Ge layer growth. It was found that the surface morphology of the Ge depended on the thickness of the first layer, and its thickness of more than 100 nm resulted in smooth surfaces. The crystalline quality of the Ge was affected by both the first and second Ge layer growth temperatures: lowering the growth temperature of the first layer and raising the growth temperature of the second layer in the epitaxial temperature range between 330 and 680°C led to further improvement in crystalline quality. Even further improvement in crystalline quality was accomplished by the high temperature annealing process. Double crystal X-ray diffraction studies showed that the full width at half maximum (FWHM) of the (400) diffraction of the 500 nm thick Ge layer was 240 s. A Ge layer with a dislocation density on the order of 10^7 cm^{-2} was obtained. A GaAs layer was subsequently grown by MOCVD. The FWHM of the 2 μm thick GaAs layer was 140 s.

1. Introduction

The possibility of integrating GaAs and Si devices in a monolithic structure and other applications involving optoelecronics or photovoltaics has motivated the recent interest in the heteroepitaxial growth of Ge layer on Si substrates [1–7]. Since GaAs is well matched to Ge in lattice parameter, the development of a high quality epitaxial growth of Ge on Si has been expected to serve as a suitable substrate for the subsequent growth of GaAs [2,4]. However, this growth includes the substantial problem of large mismatches in both the thermal expansion coefficients and lattice constants (55 and 4% respectively) between Ge and Si.

In the past several years, various techniques of growing Ge on Si have been investigated such as vacuum deposition [1,2], chemical vapor deposition [5], sputter deposition [6], and solid-phase epitaxy of a-Ge combined with ion-implantation [3,4]. However, the Ge layers reported so far have had a high density of dislocations (10^8–10^{10} cm^{-2}) [3,7]. These dislocations are the main cause of degradation in crystalline quality for the GaAs grown on Ge interlayer.

In the present work, we investigated a new approach to grow high quality Ge layers on Si by MBE. In this growth method, Ge is grown by a two-step procedure involving a thermal annealing process between the first and second Ge layer growth. The crystalline quality of the Ge layers grown by this method is compared with that of the Ge layers grown by the conventional growth method. The experimental results of GaAs growth on the Ge layers are also described briefly.

2. Experimental

The Si substrates used here were 10 Ω cm n-type (100)-oriented 3-inch wafers. Prior to loading into the MBE apparatus, the wafers were cleaned by conventional RCA solutions ($NH_4OH + H_2O_2 + H_2O$ and $HCl + H_2O_2 + H_2O$). A thin oxide layer was then formed by the method developed by Ishizaka and Shiraki [8]. Subsequently, the wafers were mounted on a Mo holder with a Ta plate, and loaded into the MBE chamber.

The growth system used here was a commercial Si MBE apparatus with two electron-beam evaporators. Prior to Ge deposition, the growth chamber was evacuated with an ion pump to a background pressure below 5×10^{-11} Torr. Next, the substrate temperature was raised to 850°C for 20 min to desorb the preformed oxide.

The polycrystalline Ge of 99.999% purity was then evaporated from the water-cooled copper crucible. The Si substrate was rotated at 30 rpm during deposition. The background pressure during deposition was about 5×10^{-9} Torr and the deposition rate was fixed at 5 Å/s.

The change in the surface morphology of the Ge layers due to variation in the growth conditions was evaluated by RHEED and Nomarski optical interference contrast microscopy. The crystalline quality was determined by transmission electron microscopy (TEM) and double crystal X-ray diffraction.

3. Results and discussion

To clarify the effects of the present growth procedure, preliminary growth of Ge was carried out by a conventional method. Table 1 summarizes growth conditions and characteristics of 500 nm thick Ge layers. Nomarski interference microscopy of the Ge layers showed smooth surface morphology if the growth temperatures were lower than 600°C. Altough the surface morphology became rough at growth temperatures higher than 600°C, the crystalline quality improved as the growth temperature increased. This was determined by examining the full width at half maximum (FWHM) of the (400) diffraction pattern of double crystal X-ray diffraction. Further increase in the growth temperature caused a slight degradation of the crystalline quality. The surface morphology and (400) diffraction pattern for the Ge layer grown at 600°C are shown in figs. 1a and 1b, respectively.

