Extended Abstracts of the 1992 International Conference on Solid State Devices and Materials, Tsukuba, 1992, pp. 641-643

Misorientation in GaAs on Si Grown by Migration-Enhanced Epitaxy

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The misorientation of GaAs grown on Si(100) by migration-enhanced epitaxy is investigated using x-ray diffraction. In addition to the well-known tilt misorientation of GaAs with respect to the Si substrate, almost all of the GaAs layers are found to exhibit a misorientation of rotation about the substrate surface normal. The misorientation systematically depends on the initial growth conditions such as the substrate off-orientation and the growth initiation. We propose a model, based on the relaxation of misfits perpendicular to the Si surface, that describes the observed tilt. Reducing unnecessary misorientation leads to better crystal quality even for thick (~4 μm) samples including strained-layer superlattices, which can provide a very low dislocation density. The surface etch-pit densities are 6.2×10^4 cm^{-2} for the thick sample with a rotation angle $\beta=2^o$, and 3.1×10^5 cm^{-2} for $\beta=12^o$, even though they are grown under the same conditions except for the initial growth conditions.

1. Introduction

The heteroepitaxial growth of GaAs on Si has attracted much attention in recent years because it is expected to play an important role in integrating Si- and GaAs-based device structures.[1] However, their different lattice constants and thermal expansion coefficients result in a high density of threading dislocations. Despite extensive efforts, it is still difficult to reduce the dislocation density of conventionally grown GaAs to less than 10^6 cm^{-2}. It was shown that most of the residual dislocations are created by thermal stress during cooling after growth, due to the difference in thermal expansion coefficients.[2] Migration-enhanced epitaxy (MEE)[3] is, thus, particularly suitable for producing low dislocation density layers, because it can grow high-quality homoepitaxial GaAs layers at growth temperatures as low as 300°C.[4-6]

Recently, it was demonstrated[6,7] that low-temperature MEE growth can produce GaAs/Si with very low dislocation density of 7×10^4 cm^{-2} with the aid of a low-temperature-grown strained-layer superlattice. This value is, indeed, comparable to that of GaAs substrates. However, one of the most important problems lies in the reproducibility. The dislocation densities are scattered from run to run over a range of an order of magnitude even with the same growth conditions. X-ray diffraction revealed that the scattering seems to be related to the GaAs misorientation, probably due to involuntary differences in growth initiation. Therefore, we intentionally varied the initial growth conditions and investigated the dependence of the misorientation on the conditions for MEE-grown samples by x-ray diffraction. It was found that the misorientation systematically depends on the initial growth conditions such as the substrate off-orientation angle and growth initiation.

2. Experimental

GaAs epitaxial growth was performed using MEE on 3" Si(100) substrates with off-orientations of 1, 1.7, 2, 3.4, and 4° toward the [011] direction. The details of the MEE growth and of the substrate preparation have been described elsewhere.[3,4] The growth sequence was as follows. Before growth, the Si substrate was heated at 1000°C for 15 min. This removes the surface oxide layer and forms a single-domain surface structure, thereby preventing the formation of antiphase domains. After the substrate was cooled to 300°C, a 100-nm-thick GaAs layer was grown as a buffer layer and the substrate was annealed for 15 min at 580°C. Then, growth was carried out at 300°C. The total film thickness was 1 μm for all samples unless otherwise specified.

For these samples, the x-ray diffraction was measured using a high-resolution double-crystal x-ray diffractometer. The diffraction rocking curves were recorded in the vicinity of the symmetric (400) peak. Some of the samples were also examined by transmission electron microscope (TEM) and etch-pit density observations. The TEM measurements were made using a JEOL400 at 100 and 200 kV. The etch-pit density was determined by Nomarski optical microscopy for samples etched in molten KOH for 4 min at 350°C.

3. Results and Discussions

As the azimuthal angle ω varies, the GaAs-Si peak separation $\Delta\theta$ shows the well-known sinusoidal variation as shown in Fig.1(a). This variation is caused by a tilt misorientation of the GaAs (100) with respect to the Si (100) surface. In this case, the angular separation $\Delta\theta$ can be expressed approximately as follows:

$$\Delta\theta=\Delta\theta_B+\alpha\cos(\omega) \quad (1),$$

where $\Delta\theta_B$ is the difference in Bragg angles and α is the tilt misorientation angle. However, this peak separation variation is rather an exceptional case than otherwise. Almost all of the GaAs/Si samples were found to exhibit an angular shift of β as shown in Fig.1 (b). This means that the GaAs has another misorientation with respect to the Si substrate. The shift β can be associated with the horizontal-axis rotation angle of GaAs about the substrate surface normal.

TEM observations substantiate this rotation. Moiré fringes can be used to observe the rotation misorientation. In a bicrystal system, when one of the crystals rotates, spaced contrast perpendicular to the Moiré lines can be seen as schematically shown in Fig.2(a). Figure 2(b) shows a plan-view TEM image near the GaAs/Si interface. It clearly exhibits such kind of the contrast in Moiré fringes.

