Journal of the Korean Crystal Growth and Crystal Technology
Vol. 12, No. 6 (2002) 299-303

Evaluation of crystallinity and defect on (100) ZnTe/GaAs grown by hot wall epitaxy

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(Received October 28, 2002)
(Accepted November 25, 2002)

Abstract The relationship of crystallinity between defects distribution with (100) ZnTe/GaAs using HWE growth was investigated by four crystal rocking curve (FCRC) and transmission electron microscopy (TEM). The thickness dependence of crystal quality in ZnTe epilayer was evaluated. The FWHM value shows a strong dependence on ZnTe epilayer thickness. For the films thinner than 6 μm, the FWHM value decreases very steeply as the thickness increases. For the films thicker than 6 μm, it becomes an almost constant value. At the thickness of 12 μm with the smallest value of 66 arcsec, which is the best value so far reported on ZnTe epilayers was obtained. Investigation into the nature and behavior of dislocations with film thickness in (100) ZnTe/(100)GaAs heterostructures grown by Hot Wall Epitaxy (HWE). This film defects range from interface to 0.7 μm thickness was high density, due to the large lattice mismatch and thermal expansion coefficients. The thickness of 0.7~1.8 μm was exists low defect density. In the thicker range than 1.8 μm thickness was measured hardly defects.

Key words TEM, HWE, Heteroepitaxy, HREM, XRD, ZnTe

1. Introduction

Zinc telluride is direct and wide band gap II-VI semiconductors (Eg = 2.26 eV at 300 K) crystallizing in the zinc-blende structure. For a single and multi-layer films of ZnTe is interesting materials with optoelectronic device such as light emitters in the pure green spectral region. This material is a promising because of its application for electro-optics, acusto-optics, green laser generation, and also as substrate material for II-VI laser diodes and as a photorefractive material for optical data processing [1].

To realize such devices, high quality epitaxial layer must be produced. For this purpose, molecular beam epitaxy (MBE) [2], metalorganic chemical vapor deposition (MOCVD) [3], and hot wall epitaxy (HWE) [4] have been employed. The lack of adequate bulk ZnTe substrates for homoepitaxy has made GaAs the substrate of choice in many cases because of its availability and high quality.

However, two problems exists in heterostructure involving ZnTe epilayer on GaAs substrate. One is lattice mismatch, the other is thermal expansion coefficients mismatch between ZnTe and GaAs. The lattice consists of ZnTe ($a_0 = 6.1037$ Å) and GaAs ($a_0 = 5.6533$ Å) at room temperature have a mismatch between ZnTe and GaAs of about 0.8 as defined by $f = (a_{ZnTe} - a_{GaAs})/a_{GaAs} \fallingdotseq 8\ \%$. On the other hand, thermal expansion coefficients mismatch of ZnTe and GaAs exists because there is a large difference in the thermal expansion coefficient between ZnTe ($8.3 \times 10^{-6}\ K^{-1}$) and GaAs ($5.8 \times 10^{-6}\ K^{-1}$).

The two problems are expect to give rise to be relaxed misfit dislocations at the film-substrate interface. In spite of this large difference, epitaxial layer has been successful. Therefore, understanding the mechanism of relaxation and nature of dislocations in ZnTe layers is important. Recently, ZnTe has received great interest because selective acceptor doping is expected to produce n-type materials that could yield p-n junctions in the heterostructure of CdTe-ZnTe, ZnSe-ZnTe [5, 6].

In this paper, we have investigated and discussed to the dependence on the film thickness with the film quality and distribution of defect by using XRD and TEM. Also we have employed cross-sectional transmission electron microscopy (XTEM) and high-resolution electron microscopy (HREM) to characterize the microstructure of the thin film of ZnTe grown by HWE directly onto (100) GaAs substrate. Film quality and interface structure observed by XTEM have been correlated with experimental growth parameters. Furthermore, it has been shown that film quality determined by four crystal X-ray diffraction data very well the quality determined by XTEM characterization. And we have investigated ZnTe films of different thickness, to determine the behavior of

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dislocations related to the lattice mismatch, thermal expansion coefficients mismatch and growth processes.

3. Experimental

The ZnTe epilayers were grown in a hot wall epitaxy (HWE) system and the experimental conditions for the growth of ZnTe layers has been in detailed elsewhere [7].