Table 1
X-ray (400) diffraction and surface morphology data for Ge layers on (100) Si grown by conventional growth method; the Ge thickness is 500 nm

Sample number	Growth temperature (°C)	X-ray diffraction FWHM (s)	Surface morphology
1	330	570	Smooth
2	510	500	Smooth
3	600	450	Slightly rough
4	680	460	Rough

A cross-sectional TEM micrograph of the same sample is shown in fig. 2. Apparently, the area near the highly mismatched Si–Ge interface includes a high density of dislocations. The dislocation density near the Ge surface is over 10^{10} cm^{-2}. The contrast in the micrograph is also significant. It may be due to the residual lattice strain in the Ge layer.

These results demonstrate that it is difficult to grow high quality Ge layers on Si by the conventional growth method.

Table 2 summarizes the measurements results for Ge layers grown by the two-step procedure. Growth was performed at various layer thicknesses, growth temperatures for the first and second Ge layers, and thermal annealing temperatures. Annealing time was 20 min. In contrast with the Ge layers grown by the conventional method, a great improvement in crystalline quality was accomplished using this growth method.

The surface morphology varied with the thickness of the first Ge layer rather than that of the second Ge layer, as seen in the optical micrographs in fig. 3. The first Ge layer thickness over 100nm was found to be necessary to obtain mirror-surface finished growth.

The crystalline quality of the Ge layers was strongly dependent on both the first and the second Ge layer growth temperatures, and on the annealing temperature. In general, lowering the growth temperature of the first layer and raising the growth temperature of the second layer led to a further improvement in crystalline quality. Besides these effects, the crystalline quality was considerably improved by the thermal annealing process. The FWHM of the Ge layer was reduced by increasing the annealing temperature from 600 to 680°C. The surface morphology and the (400) diffraction pattern for sample 11 are shown in figs. 4a and 4b, respectively. In comparison with sample 3 shown in fig. 2, the surface of the sample is very smooth, and the (400) diffraction pattern is sharper and stronger.

A cross-sectional TEM micrograph of sample 8 is shown in fig. 5. Various distinctions can be

