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CHARACTERISTICS OF MOCVD-GROWN HIGH-QUALITY CDTE LAYERS ON GAAS SUBSTRATES

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CdTe epitaxial layers are grown successfully on a (100)-GaAs substrate by metalorganic chemical vapor deposition (MOCVD) using dimethylcadmium (DMCd) and diethyltelluride (DETe) as alkyl sources. The CdTe epilayers grown between 365°C and 380°C possess the best surface morphology. DETe is used as the controlling species of this growth system. Typical growth rates are varied from 2.5μm/hr to 5.3μm/hr. Low-temperature (12K) photoluminscence (PL) measurements reveal that 380°C is the best growth temperature and the full width at half maximum (FWHM) of the dominated peak is about 1.583eV by the bound-exciton emission of 9.38meV. The double crystal X-ray rocking curves (DCRC) indicate that the FWHM decreases while increasing the epilayer thickness and approaches a stable value about 80 arc sec under the growth rate of 5.2μm/hr, the growth temperature of 380°C and the DETe/DMCd concentration ratio of 1.7. The value of 80 arc sec in FWHM is the smallest one ever reported to date.

INTRODUCTION

CdTe is a large bandgap, versatile II-VI compound semiconductor known for its wide use in infrared detectors[1], γ-ray nuclear detectors[2] and solar cells[3]. Because of its small lattice mismatch and the inherent high resistivity with $Hg_xCd_{1-x}Te$, CdTe is used as a substrate in preparing $Hg_xCd_{1-x}Te$ infrared detectors. However, the CdTe substrate material contains microscopic crystal defect such as subgrain boundaries and twins, which degrade the performance[4] of infrared detectors made on the wafers containing such defects. Moreover, a large and high quality $Hg_xCd_{1-x}Te$ wafer is the suitable candidate for the next generation of two-dimensional infrared detector arrays. Therefore, the selection of alternative substrates, such as Si[5], InSb[6], GaAs[7] and sapphire[8], is useful for growing CdTe thin film as a buffer layer to reach this purpose. Among these substrates mentioned above, GaAs is the most popular one due to its high resistivity and ease of

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compatibility with high-speed III-V semiconductor devices. It also has been proved that high-quality CdTe epilayers could be grown on GaAs substrates, in spite of the large mismatch (14.6%) between them.

To date, several methods including pulse laser evaporation (PLE)[9], laser-assisted deposition and annealing (LADA)[10], photo-assisted molecular beam epitaxy (PAMBE)[11], hot-wall epitaxy (HWE)[12], and metalorganic chemical vapor deposition (MOCVD)[13] have been reported on the preparation of CdTe epitaxial layers. In the present work, under the consideration of easy control, lower growth temperature, and high quality of in-situ growth of $Hg_xCd_{1-x}Te$, a promising low temperature MOCVD method is adopted for growing CdTe buffer layer. Experimental measurements including surface morphology, film growth rate, X-ray diffraction, PL, and DCRC properties are investigated to analyze the film quality.

EXPERIMENTAL

The CdTe epilayers were grown at approximately atmospheric pressure in a rf-heated cold wall vertical reactor. Fig. 1 schematically shows an experimental apparatus. DETe and DMCd were used as source materials. They were separately kept at 20°C and 10°C in different temperature reservoirs for supplying the equilibrium vapor pressure of 7.1 torr and 16.8 torr, respectively. By using the mass flow controller, the amount of reactants put into reactor could be precisely adjusted. Palladium-diffused ultra-pure hydrogen was used as carrier gas and the total gas kept at 1.4SLM. The susceptor was rotated at 60 rpm to get the uniform epilayers. The waste gases at the outlet of the growth chamber were passed through a resistance-heated furnace held at 800°C, an activated carbon cell, and a burn-off unit to eliminate the harmful residual metal alkyls.

