Structural properties and interfacial atomic arrangements in CdTe thin films grown on GaAs (211) B substrates

Y. S. RYU, T. W. KANG*
Quantum-Functional Semiconductor Research Center, Dongguk University, 3–26 Pil-dong, Chung-gu, Seoul 100-715, Korea
E-mail: twkang@dgu.ac.kr

T. W. KIM
Advanced Semiconductor Research Center, Division of Electrical and Computer Engineering, Hanyang University, 17 Haengdang-dong, Seongdong-gu, Seoul 133-791, Korea

CdTe thin films have attracted attention for their potential applications in solar energy conversion, gamma-ray detection, and electro-optic modulation due to their low thermal noise and large absorption coefficient [1–3]. The growth of CdTe epitaxial layers by molecular beam epitaxy (MBE) has been performed because CdTe epilayers can be used as buffer layers for the growth of $Hg_{1-x}Cd_xTe$ thin films [4–6]. However, since CdTe thin films grown on GaAs (211) B substrates have inherent problems with obtaining high-quality epitaxial growth due to their large lattice mismatch ($\Delta a/a = 14.6\%$), studies concerning the structural properties and the atomic arrangements of CdTe/GaAs (211) B strained heterointerfaces are very important for obtaining high-quality $Hg_{1-x}Cd_xTe$ epilayers [7–10]. Even though investigation of the microstructural properties and the atomic arrangements of the CdTe/GaAs (211) B heterointerfaces are necessary for obtaining high-quality $Hg_{1-x}Cd_xTe$ epilayers, systematic studies of the dependence of the structural properties and the interfacial atomic arrangement on the growth temperatures in CdTe thin films grown on GaAs (211) substrates have not been performed.

This communication reports the dependences of the structural properties and the interfacial atomic arrangement on the growth temperatures in CdTe thin films grown on GaAs (211) B substrates. X-ray diffraction (XRD) measurements were performed to investigate the structural and the surface properties of CdTe thin films grown on GaAs (211) B substrates at several temperatures by using molecular beam epitaxy. High-resolution transmission electron microscopy (HRTEM) measurements were performed in order to investigate the microstructural properties of the CdTe thin films, and possible interfacial atomic arrangements for the CdTe/GaAs (211) B heterointerfaces are presented on the basis of the experimental results.

The samples used in this study were grown on undoped semi-insulating GaAs (211) B orientated substrates by using MBE in a facility with a Riber 32P MBE chamber for the growth of the CdTe thin films. The GaAs substrates were degreased in warm trichloroethylene (TCE), etched in a mixture of H_2SO_4, H_2O_2, and H_2O (5:1:1) at 40 for 1 min, and rinsed in deionized water thoroughly. After the GaAs substrates had been thermally cleaned at 200 °C for 5 h in the introduction chamber, they were transferred into the growth chamber. Before CdTe growth, the GaAs substrates were thermally cleaned at 580 °C in a Te atmosphere for 5 min in the growth chamber. The 2 μm CdTe thin films were grown on the GaAs substrates at various temperatures.

Cross-sectional TEM specimens were prepared by forming a sandwich with epoxy, followed by mechanical cutting and polishing with diamond paper to an approximately 30 μm thickness, and then argon-ion milling at liquid-nitrogen temperature to electron transparency. High-resolution micrographs were obtained using a JEOL JEM 2000EX transmission electron microscope operating at 200 kV with a high-resolution pole piece.

The 50-keV RHEED patterns observed along the [100] direction of the CdTe/GaAs (211) B heterostructures grown at 300 show a mixture of spots and streaks, which is indicative of a two-dimensional growth process. The SEM images for the 2 μm CdTe layers grown at 300 show that the CdTe layers have mirror-like surfaces without any indication of pinholes and defects.

Fig. 1 shows XRD data for CdTe thin films grown on GaAs (211) B substrates at various temperatures of (a) 270 °C, (b) 300 °C, and (c) 340 °C. The peaks at 62.5° and 71° corresponding to CdTe (133) and CdTe (422), respectively, together with the peak at 84° related to GaAs (422), are dominant. When the growth temperature is 270 °C, the peak intensity at 62.5° corresponding to CdTe (133) is dominant, and the peak intensity at 71° related to CdTe (422) is very small. When the growth temperature increased to 300 °C, the intensity of the CdTe (133) peak is comparable with that of the CdTe (422) peak. However, when the growth temperature is 340 °C, the CdTe (133) peak almost disappears, and a broad CdTe (422) peak is dominant. Therefore, when the growth temperature is low, the orientation of the grown CdTe thin film is (133), but when the growth temperature is high, the orientation of the grown CdTe thin film is (211). These results indicate that the

* Author to whom all correspondence should be addressed.