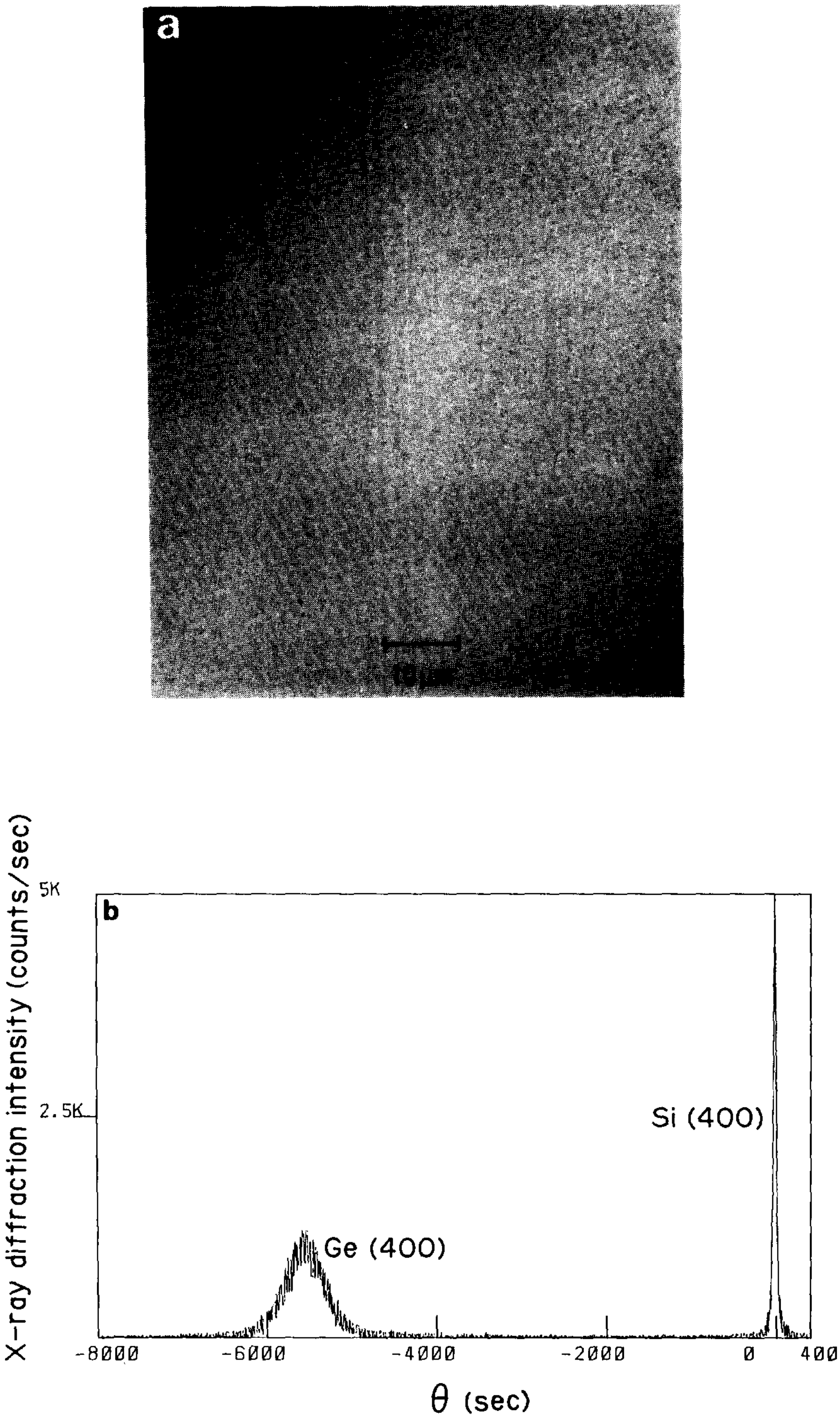


Fig. 1. (a) Nomarski interference micrograph and (b) X-ray (400) diffraction pattern of Ge layer (sample 3) grown at 600 °C.

Fig. 2. A cross-sectional TEM micrograph of Ge layer (sample 3) grown at 600 °C.

pointed out by comparing this micrograph with the micrograph shown in fig. 2. The defect density of the Ge drops rapidly toward the surface and a transition region where there is a high density of dislocations is restricted to several tens of nm from the Si–Ge interface. The background contrast evenness shows that the large lattice mismatch is effectively relaxed in this narrow transition region. Furthermore, the propagating dislocations which arise from this transition region are greatly reduced, and some parts of these dislocations are truncated near or at the interface between the first and second Ge layers, as shown in fig. 6. The dislocation density near the Ge surface is on the order of 10^7 cm^{-2}. This is two or three orders of magnitude lower than the value of the Ge layers grown by the conventional growth method.

As an initial step in determining the usefulness of these Ge layers as substrates for the growth of GaAs, the GaAs epitaxial layers with about 2 μm thickness were grown by the low-pressure MOCVD using trimethylgallium (TMG) and AsH_3 as source gases. The V/III ratio was about 70 and the growth temperature was 700 °C. The single-domain GaAs layers were successfully grown, and in most cases, their crystalline quality was superior to that of the underlying Ge layers. Fig. 7 shows the (400) diffraction pattern of the grown GaAs layer. The FWHM is 140 s, which seems to be sufficiently narrow. This result means that the large lattice mismatch between GaAs and Si is effectively relaxed in the intermediate Ge layer.