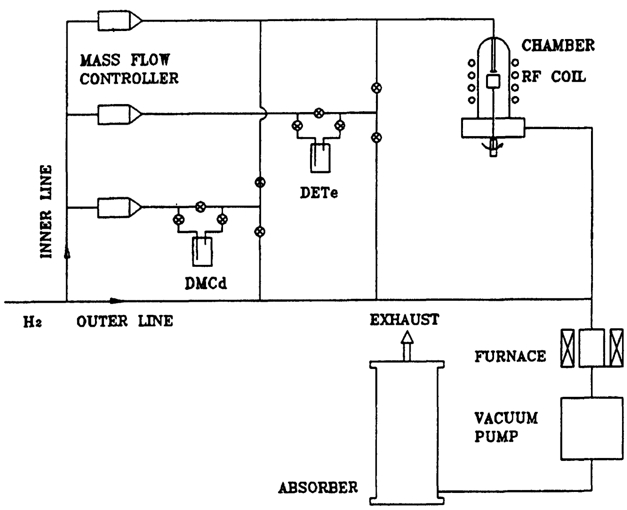

FIGURE 1 Schematical experimental apparatus.

After degreasing, the GaAs substrate was etched by H_2SO_4 for 2–3 minutes and then loaded into the reactor at a growth temperature of 380°C. In preliminary experiments, source gases with the same DETe/DMCd ratio of 1.0 were ejected from a quartz tube and then modulated by the different temperatures. After selecting the suitable growth temperature by a PL measurement, different DETe/DMCd ratios were used to find the best growth condition.

The surface morphology and the thickness of CdTe epilayers grown on GaAs substrates were examined by using an optical microscope. To evaluate the CdTe film crystalline condition, we measured the X-ray diffraction of (400) reflection with a spot size of 2mm × 2mm. Low temperature (12K) PL measurements were carried out with a 25mW argon laser source (5145Å). Finally, DCRC were checked to investigate the CdTe film quality.

RESULTS AND DISCUSSION

Surface morphology

The photomicrographs of CdTe epilayers grown on (100)-GaAs at 335°C, 350°C, 365°C, 380°C, and 395°C with equal amount of DETe and DMCd are shown respectively in Fig. 2. It has been reported that the existence of an oxide layer on the GaAs surface would lead to 3D growth for (100)-CdTe epilayers and form pyramids[14]. In Fig. 2, we find that the surface morphology of CdTe epilayers are strongly dependent on the growth temperature. The volume of pyramids are larger as the growth temperature increases and the best morphology is observed at 380°C. At 380°C, the pyramids are nearly the same and arrange in order. Below 365°C, the epilayer shows a smooth surface with only a few pyramids due to the lack of surface kinetics for the deposited molecules. For growth temperature above 395°C, a rugged and different volume of pyramidal surface is obtained owing to the escaping of Cd or Te atoms from the deposited surface at higher temperature.

Growth rate

In an MOCVD growth processes, the epilayer growth rate plays an important role on understanding the growth mechanism and predicting film quality. Fig. 3 shows the relationship between growth rates and 9.8×10^{-4}mole% DETe/DMCd concentrations. The growth rates almost increase linearly with temperature between 335°C and 380°C and approach a maximum growth rate of 4μm/hr. In this temperature range, the growth rates are controlled by the reaction kinetics and the reaction activation energy is above 21.3Kcal/mole by calculating the Arrhenius equation. About 380°C, the growth rates fall off gradually. The decrease of growth rate at higher temperature in this work is attributed to the increased tendency of gas phase dissociation of metal alkyls[15].

To examine whether the growth of a CdTe epilayer is reached to the mass transport limit or not, the test would be done by keeping the DETe/DMCd concentration ratio at a constant value of 1.0 and the growth temperature at 380°C. The result is shown in Fig. 4. Initially, the growth rate increases linearly with the total concentration of metal alkyls. Above 2.86×10^{-3}mole% concentration, the growth rate decreases gradually. This indicates that the total concentration of metal alkyls reaches that of transport-limited condition. Because the films tend to degrade at a total concentration of 3.42×10^{-3}mole%, we therefore selected the value of 2.86 $\times 10^{-3}$mole% as the total concentration of metal alkyls in this experiment.