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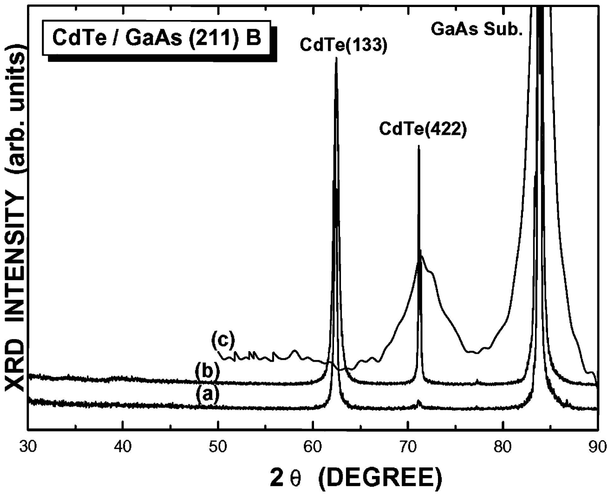

Figure 1 X-ray diffraction data for CdTe thin films grown on GaAs (211) B substrates at temperatures of (a) 270 °C, (b) 300 °C, and (c) 340 °C.

orientation of the grown CdTe epilayers depends significantly on the growth temperature. When CdTe (133) epilayers are grown on GaAs (211) B substrates, twinned crystals are formed in the epilayers [7]. The existence of the twinned crystals in the CdTe (133) epilayers reduces the lattice mismatch between the CdTe (133) epilayer and the GaAs (211) B substrate. However, when the thickness of the CdTe (133) epilayer is above a critical value, the twinned crystals existing in the CdTe (133) epilayer disappear due to the lattice mismatch. Since the lattice mismatch and the generation of dislocations in the CdTe (133) epilayer change with the interface bonding state, investigations of the atomic arrangements between CdTe (133) epilayers and GaAs (211) B substrates are necessary.

Fig. 2 shows a HRTEM image of a CdTe (133) epilayer grown on GaAs (211) B substrate at low temperature. The incident electron beam is parallel to the [011] GaAs axis and to the [011] GaAs interface [11]. The HRTEM image of the CdTe (133) epilayer indicates

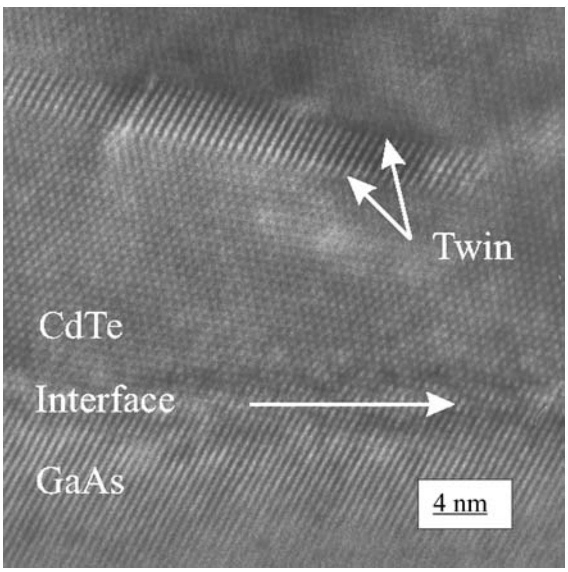

Figure 2 High-resolution transmission electron microscopy image of CdTe (133) epilayers grown on GaAs (211) B substrates at 270 °C.

the formation of twinned defects in the CdTe (133) thin film. The HRTEM image suggests that the tetrahedral bond network continues from the GaAs substrate to the CdTe epitaxial layer without severe distortion, in contrast to the $(\dot{2}\,\dot{1}\,\dot{1})$CdTe/$(\dot{2}\,\dot{1}\,\dot{1})$ GaAs interface [11].