Next, we discuss the relationship between the misorientation and the initial growth conditions. Figure 3 shows the relationship between the GaAs misorientation and the Si substrate off-orientation angle ϕ. The most important point is the reproducible dependence of the misorientation on the substrate off-orientation angle. The tilt α increases as ϕ increases. This tendency is similar to the result reported for conventional MBE-grown samples.[8] In contrast to growth on a just-oriented substrate, the lattice mismatch along the [100] direction, that is, the difference between d_0 and d in Fig.4, should be taken into consideration in case of growth on off substrates. It is likely that GaAs (100) plane inclines in order to absorb the difference and to relax the misfit as shown in Fig.4. Based on this hypothesis, simple geometrical consideration provides the relationship between α and ϕ,

$$\alpha=\sin^{-1}(d\sin\phi/d_0)-\phi \quad (2).$$

In Fig.3, the solid line is obtained from the calculation using this equation. The experimental results (shown as solid circles) coincide approximately with the calculation, although ignoring effect of the rotation leaves some ambiguity. The tilt generates dislocations at the step edges. The Burgers vector for the dislocations can be resolved into components vertical and horizontal to the Si surface. The tilt, therefore, contributes to the misfit relaxations along the [100] and [011] directions but not the $[0\bar{1}1]$ direction. The rotation must be responsible for the relaxation along the direction parallel to the step ($[0\bar{1}1]$), since the rotation will break Ga-Si or As-Si bonds along $[0\bar{1}1]$ as well as along [011]. The rotation β decreases as the substrate off-orientation angle increases, as shown in Fig.3 (open squares). This tendency could be explained as follows, although a quantitative explanation has not yet been determined. As ϕ increases, α increases and the lattice distortion along the orthogonal direction to the Si surface becomes larger. Suppose that the smaller distortion makes rotation more easy, then increasing ϕ will result in more restricted rotation. Therefore, as a rule, the samples with a larger α will exhibit a smaller β.

If the misfit relaxation takes place ideally, dislocations will systematically nucleate at the surface and will finally be absorbed at the interface. In such a case, there is no more need to rotate, so β will approach zero. On the other hand, α should be as low as possible, and is uniquely determined by the substrate off-orientation angle.

Only the growth conditions of the first GaAs monolayer on Si (2^o off) affects the misorientation. Growth initiation by Ga-supply first or simultaneous supply of Ga and As_4 with as low an As_4 flux as possible can reduce β (see Fig.5). This indicates that the relaxation can approach ideal by optimizing the growth initiation.

We also grew thicker layers (~4 μm) under the same growth conditions to show how the surface dislocation-density dispersion depends on the GaAs misorientation. Each of the layers has a strained-layer superlattice to minimize the surface dislocation density. The layer structure is described elsewhere.[6,7] Only the growth conditions of the first GaAs monolayer was varied. Therefore each sample has a different misorientation. The surface etch-pit densities were 6.2×10^4 cm^{-2} for the sample with $\beta=2^o$, and 3.1×10^5 cm^{-2} for $\beta=12^o$. The crystal quality of the sample with a lower β is better, even though both are grown under the same conditions. This result indicates that the optimizing the initial growth conditions can open the way for controlling the reproducibility of low dislocation density GaAs/Si.

4. Summary

In this study, we investigated the misorientation of MEE-grown GaAs on Si(100) by x-ray diffraction. In addition to the well-known tilt misorientation of GaAs, it was found that the MEE-grown GaAs/Si layers have a misorientation of rotation about the substrate surface normal. The misorientation systematically depends on the initial growth conditions. Reducing unnecessary misorientation leads to better crystal quality even if many GaAs layers are grown under the same conditions.

References

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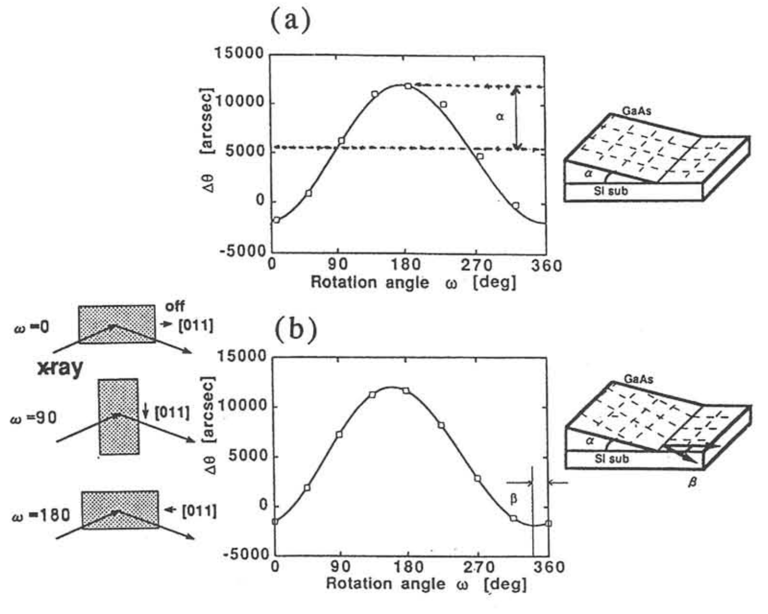

Fig. 1. GaAs-Si peak separation as a function of azimuthal angle ω.

