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In situ Synchrotron X-ray Observation of Anisotropy in the initial stage Lattice Relaxation Processes of GaAsSb/GaAs(001)

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Abstract

In a multijunction solar cell, lattice-mismatched materials are stacked; however, the propagation of threading dislocations to the active layer due to strain relaxation is a major drawback. To understand the mechanism of strain relaxation, the anisotropic formation of misfit dislocations (MDs) during GaAsSb growth on the GaAs(001) substrate was observed by in situ three-dimensional reciprocal lattice mapping using synchrotron X-rays. In the initial stage of the relaxation process, anisotropic generation of α- and β- MDs was observed. Therefore, we suggested that a high anisotropy in the initial stage is required to grow lattice-mismatched solar cells.

1. Introduction

To optimize the bandgap energy of III-V multijunction solar cells for the solar spectrum, lattice-mismatched layers are stacked on the substrate. However, in such lattice-mismatched systems, misfit dislocations (MDs) are formed at strained heterointerfaces, which in turn cause threading dislocations. Therefore, it is important to understand the strain relaxation mechanism to reduce such dislocations. There are two types of MDs depending on the crystal structure of the III–V semiconductors. For the III and V core atoms, MDs are called α- and β-MDs, and their line directions are [110] and $[1\bar{1}0]$, respectively. Recently, MD strain relaxation processes were observed via in situ measurements during the growth of InGaAs and GaAsSb on GaAs(001) [1-2]. These studies showed that the anisotropy of α- and β-MDs at the initial stage of lattice relaxation may affect the crystallinity after growth.

In this study, we focused on the satellite peaks near the Bragg diffraction peak that occur at the initial stage of lattice relaxation. The anisotropy of the relaxation process was analyzed in situ via three-dimensional reciprocal space mapping (3D-RSM) using synchrotron radiation X-rays during GaAsSb/GaAs(001) growth.

2. Experimental details

The experiments were performed at the 11XU beamline of the synchrotron radiation facility, SPring-8 in Japan, using a molecular beam epitaxy (MBE) system directly coupled to an X-ray diffractometer [1]. Three GaAsSb films were grown on GaAs(001) substrates at 520 °C, 540 °C, and 560 °C, respectively. The other growth conditions are summarized in Table I. During the growth of the films, real-time X-ray measurements were performed at the 004 diffraction point. The Sb composition was estimated as 5.9 %, 7.5 %, and 5.8 % via ex situ X-ray diffraction (XRD) measurements.

3. Results and discussion

A typical 3D-RSM around the 004 point is shown in Fig. 1. The growth temperature and film thickness were 540 °C and 71 nm, respectively, and a 004 Bragg peak of GaAsSb was observed below that of GaAs. In addition to this, satellite peaks [3] due to MDs were observed along the [110] and $[1\bar{1}0]$ directions, which represent the formation of α- and β-MDs, respectively.

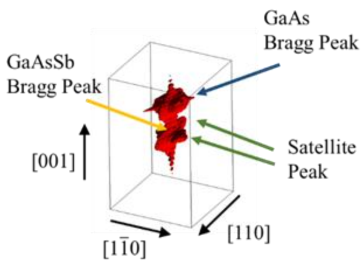

Fig.1 Typical 3D-RSM around 004 of GaAsSb grown on GaAs(001).

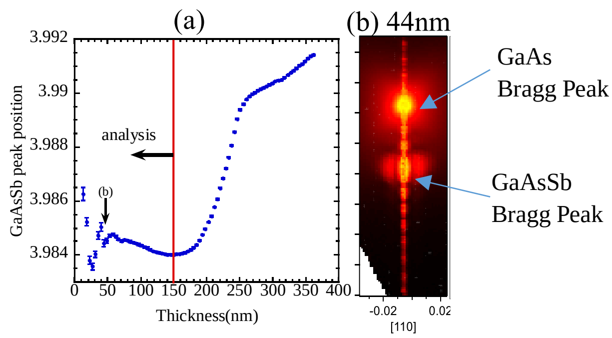

Fig. 2 (a) Variation of the positions of GaAsSb Bragg peaks with the GaAsSb film thickness. (b) Out of plane RSM of GaAsSb with a 44 nm thick film.

The evolution of the GaAsSb peak position along the [001] direction during growth is illustrated in Fig. 2(a) and 2D-RSM at a thickness of 44 nm is shown in Fig. 2(b). At 170 nm, the peak position begins to shift due to lattice relaxation and tends to saturate beyond 250 nm. Although peak shifts did not occur below 170 nm, satellite peaks were observed along the [110] direction, as shown in the RSM at 44 nm (Fig.2 (b)). This implies that α- and β-MDs were already formed below 170 nm. In other words, the anisotropic formation processes of MDs at an early stage of lattice relaxation can be observed by analyzing the satellite peaks.

