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Formation of High Quality $Si_{1-x}Ge_x/Si$ Crystals Heterostructure Limited Area MBE Growth

A. Nishida, K. Nakagawa, E. Murakami, and M. Miyao

Central Research Lab., Hitachi,Ltd.
Kokubunji, Tokyo 185, Japan

Limited area molecular beam epitaxial (MBE) growth, in which $Si_{1-x}Ge_x$ film grows on an Si region surrounded by SiO_2, is studied in order to obtain high quality $Si_{1-x}Ge_x$ / Si heterostructures. This method drastically reduces misfit dislocations in the film growth and remarkably improves thermal stability. This phenomenon is attributed to relaxation of the strain in the film growth around the pattern edge and to limited dislocation extension.

1. INTRODUCTION

Si-Ge heteroepitaxy is a key technology for introducing the concept of band engineering into Si LSIs. However, strained $Si_{1-x}Ge_x$ / Si heterostructures are unstable due to lattice mismatch between the $Si_{1-x}Ge_x$ film and Si substrate[1]. Therefore, both misfit and threading dislocations are introduced to relax the strain in the $Si_{1-x}Ge_x$ film grown on a Si substrate during MBE growth or post annealing. A detailed study about limited area MBE growth, in which a strain $Si_{1-x}Ge_x$ film is grown on Si region surrounded by SiO_2[2], was performed to reduce the dislocation density and to improve thermal stability of the growth film. Results show that the dislocation density reduced as the area of the SiO_2 opening decreased. Dislocation free $Si_{0.8}Ge_{0.2}$ film was produced at the area smaller than 2.5 x 2.5 μm^2. It was also found that the thermal stability of the growth film was remarkably improved.

This paper describes the results of the limited area MBE growth. In addition, it discusses to the mechanisms of reduction of the dislocation density and improvement of the thermal stability of the $Si_{1-x}Ge_x$ film.

2. EXPERIMENTS

N-type Si (100) wafers were used in the experiment. A thermal oxide layer (about 80 nm thick) was formed on the Si substrate. Then, square (1 x 1 - 100 x 100 μm^2) or stripe shaped (1 - 100 μm width and 9 mm length) seed openings were formed on a SiO_2 layer by conventional lithography and a wet etching technique. Figure 1 shows a schematic illustration of the samples.

$Si_{1-x}Ge_x$ layers were grown with VG - 366 MBE equipment. The base pressure of the growth chamber was below 1 x 10^{-10} mbar. Before introducing the Si substrate to the growth chamber, the substrate surface was precleaned by chemical treatment, and a protective thin oxide layer was formed[3]. Next, the thin oxide layer was sublimated at 850 °C for 20 minutes in the growth chamber to obtain a clean surface. After the substrate temperature was lowered to 520 °C, Si and Ge

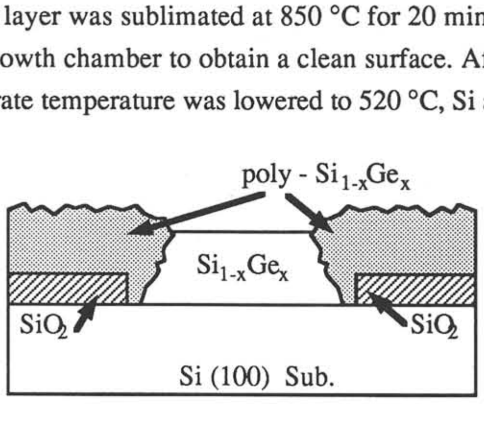

Fig.1 A schematic cross - sectional view of samples

were codeposited using E - gun evaporator and Knudsen cell, respectively. Beam fluxes were monitored by quartz thickness monitors to control the alloy ratio. Thus, $Si_{1-x}Ge_x$ films with different alloy ratios were grown on patterned Si substrates. The growth conditions are shown in Table 1. The thicknesses of film growth were fixed at 150 nm. Under these conditions, the $Si_{1-x}Ge_x$ films were grown incommensurately on unpatterned Si substrates, and dislocations were introduced to the growth films[4,5].