High resolution X-ray diffraction was measured with a Phillips. X'Pert-MRD 188/HR having a 3 kV Cu radiation source. The X-ray beam from a Cu tube is monochromated by the four reflections of a Bartels monochromator at the (220) face of perfect channel-cut germanium (Ge) single crystals. The resultant beam has a divergence of 12 arcseconds.

For TEM study, three specimens with different thickness (4.3, 12, 24 μm) were used. Thin specimens for TEM observation were prepared by mechanical polishing and ion milling. Low magnification was obtained by using JEM-2000EX of accelerating voltage of 200 kV, and then a HREM study was carried out by using JEM-ARM1250 with an accelerating voltage of 1250 kV and a point-to-point resolution of 0.1 nm.

2. Results and Discussion

High quality ZnTe epitaxial layers were grown on (001) GaAs substrates with HWE. The thickness dependence of the crystal quality and distribution of defects for ZnTe/GaAs grown under the optimum condition is discussed [7, 8].

Figure 1 shows the FWHM value of the four crystal rocking curves (FCRC) as a function of the thickness of the ZnTe epilayer. As shown Fig. 1, FWHM decrease rapidly as the thickness increases up to about 6 μm. It still decreases slowly to 12 μm thickness in epilayer is finally saturated with the best FWHM value. This result indicates that the crystallinity of the epilayer gets better at the 12 μm in epilayer thickness. A FWHM value from 12 μm of ZnTe epilayer is 66 arcsec, which is the best value so far reported on ZnTe epilayers [7], as shown in the inset. In order to clarify relationships between the crystallinity and distribution(kinds) of defect on the ZnTe epilayer of different thickness related to lattice mismatch and thermal expansion coefficient, we investigate the distribution of defect on ZnTe epilayer and GaAs substrate using TEM.

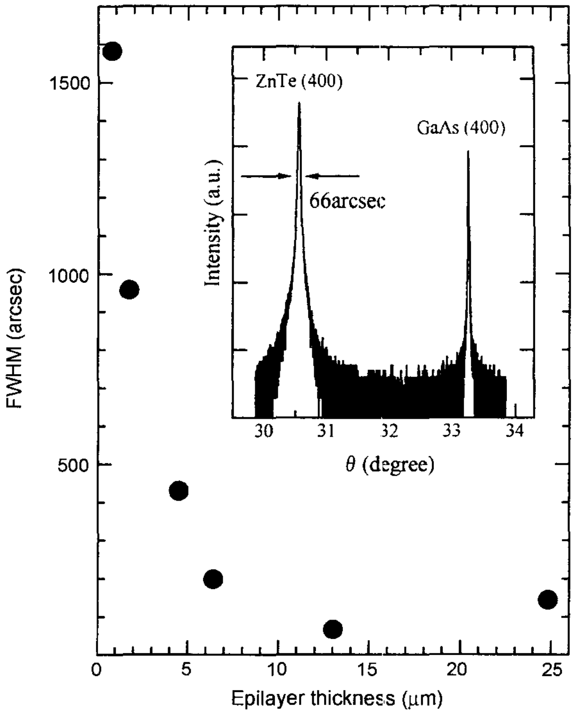


Fig. 1. The film thickness dependence of the FWHM. The insert is the four crystal rocking curves (FCRC) measured on the best of a good quality ZnTe epilayer.