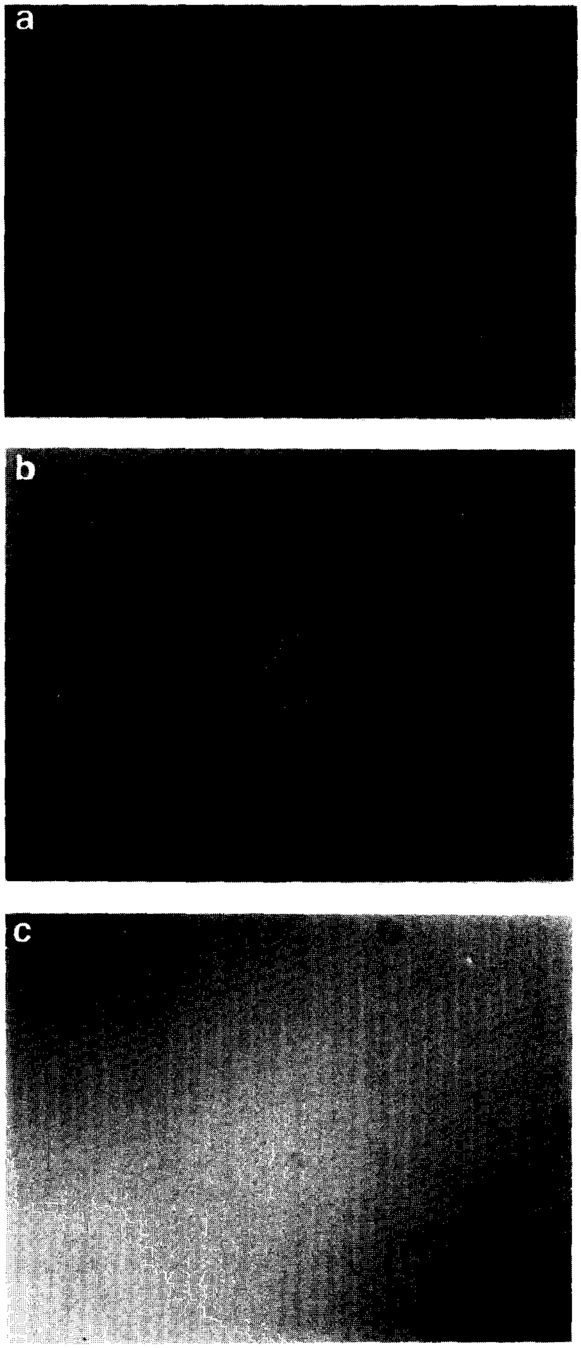
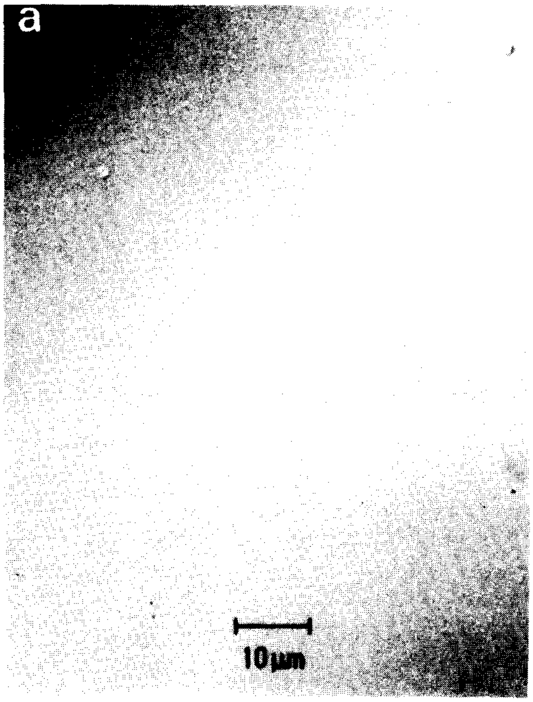


Fig. 3. Nomarski interference micrographs of Ge layers with various first Ge layer thickness. The surface morphology changes with first Ge layers thickness: (a) 20 nm (sample 5); (b) 70 nm (sample 6), (c) 100 nm (sample 7).



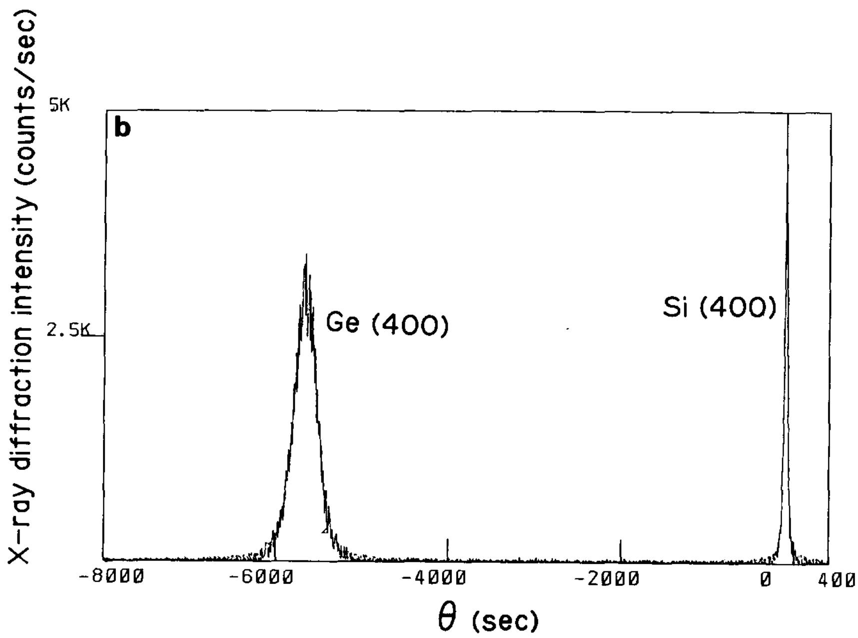


Fig. 4. (a) Nomarski interference micrograph and (b) X-ray (400) diffraction pattern of Ge layer (sample 11).