Fig. 3 shows cross-sectional and top-view interfacial atomic arrangements of a CdTe (211) epilayer grown on a GaAs (211) B substrate at high temperature. When the growth temperature is high, since the migration length of the adatom is long enough, Cd atoms start to adsorb at the ledge area of the terrace. After Cd and Te atoms are absorbed at the step 1 region, denoted by the dotted line, the atoms are absorbed at step 2. Therefore, the orientation of the CdTe initial epilayer is the same as that of the (211) GaAs substrate, and the CdTe thin film forms a two-dimensional mode. Since the lattice mismatch between the CdTe (211) epilayer and the GaAs (211) B substrates is very large ($\Delta a/a = 14.6\%$), misfit dislocations or twin defects occur near the CdTe/GaAs heterointerface. Therefore, when the growth temperature is high, the crystallinity of the CdTe (211) thin film deteriorates, which is verified by the XRD result.

Fig. 4 shows cross-sectional and top-view interfacial atomic arrangements of a CdTe (133) epilayer grown on a GaAs (211) B substrate at low temperature. When the growth temperature is low, since the migration length of the adatom is small, Cd atoms, denoted by a dotted line, are absorbed on the 1 region in Fig. 4. The direction of the dangling bond Cd atoms is the same as that of the As atoms. The variation of the dangling bond direction of the Cd atom depends on the bonding position and originates from one dangling bond of the As-terminated GaAs (211) B surface. The second Cd atoms are absorbed on the 2 region in Fig. 4. The orientation of the CdTe epilayer changes from the (211) to the (133) direction due to the absorption of the second Cd atom on the GaAs (211) B surface. Therefore, the orientation of the CdTe (133) epilayer is attributed to the orientation of the GaAs (211) B substrates.

The distance between the bonding atoms of the CdTe (133) epilayer and those of the GaAs (211) B substrate is different due to the lattice mismatch. Since the lattice constant of the GaAs (211) B substrate is smaller than that of the CdTe (133) epilayer, a distance of 8 periods of the GaAs (211) B substrate is almost the same as that of 7 periods of the CdTe (133) epilayer grown above the critical thickness. Even though the buried region of the Te atoms forms twin defects [7], the twin defects no longer that exist near the CdTe (133)/GaAs (211) heterointerface. The elimination of the dislocations or twin defects relaxes the strain due to the lattice mismatch, so a CdTe (133) epilayer with high quality can be obtained, as shown in Fig. 5.

In summary, the results of XRD measurements on CdTe thin films on GaAs (211) B substrates showed that the structural properties of the CdTe epilayers depend significantly dependent on the growth temperature. The HRTEM image showed the formation of twinned defects in the CdTe (133) thin film. The interfacial atomic arrangements of the CdTe (211) and the CdTe (133) epilayers grown on GaAs (211) B substrates

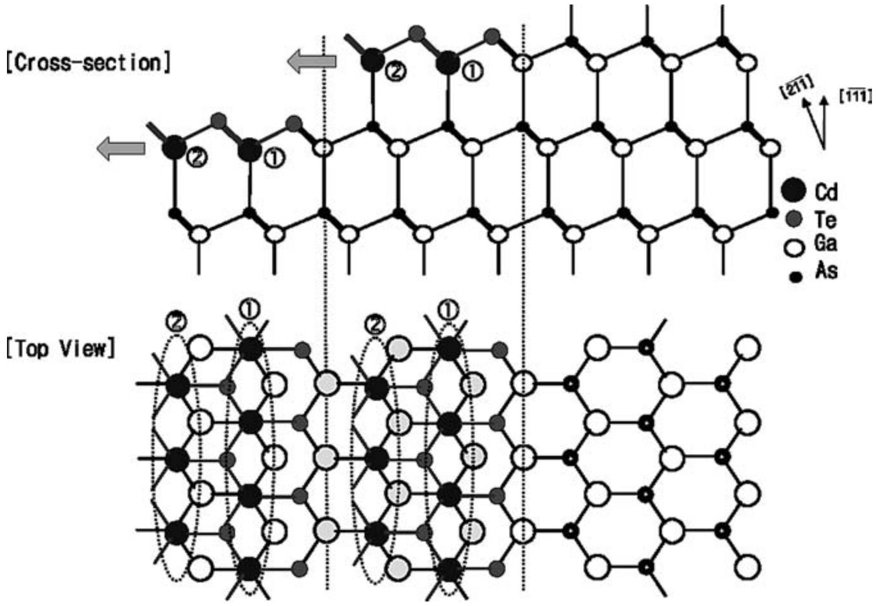

Figure 3 Interfacial atomic arrangement of CdTe (211) epilayers grown on GaAs (211) B substrates at high temperature.

