Extended Abstracts of the 1992 International Conference on Solid State Devices and Materials, Tsukuba, 1992, pp. 647-649

Behavior of Misfit Dislocations in GaAs Layers Grown on Si at Low Temperature by Molecular Beam Epitaxy

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The behavior of misfit dislocations in GaAs layers grown on Si substrates is studied using optical interferometry and transmission electron microscopy. After the growth at 250℃ buffer layers with thickness from 0.05μm to 0.2μm are annealed at 500℃. The anisotropic residual strains are observed in the layers with buffer layer thickness below 0.1μm. With increasing the buffer layer thickness, the anisotropic strains become isotropic. These results indicate that the buffer layer thickness is an important factor to form the misfit dislocations in addition to the annealing temperature.

1 Introduction

The heteroepitaxial growth of GaAs on Si substrates has been studied because it will lead to the monolithical integration of GaAs devices with Si devices. In conventional growth at high temperatures, however, a large number of threading dislocations are induced during the cooling process after the growth by tensile stress which is caused by the difference in thermal expansion coefficients[1]. Therefore, the growth at low temperature such as migration-enhanced epitaxy[2] is very effective to reduce the threading dislocation density.

In addition to the threading dislocations, we should pay attention to the generation of misfit dislocations at the initial stage of the growth. The misfit dislocations are formed to relax the compressive stress in the epitaxial layers due to the lattice mismatch[3]. However, if the process temperature is low or GaAs layers are thin, the misfit dislocations are formed incompletely. The incomplete formation of the misfit dislocations results in the compressional residual stress and often brings many defects at the GaAs/Si interfaces. To grow the high quality GaAs layers on Si, it is important to understand the behavior of the misfit dislocations. In this work, we investigate the formation process of the misfit dislocations in GaAs layers grown at low temperature. In particular, the residual stress studied in the epitaxial layers with various thicknesses.

2. Experimental

GaAs layers on Si substrates were grown by conventional molecular beam epitaxy (MBE) method. Silicon substrates were misoriented by 3° off towards [011] direction. The Si substrates were cleaned by a HF solution before loading into a vacuum chamber. The growth sequence is shown in Fig.1. After heating at 800℃, GaAs buffer layers with the thickness from 0.05μm to 0.2μm were grown at 250℃. Subsequently, these samples were annealed at 500℃ for 5 minutes. Finally, 1.4μm-thick GaAs overlayers were grown at 300℃. The change of the strains during this growth is considered to be negligible as discussed later.
The annealing temperature dependence was also studied for the sample with 0.1μm buffer layer from 500℃ to 600℃.

The wafer warpage of the samples was measured using an optical interferometer. The residual strains in GaAs layers were estimated from the wafer warpage. We also carried out the transmission election microscope observation of the GaAs/Si interface.

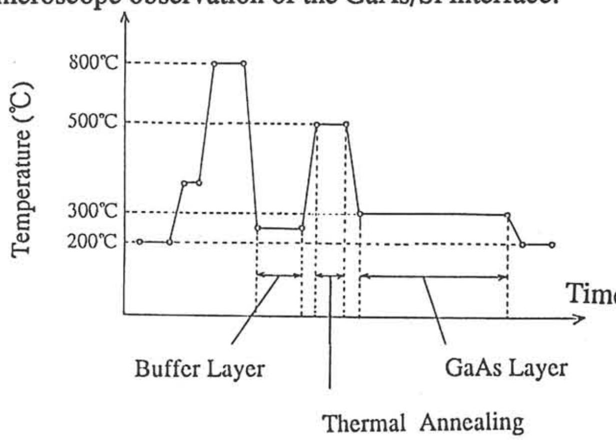

Fig.1 Growth sequence of GaAs/Si.

3. Results and Discussion

The residual strains in the GaAs layers grown at low temperature remarkably depend on the buffer layer thickness. Figure 2 shows the typical optical interference images of GaAs/Si with (a) 0.05μm and (b) 0.2μm, where 1 fringe corresponds to 2μm warpage. The sample with 0.2μm buffer layer exhibited concave deformation which is usually observed in the conventionally grown GaAs/Si, and the residual strain in the GaAs layers was tensile. On the other hand, extremely anisotropic strains were observed in the sample with 0.05μm buffer layer; the strain parallel to [0$\bar{1}$1] direction was tensile and that parallel to [011] was compressive. It is noted that the step edge of the misoriented Si substrate is parallel to [0$\bar{1}$1] direction.