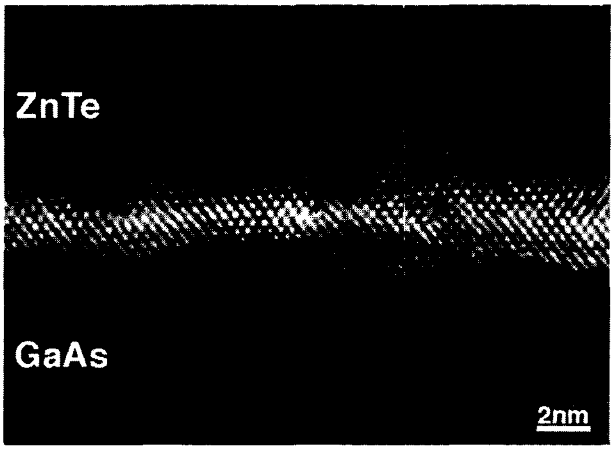
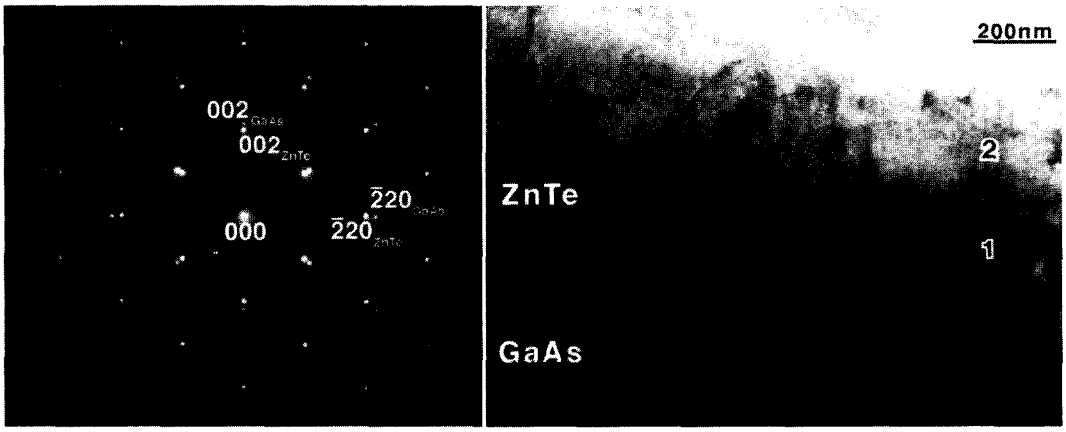


Fig. 2. HREM image of the ZnTe-GaAs interface projected along [110] direction.

A HREM image of interface between ZnTe epilayer and GaAs substrate obtained with the incident electron beams parallel to the [110] direction is shown in Fig. 2. This HREM image is representative of all the interfaces of epitaxial layers observed. The interface appears well defined without the presence of oxide or foreign layer over the area examined. Arrows in Fig. 2 indicate the misfit dislocations due to the lattice mismatch. An array of misfit dislocations is responsible for the relaxation of the elastic strain. In the Zinc-blend lattice, the Burgers



(a) Electron diffraction pattern (b) A bright-field image

Fig. 3. Cross-sectional transmission electron microscope image of a ZnTe layer on GaAs substrate.

vectors of misfit dislocations are parallel to the interface (screw and sessile edge dislocation) or are inclined 45° with respect to the interface (60° dislocation) [9-11]. A small fraction of misfit dislocation in the thinnest film were of the 60° dislocation, which are only half as effective in relaxing the strain as the edge type dislocation [9-11]. The 60° dislocations can interact with each other to produce the edge type after they glide in from the surface of the film along <111> planes [9, 10]. By previous reports [9], an average separation spacing of these misfit dislocation for all ZnTe epilayer grown by MBE is estimated to by about 5.4 nm, whereas equilibrium spacing is 5.9 nm for edge type dislocation. In our samples, these misfit dislocations, which are not periodic, for all ZnTe epilayer have an average separation of about 6.3 nm and run parallel to [110] direction in the interface plane. The measured spacing in our samples is not close to the equilibrium spacing. Consequently, these misfit dislocations in the interface plane are existent as three types of dislocation, which are screw, sessile edge and 60° dislocation [9].

Figure 3 shows electron diffraction pattern (a) and a bright-field image (b) of the 1.7 μm film on ZnTe-GaAs epilayer. Figure 3(a) shows a selected area diffraction (SAD) pattern of the ZnTe film/GaAs interface taken with the incident beam parallel to $[110]_{ZnTe/GaAs}$ directions. This SAD pattern indicates that the ZnTe film grown on GaAs substrate was single crystalline epilayer. Figure 3(b) can be divided into two distinct zones with regard to the dislocation density. A first region, about 700 nm extending from the interface towards the surface, indicated by an arrow has high dislocation density, whereas a second region has low dislocation density. These new dislocations were probably nucleated at the surface during growth and glide toward the interface along <111> planes driven by the residual elastic strain. The density of these new dislocations [9] increases with increasing the thickness of the epilayer and does not affect the density of misfit dislocations at the interface. The present observation is similar to the previous investigations of II-VI on III-V heterostructures with large lattice mismatch and thermal expansion coefficient. In Fig. 3, the new dislocations in 1.7 μm epilayer is exist from interface to surface and relax the remaining stress either themselves or by interacting with existing misfit dislocation. Because of the distribution of these new dislocations above interface, the FWHM of FCRC on 1.7 μm epilayer is wide than thicker epilayer.