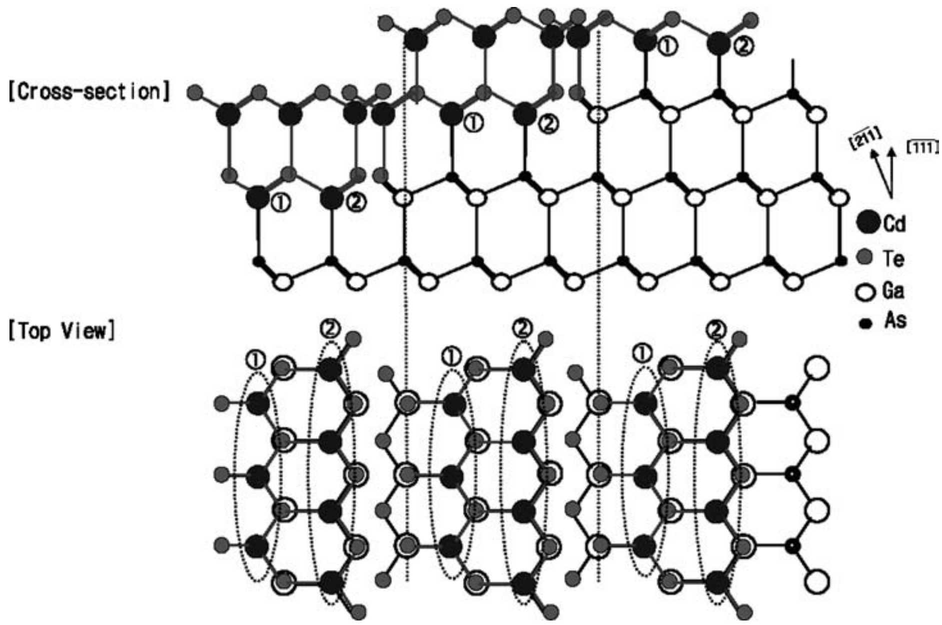

Figure 4 Interfacial atomic arrangement of CdTe (133) epilayers grown on GaAs (211) B substrates at low temperature.

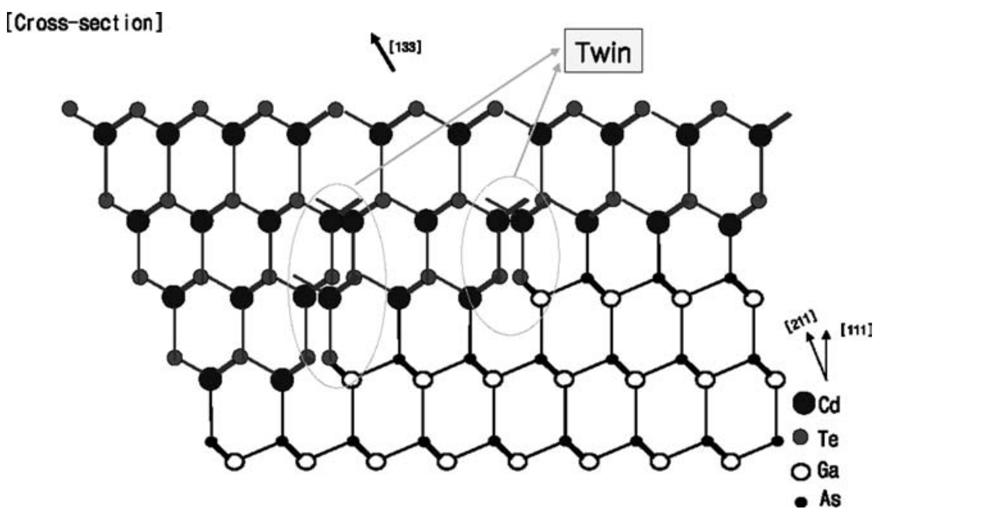

Figure 5 Interfacial atomic arrangement of CdTe (133) epilayers with twin defects grown on GaAs (211) B substrates at low temperature.

at low and high temperatures have been presented on the basis of the experimental results. These present observations can help improve understanding of the interfacial atomic arrangements of CdTe epilayers grown on GaAs (211) B substrates.

Acknowledgment

This work was supported by the Korea Science and Engineering Foundation through the Quantum-functional Semiconductor Research Center at Dongguk University.

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Received 23 September
and accepted 17 November 2004