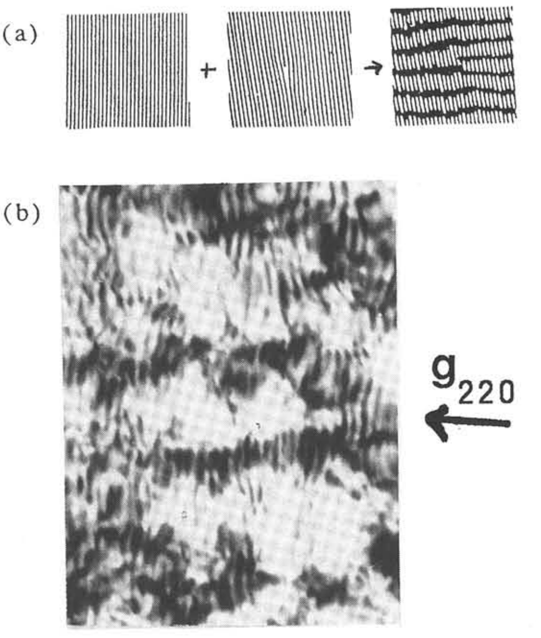

Fig. 2. (a) Schematic illustration of Moiré fringes in a bicrystal system when one of the crystals rotates.
(b) Plan-view TEM phtomicrographs of GaAs/Si interface.

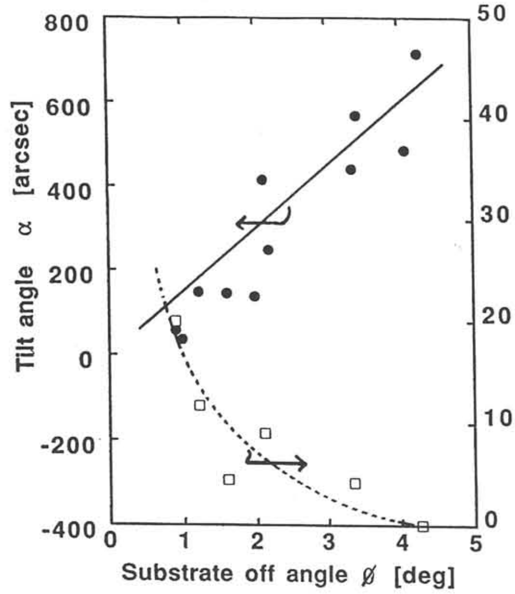

Fig. 3. Relationship between the GaAs misorientation and substrate off-orientation angle ϕ.

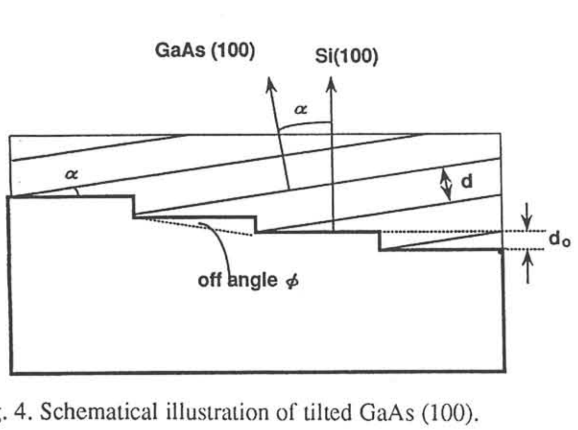

Fig. 4. Schematical illustration of tilted GaAs (100).

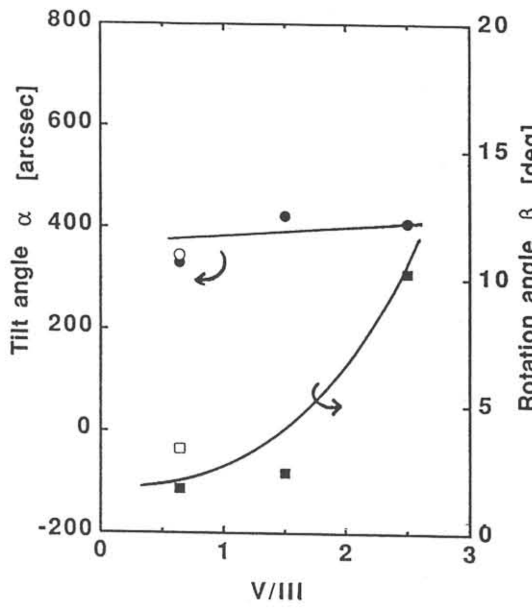

Fig. 5. Relationship between the GaAs misorientation and growth conditions of the first monolayer of GaAs on Si. Solid symbols indicate simultaneous supply of Ga and As_4, open symbols indicate Ga-first supply.