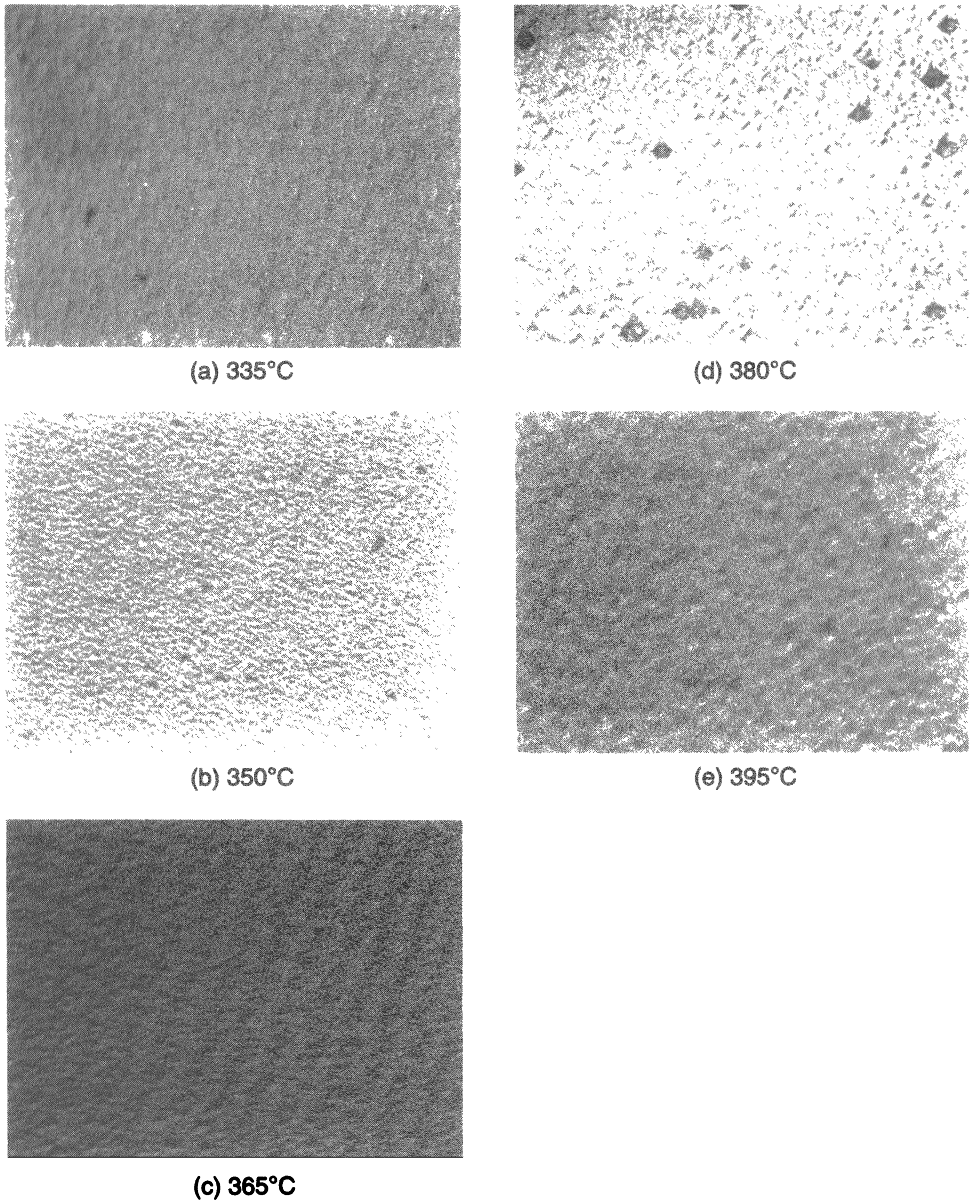

FIGURE 2 Morphology of CdTe film on (100) GaAs substrate; (a) 335°C, (b) 350°C, (c) 365°C, (d) 380°C, (e) 395°C, where the concentration of DCMd is $9.8*10^{-4}$ mole% and the DETe/DMCd ratio is equal to 1.0.