Figure 4 shows a bright-field image of the 12 μm film that displays the dislocation structure above interface. Figure 4 can be divided into three distinct zones with regard to the dislocation structure. The first region being from the interface and extending about 720 nm towards the surface, a high density of these new dislocations is found. Contrary to the case of the 1.7 μm film, the first region wide of high dislocation density has decrease as shown Fig. 4. This is a very interesting feature of ZnTe epilayer with changes of the first region, the widely distribution of defect. This special phenomenon is expected that the epilayer strain for lattice mismatch and thermal expansion coefficient may be relaxed toward the substrate at optimum growth condition. This relaxation mechanism is yet investigated by reciprocal lattice mapping method using X-ray spectroscopy, nano-beam diffraction method and high-resolution electron microscopy with TEM. Consequently, the crystallinity for a 12 μm epilayer gets better than thinner epilayer such as 1.7 μm in thickness. In addition, the second region is very low

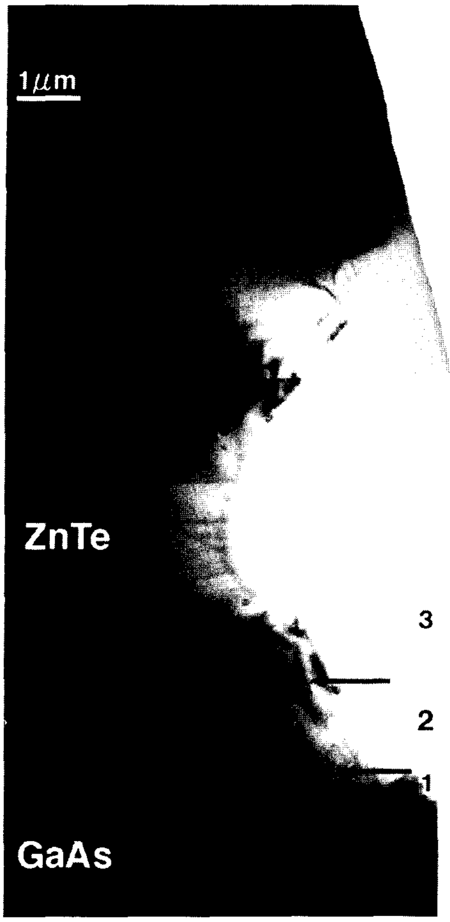


Fig. 4. Bright-field image of the 12 μm thick ZnTe film in cross section displaying three regions of dislocation structure.

density of dislocations from 720 nm to 1860 nm. This low density of dislocations is not surprising since the bulk of the lattice mismatch and thermal expansion coefficient has been accommodated by the dislocations near the interface. Figure 4 shows very important features concerning the behavior of dislocations in the ZnTe epilayer. The important feature occurs in the third region from 1.86 μm to the surface where no density of dislocation is present. It is evident that elastic strain for lattice mismatch and thermal expansion coefficient between ZnTe epilayer and GaAs substrate has been relaxed perfectly by these new dislocation [9] in the region from interface to 1.86 μm. The region of no dislocation density from 1.86 μm to the surface is perfectly the same with the bulk of ZnTe.

4. Conclusions

We have studied the relationship between crystallinity and defects distribution. The nature and the behavior of dislocations heterostructures growth were investigated on (100) ZnTe/GaAs by HWE using four crystal rocking curve (FCRC) and transmission electron microscopy (TEM). No evidence of oxide or foreign interface layer was found in these samples. The relaxation steps include the creation of dislocations away from the interface in the fashion that appear to be dependent on the epitaxial layer thickness. A correlation between the dynamic of dislocation generation and growth stage is presented. These results provide an experimental for theoretical models about the growth and misfit relaxation in high strained semiconductor hetero-structures. In our samples, the misfit dislocations, which are not periodic, for all ZnTe epilayer have an average separation of about 6.3 nm and run parallel to [110] direction in the interface plane. Consequently, these misfit dislocations in the interface plane are existent as three types of dislocation, which is screw, sessile edge and 60° dislocation. The perfect growth of ZnTe epilayer (12 μm sample) with similar to bulk was convinced that the elastic strain for lattice mismatch and thermal expansion coefficient between ZnTe epilayer and GaAs substrate has been relaxed perfectly by these new dislocation in the region from interface to 1.86 μm.

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