Dislocations in the $Si_{1-x}Ge_x$ films were observed using transmission electron microscopy (TEM) with an accelerated voltage of 200 kV.

To check the thermal stability of the $Si_{1-x}Ge_x$ films, the films grown on both patterned and unpatterned substrates were annealed at 700 - 900 °C for 15 minutes in N_2 ambient. The change of misfit dislocation density caused by annealing was also observed using TEM.

Table 1 List of growth samples

ratio	thickness (nm)	
0.1	150	commensulate growth
0.12	150	incommensulate growth
0.2	150	incommensulate growth
0.3	150	incommensulate growth

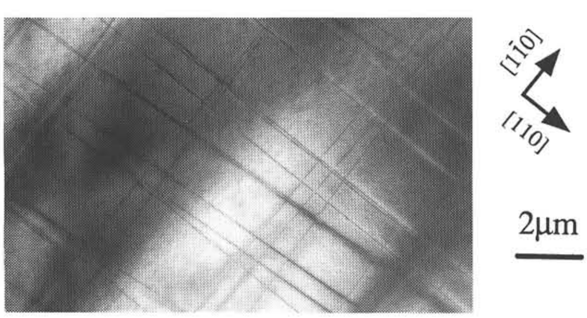

Fig.2 Plan-view TEM micrograph of the $Si_{0.8}Ge_{0.2}$ film grown on an unpatterned substrates.

3. RESULTS AND DISCUSSION

(1) $Si_{1-x}Ge_x$ film growth on patterned substrate

Figure 2 shows a plan-view TEM micrograph of the $Si_{0.8}Ge_{0.2}$ layer grown on an unpatterned substrate. This micrograph includes both the $Si_{0.8}Ge_{0.2}$ layer and the herero-interface. Defects in the growth film are mainly misfit dislocations extended along both the [110] and [1$\bar{1}$0] direction. The linear dislocation density (the reciprocal number of misfit dislocation spacing) is about 10,000 cm^{-1}. This value is much lower than the one estimated from the lattice mismatch. This means that strain is still in the $Si_{0.8}Ge_{0.2}$ film. The TEM micrograph of the $Si_{0.8}Ge_{0.2}$ grown on SiO_2 patterned substrate is shown in Figure 3. A crystal $Si_{0.8}Ge_{0.2}$ film grew on a Si layer surrounded by SiO_2, and a polycrystalline $Si_{0.8}Ge_{0.2}$ film grew on a SiO_2 layer. Dislocation density reduced as the growth area of the SiO_2 opening decreased, and no dislocation was observed in the 2.5 x 2.5 μm^2 square SiO_2 opening (Figure 3 (c)). In Figure 4, the linear misfit dislocation densities from the TEM results above are plotted as a function of the size of square SiO_2 opening. These densities are the average values of misfit dislocations extended along both the [110] and [1$\bar{1}$0] directions. As seen in this figure, the density drastically reduced when the area was reduced to less than 5 x 5 μm^2. On the other hand, the density was not affected when the area was lager than 5 µm.