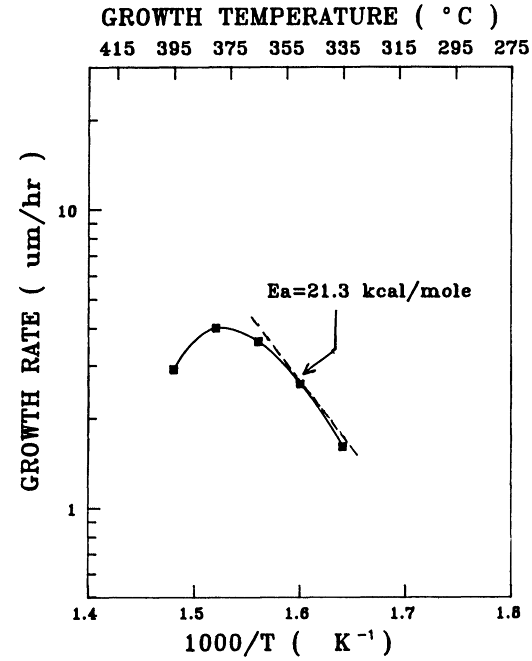

FIGURE 3 Variation of the growth rate as a function of growth temperature, where the concentration of DMCd is $9.8*10^{-4}$ mole% and the DETe/DMCd ratio is equal to 1.0.

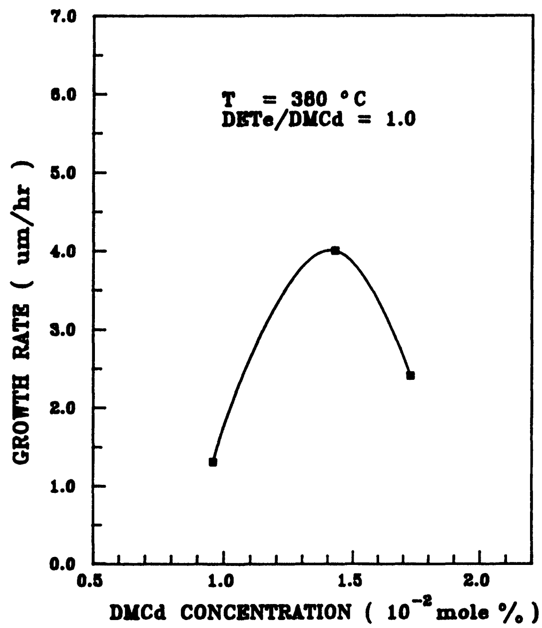

FIGURE 4 Variation of the growth rate at 380°C as a function of the total alkyl concentrations, where the concentration of DMCd is $9.8*10^{-4}$ mole% and the DETe/DMCd ratio is equal to 1.0.