Figure 3 shows the relation between the wafer warpage and the buffer layer thickness; the solid line represents the wafer warpage parallel to [011] and the broken line represents that to [0$\bar{1}$1]. Here positive wafer warpage is defined to correspond to the concave deformation as shown in Fig.3. With increasing the buffer layers thickness, the strain in [011] direction changed from compressive to tensile and the tensile strain in [0$\bar{1}$1] direction increased slightly. The strain became isotropic in the sample with 0.2μm buffer layer. The residual stress in the layer with 10 μm warpage is estimated to be $5x10^8$ (dyn/cm^2) by applying the simple model[4].

The behavior of the residual strains also depends on the annealing temperature. Wafer warpage of the samples with 0.1μm buffer layers is shown in Fig.4 as a function of the annealing temperature from 500 ℃ to 600℃. The annealing at 600℃ for 5 minutes resulted in the isotropic strains in the sample.

The complicated behavior of the residual strains may be related to the formation of the misfit dislocations during the annealing. The equilibrium model[5,6] is well used to explain the formation of misfit dislocations; the introduction of the misfit dislocation occurs in the layers with the thickness above the critical thickness. With increasing the layer thickness, the strain is gradually relaxed. The dependence of the strain on the buffer layer thickness qualitatively corresponds to the behavior predicted by the equilibrium model. In this model, it is assumed that the dislocations in the epitaxial layers can move fast to minimize the total energy. The temperature dependence of the dislocation velocity v is given by

$$v = B \exp(-U/kT)\, \sigma^{1.6} \qquad (1)$$

where U is the activation energy for dislocation motion, and σ is the stress. The assumption is

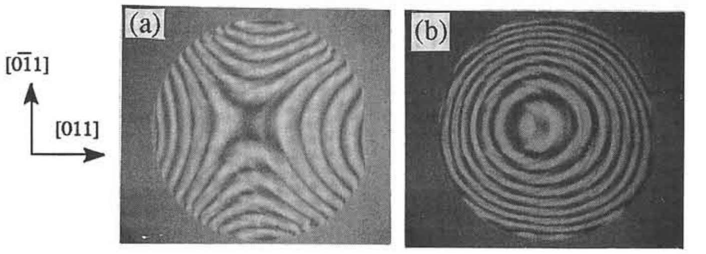

Fig.2 Optical interference images of GaAs/Si with (a) 0.05μm and (b) 0.2μm buffer layers. 1 fringe corresponds to 2μm warpage.

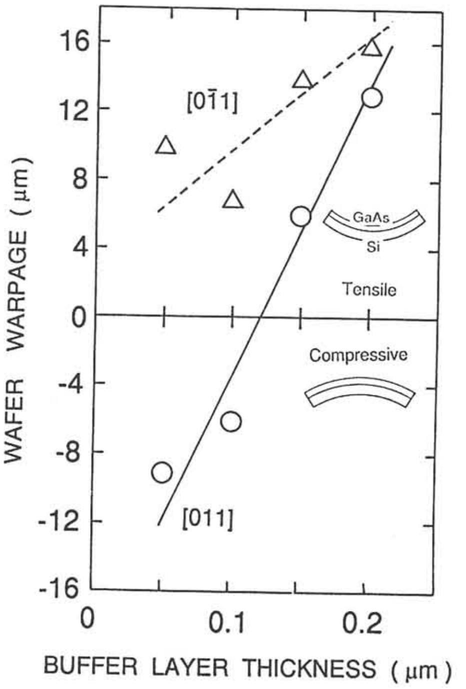

Fig.3 Wafer warpage of GaAs/Si with various buffer layer thicknesses annealed at 500℃ in [011] (○) and [0$\bar{1}$1] (△)derections.