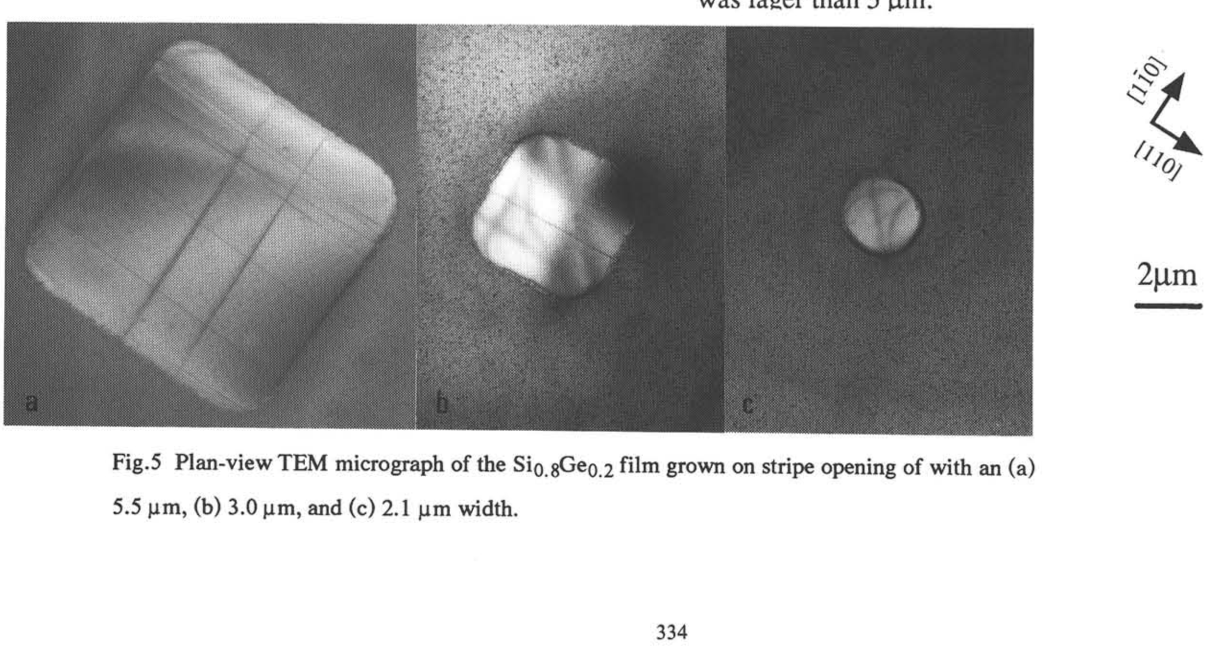

Fig.5 Plan-view TEM micrograph of the $Si_{0.8}Ge_{0.2}$ film grown on stripe opening of with an (a) 5.5 µm, (b) 3.0 µm, and (c) 2.1 µm width.

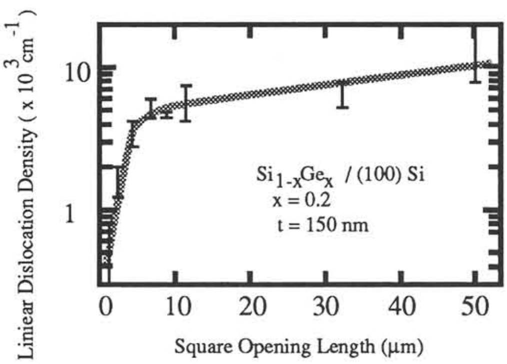

Fig.4 The linear dislocation density in the $Si_{0.8}Ge_{0.2}$ film as a function of square SiO_2 opening dimension. The density is the average value of the dislocations extended along both the [110] and the [1$\bar{1}$0] direction.

(a) (b) (c)

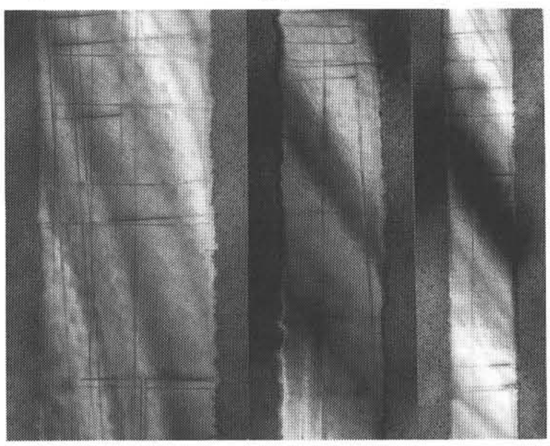

Fig.5 Plan-view TEM micrograph of the $Si_{0.8}Ge_{0.2}$ film grown on stripe opening of with an (a) 5.5 μm, (b) 3.0 μm, and (c) 2.1 μm width.