In-plane RSMs around the GaAsSb Bragg peaks, taken from the 3D-RSMs observed during growth, are shown in Fig. 3. At 40 nm, satellite peaks were observed only along the [110] direction, whereas at 62 nm, they were observed along both [110] and $[1\bar{1}0]$. In addition, the peak intensity along [110] was higher than that of the other. This implies that α-MDs form at a lower thickness and their density is higher than that of the β-MDs at these thicknesses. Thus, the dislocation anisotropy was evaluated using the intensity of the satellite peak in each direction.

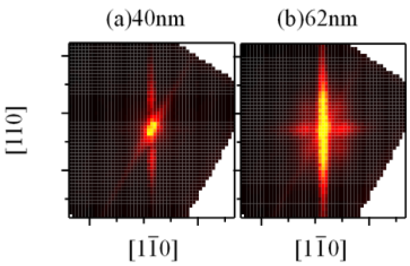

Fig. 3 In-plane RSMs of GaAsSb with film thickness of (a) 40 nm and (b) 62 nm. The growth temperature was 540 °C.

The evolution of the satellite peak intensity in each direction as a function of GaAsSb thickness grown at 540 °C is illustrated in Fig. 4. For the [110] direction, the slope changes at 42 nm, which implies that α MDs started to form at 42 nm. For the $[1\bar{1}0]$ direction, the β MDs started forming at 46 nm. (Hereafter, the formation thicknesses for α- and β-MDs are referred to as d_α and d_β, respectively.) In this film, the difference between d_α and d_β (d_β–d_α) was 4 nm. Moreover, at 120 nm, the intensity ratio along [110] to $[1\bar{1}0]$ (I_α/I_β) was 1.3. These results indicate that α-MDs occur at a film thickness of approximately 4 nm thinner than that in the case of β-MDs, and the density of α-MDs is approximately 1.3 times higher than that of β-MDs at 120 nm.

The observed d_α, d_β, and I_α/I_β at each growth temperature are summarized in Table I. In all the films, α-MDs were observed at a thickness lower than that in the case of β-MDs. No systematic correlation was observed between these parameters (d_α, d_β, and I_α/I_β) and the corresponding growth temperatures. However, a clear positive correlation was observed between (d_β–d_α) and I_α/I_β, as shown in Fig. 5. The anisotropy in MD density increases when (d_β–d_α) is high. This occurs because β-MDs are blocked by α-MDs, which are already formed and running freely. However, in the case of small (d_β–d_α), α and β MDs form and run simultaneously, and thus, get blocked by each other. Therefore, the anisotropy in MD density decreases. In our previously reported investigations [2], films with low (d_β–d_α) showed lower relaxation ratios compared to those with high (d_β–d_α) at 500 nm thickness. This indicates that thick films are required to release the strain caused by lattice mismatch. This further suggests that a high (d_β–d_α) is advantageous to grow lattice-mismatched solar cells.

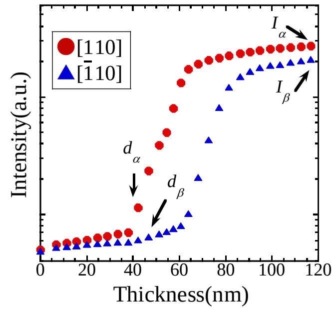

Fig. 4 Relationship between the film thickness of GaAsSb and the intensities of the satellite peaks along [110] and $[1\bar{1}0]$.

Table I Summary of the growth conditions, d_α, d_β and I_α/I_β

T_g (°C)	**520**	**540**	**560**
Sb composition(%)	5.9	7.5	5.8
Growth rate (ML/sec.)	0.11	0.09	0.09
d_α(nm)	56.7	39.7	42.2
d_β(nm)	62.4	48.4	46.6
d_β-d_α(nm)	5.7	8.7	4.4
I_α/I_β	2.0	3.5	1.3

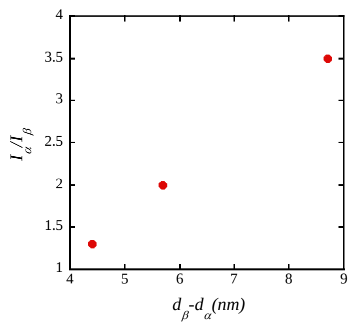

Fig. 5 Relationship between MDs generation film thickness difference and intensity ratio.

4. Conclusions

In this study, lattice relaxation anisotropy during GaAsSb/GaAs(001) growth at 520 °C, 540 °C, and 560 °C was analyzed using a 3D-RSM technique. In the initial stage of the relaxation process, anisotropic generation of α- and β-MDs was observed. Therefore, we suggested that high anisotropy in the initial stage is required to grow lattice-mismatched solar cells.

References

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