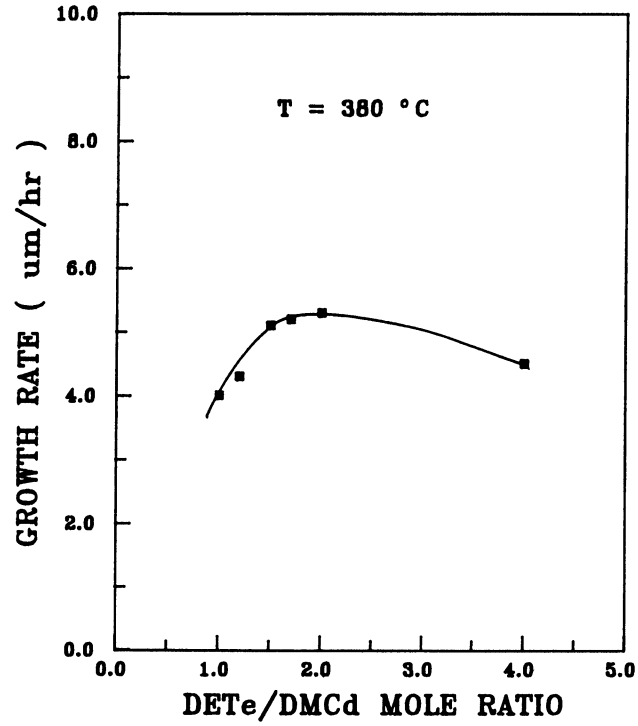

FIGURE 5 Variation of the growth rate at 380°C as a function of the DETe/DMCd ratio, where the concentration of DMCd is $9.8*10^{-4}$ mole% and the DETe/DMCd ratio is equal to 1.0.

To find out the effect of DETe/DMCd ratio versus growth rate, a series of experiments were carried out at 380°C. Here, we modulated the DETe concentration by fixing DMCd concentration and the result is shown in Fig. 5. Basically, the maximum growth rate occurs at the ratio of 1.5 ~ 2.0. Below the ratio of 1.5, the growth rate decreases. It is evident that DETe is the rate-controlling species during CdTe epitaxial growth. Above the ratio of 2.0, the growth rate also decreases. The reason is that the decomposition efficiency of the excess DETe alone is small at 380°C when the gas phase molecules are dominated by DETe[16]. Besides, there are the least defects on the top of pyramids in the range of 1.5 ~ 2.0.

X-ray diffraction (XRD) analysis

To examine the orientation and crystallization of CdTe epilayers, XRD analysis is used and diffraction patterns are shown in Fig. 6. Three diffraction peaks observed at $2\theta = 27.65°$, 56.95° and 66.1° under three temperature (350°C, 365°C, and 380°C) belong to (111)-GaAs, (400)-CdTe, and (400)-GaAs, respectively. It means that the CdTe epilayers are single crystal in (100) orientation. For the three deposition temperatures examined, no correlation between film orientation and growth temperature is evident. Similarly, there is no apparent relation between growth rate and film orientation when the growth rate varies from 2.6μm/hr to 4.0μm/hr.