Figure 5 shows a plan-view TEM micrograph of $Si_{0.8}Ge_{0.2}$ film grown on SiO_2 stripe shaped openings. Defects in the growth films are also misfit dislocations extended along both the [110] and [1$\bar{1}$0] direction. Figure 6 shows the relationships of the linear dislocation densities of the $Si_{0.8}Ge_{0.2}$ films grown on Si substrate in a stripe opening to the width of the stripe opening. Dislocation density reduction occured when the stripe opening width was less than 10 μm. This reduction was especially remarkable when the dislocations extended perpendicular to the stripe ([1$\bar{1}$0] direction). When the width opening was more than 10 μm, the density did not reduce and had the same value as films grown on unpatterned substrates.

Fitzgerald et al proposed the model[6] for the

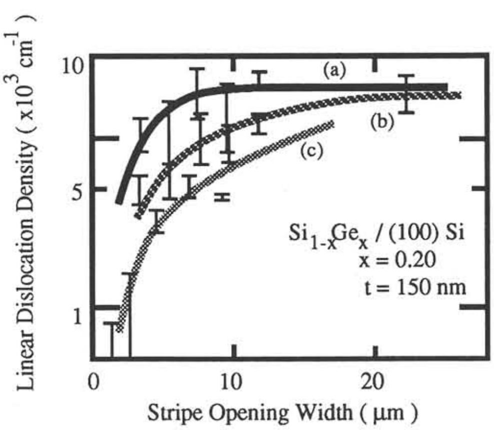

Fig.6 The relationship of the linear dislocation density of the $Si_{0.8}Ge_{0.2}$ film to the width of the stripe opening. All densities were estimated from dislocations extended perpendicular to the stripe (line (a)) and parallel to the stripe (line (b)). Line (c) is the replotted data of Figure 4.

reduction of dislocation density for InGaAs / GaAs strained systems. That is,the extension of dislocation was limited, and the dislocation multiplication was prevented by the patterned substrate. For stripe patterned substrates, the reduction of the density of dislocation extended perpendicular to the stripe was thought to be due to the limited dislocation extension caused by SiO_2. However, it is impossible to explain the reduction extended parallel to the stripe (Figure 6 (b)) using this model.

TEM was used to observe the cross - sections of the growth film to clarify the reduction mechanism. Figure 7 shows the cross - sectional TEM micrograph of the $Si_{0.8}Ge_{0.2}$ / Si heterostructure. Misfit dislocations were introduced at the hetero-interface to relax the strain in the $Si_{0.8}Ge_{0.2}$ film in the center of the stripe opening (Figure 7 (a)). On the other hand, there was no misfit dislocation at the interface around the SiO_2 pattern edge, i.e. the boundaries between crystal and polycrystalline $Si_{0.8}Ge_{0.2}$ film. This result suggests that the relaxation of the strain in the $Si_{0.8}Ge_{0.2}$ film occured around the SiO_2 pattern edge, and, as a result, there was no dislocation . Therefore, the drastic reduction of the misfit dislocation in the $Si_{0.8}Ge_{0.2}$ film grown on patterned substrate must be due to the strain relaxation around the SiO_2 pattern edge as well as to limited misfit dislocation extension