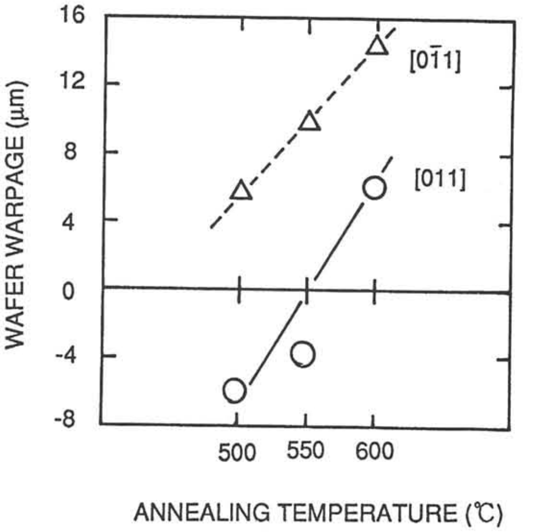

Fig.4 Wafer warpage of GaAs/Si with 0.1μm buffer layer thickness annealed from 500℃ to 600℃in [011] (○) and [0$\bar{1}$1] (△)derections.

satisfied if the substrate temperature is high. However, in the low temperature growth, the velocity of the dislocations is not so fast that the misfit dislocation formation is kinetically controlled by the motion of dislocations in the GaAs layers. For example, the activation energy of β dislocation in GaAs bulk crystal is 1.35eV[7]. The velocity at 300℃ is three orders of magnitude smaller than that at 500℃. Therefore, the motion during the overlayer growth at 300℃ can be negligible. The increase of the tensile strain in Fig.3 induced by the increase of the velocities of the dislocations. From the dependence of the residual strains on the buffer layer thickness in Fig.2, it is considered that the dislocation velocities in the epitaxial layers increase with the layer thickness.

Next, we discuss the anisotropy of the strains. The anisotropy of the velocities in the GaAs layers is not expected between [011] and [0$\bar{1}$1] directions, so that the observed anisotropic strain is caused by other factors. For the formation of the misfit dislocations, the nucleation and multiplication of the dislocations are important factors in addition to the motion in the epitaxial layers[3]. In the misoriented substrates used in the growth, the atomic steps parallel to [0$\bar{1}$1] exist on the substrates. Thus, these steps may play an important role in the dislocation nucleation or multiplication process. If the dislocation nucleation is enhanced by the atomic steps parallel to [0$\bar{1}$1] at the interface or the growing surface, more misfit dislocations in [011] may be formed, because their line vectors are parallel to the atomic steps. However, this prediction was not consistent with the experimental results; the anisotropic strains in Fig.2 revealed that more misfit dislocations in [011] direction were formed.

The transmission election microscopy (TEM) observation is very useful to study the misfit dislocations at the GaAs/Si interface[8]. We carried out the TEM observation of the samples with the 0.1μm buffer layer annealed at 500℃. From the number of the misfit dislocations at the interface, we calculated the residual strains as shown in Table 1, assuming that the lattice relaxation is caused by only the misfit dislocations[9]. Since the number of the misfit dislocations observed in [0$\bar{1}$1] is larger than that in [011], more lattice relaxation is occurred. This anisotropic behavior is qualitatively consistent with the results from the wafer warpage. However, the compressive strain calculated from the TEM observation is much larger than that from the wafer warpage. This result suggests that many dislocations which is not able to move to the interface exist in the epitaxial layers and that they also contribute to the lattice relaxation. To clarify the reason of the anisotropic strains, the misfit dislocations in the samples with various misoriented angles should be investigated.

Table1 Residual strains estimated from the wafer warpage and the number of misfit dislocations at the interface observed by TEM.

	warpage	TEM
[011](compressive)	-3.2×10^{-4}	-4.9×10^{-3}
[0$\bar{1}$1](tensile)	3.5×10^{-4}	0.9×10^{-4}

4 Summary

The behavior of the misfit dislocation is studied in the GaAs/Si epitaxial layers grown at low temperature. In addition to the annealing temperature, the buffer layer thickness influences the misfit dislocation formation. With increasing the buffer layer thickness, the anisotropic residual strains change to isotropic. The anisotropy may be related to the atomic steps at the growing surface or the interface. These results indicate that the buffer layer thickness is an important factor to improve the crystal quality of GaAs/Si.

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