Table 2
X-ray (400) diffraction and surface morphology data for Ge layers on (100) Si grown by two-step procedure with thermal annealing process between first and second Ge layer growth; annealing time is 20 min

Sample number	First layer		Annealing (°C)	Second layer		FWHM (s)	Surface morphology
	Thickness (nm)	Temp. (°C)		Thickness (nm)	Temp. (°C)		
5	20	330	600	300	600	490	Rough
6	70	330	600	300	600	406	Slightly rough
7	100	330	600	400	600	345	Smooth
8	300	330	600	200	600	318	Smooth
9	300	510	600	200	600	374	Smooth
10	300	330	680	200	330	294	Smooth
11	300	330	680	200	600	270	Smooth
12	300	330	680	200	680	240	Slightly rough

Fig. 5. A cross-sectional TEM micrograph of Ge layer (sample 8).

Fig. 6. A magnified cross-sectional TEM micrograph of a Ge layer (sample 8). Note that some propagating dislocations are truncated at the interface between first and second Ge layers.

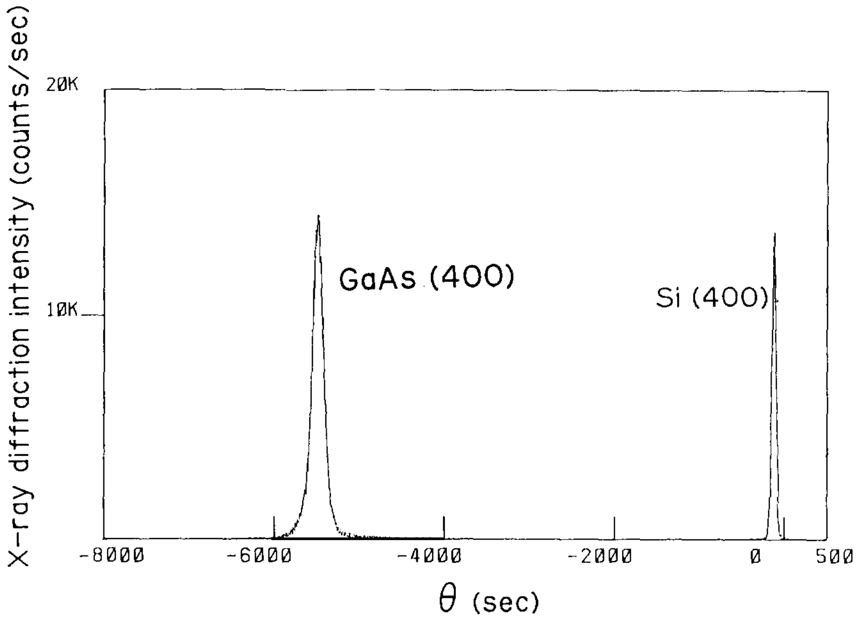


Fig. 7. X-ray (400) diffraction pattern for GaAs layer grown by MOCVD.

4. Summary

A new approach to grow high quality Ge layers on Si substrates has been demonstrated. A great improvement in the crystalline quality of the Ge layers was achieved by the growth method studied here.

The thickness of the first Ge layer was found to be critical to obtain the mirror-surface finished morphology. A layer with a thickness over 100 nm came out to have a smooth surface without any relief. The crystalline quality of the Ge layer was considerably improved by controlling the first and second Ge growth temperatures, and the thermal annealing temperature. TEM observations revealed that the large lattice mismatch between Si and Ge was effectively relaxed in the narrow transition region within several tens of nm from the Si–Ge interface. Moreover, some propagating dislocations were truncated near the interface between the first and second Ge layers. Ge layers with dislocation density on the order of $10^7\ cm^{-2}$ were obtained. Epitaxial GaAs layers of good crystalline quality were successfully grown on the Ge layers by MOCVD.

On the basis of these results, it is highly probable that the Ge layer grown by the method studied here can serve as a suitable substrate for the subsequent growth of GaAs.

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