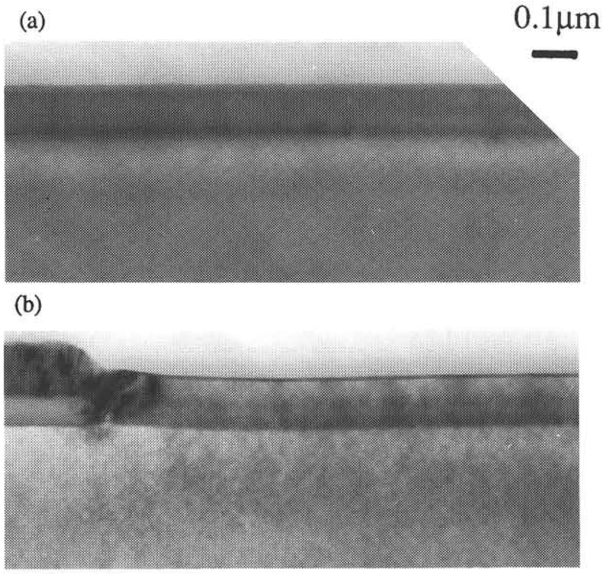

Fig.7 Cross-sectional TEM micrograph of $Si_{0.8}Ge_{0.2}$ film grown (a) in the center of the stripe opening and (b) in around SiO_2 pattern edge.

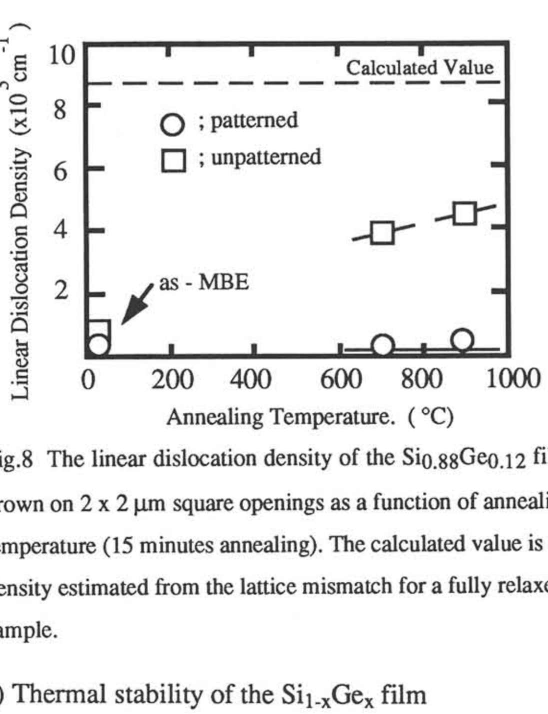

Fig.8 The linear dislocation density of the $Si_{0.88}Ge_{0.12}$ film grown on 2 x 2 μm square openings as a function of annealing temperature (15 minutes annealing). The calculated value is the density estimated from the lattice mismatch for a fully relaxed sample.

(2) Thermal stability of the $Si_{1-x}Ge_x$ film

For film grown on patterned substrates, the dislocation density can be reduced as mentioned above. Annealing experiments were carried out to check the thermal stability of the films. Figure 8 shows the relationship between the linear dislocation density of the $Si_{0.88}Ge_{0.12}$ film and the annealing temperature. The annealing was performed between 700 and 900 °C for 15 minutes. For growth on unpatterned substrates (Figure 8 (a)), linear misfit dislocation density was increased with annealing temperature. On the other hand, the density is not affected by annealing at any temperature in the case of growth on 2 x 2 μm^2 square SiO_2 opening (figure 8 (b)). This result implies that the film is thermally stable due to the relaxation of the strain at the SiO_2 pattern edge as mentioned above. A detailed study of the strain in the $Si_{1-x}Ge_x$ film is now underway.

4. SUMMARY

Limited area MBE growth, in which $Si_{1-x}Ge_x$ film is grown on a Si region surrounded by SiO_2, was studied. As the area of the SiO_2 opening decreased, the dislocation density reduced, and no dislocation was observed when the area was below 2.5 x 2.5 μm^2. This phenomenon is a result of the relaxation of the strain around the SiO_2 pattern edge as well as the limitation of the dislocation extension. Thermal stability of the $Si_{1-x}Ge_x$ film grown on patterned substrate can be improved remarkably.

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