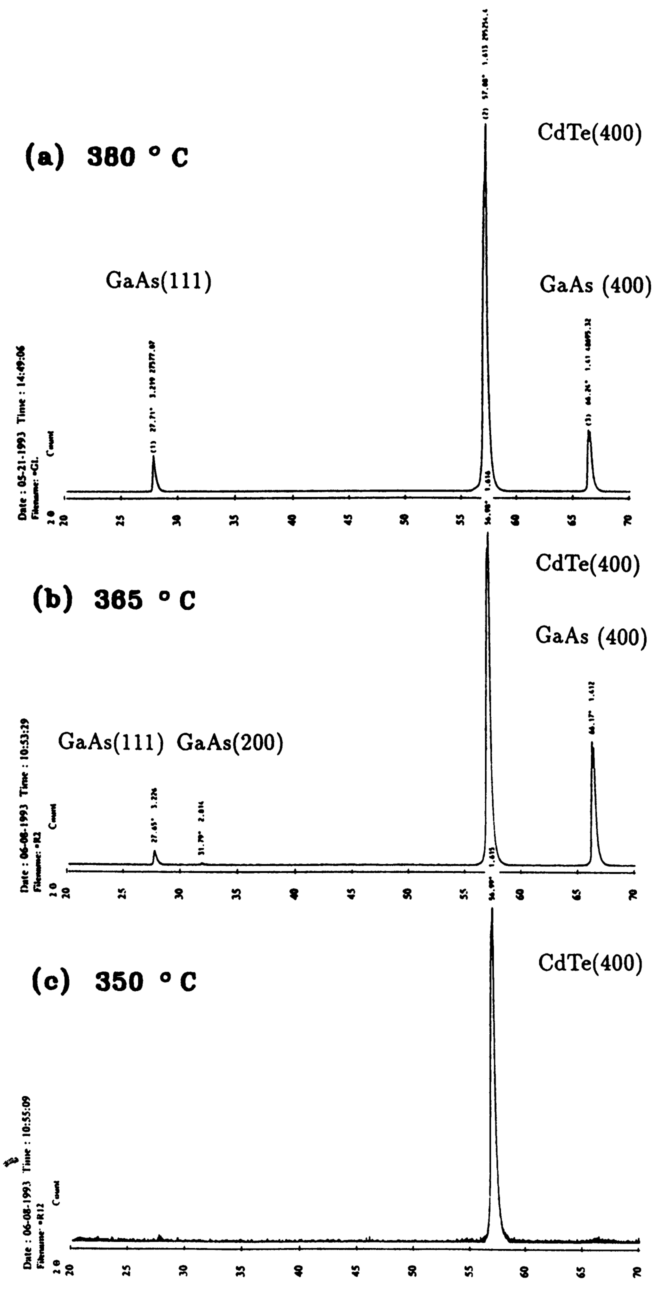

FIGURE 6 XRD patterns of CdTe epitaxial layers on GaAs substrate at (a) 350°C, (b) 365°C, (c) 380°C, where the concentration of DMCd is $9.8*10^{-4}$ mole% and the DETe/DMCd ratio is equal to 1.0.

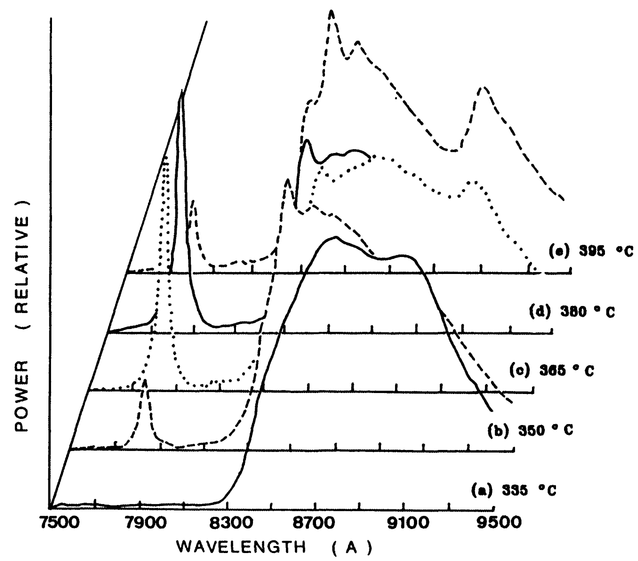

FIGURE 7 Low-temperature (12k) photoluminescence spectra of CdTe epilayers grown on GaAs substrate at (a) 335°C, (b) 350°C, (c) 365°C, (d) 380°C, (e) 395°C, where the concentration of DMCd is $9.8*10^{-4}$ mole% and the DETe/DMCd ratio is equal to 1.0.

Optical properties

The optical properties of CdTe epilayers grown at different temperatures with equal amount of DETe and DMCd are characterized by a 5145Å argon laser with output power of 25mW under 12K. Fig. 7 shows the PL spectra of CdTe layers grown on GaAs substrates at different temperatures. A relative sharp peak at about 7820Å due to the bound exciton emission[17] and a broad peak at long wavelength of 8500Å due to the so-called defect luminescence[18] are observed. They also can be seen from the ratio of exciton intensity (I_{exc} = 1.583eV) to the defect intensity (I_{def} = 1.463eV) shown in Fig. 8 which indicates that the best growth temperature appears at 380°C. Simultaneously, Fig. 9 shows the FWHM of dominated peak at different temperatures and the minimum value of 9.38eV is obtained at 380°C.

DCRC analysis

In this section, a DCRC analysis is used with a scan speed of 0.2mm/sec to identify the CdTe crystal quality. Fig. 10 shows the FWHM of the (400)-CdTe bragg reflex from (100)-CdTe/(100)-GaAs as a function of the CdTe thickness. A decrease of FWHM with increasing layer thickness is observed. Since the width of the X-ray rocking curve is sensitive to the extended crystal defects (e.g., dislocation lines) in the epilayer, thus, the data in Fig. 10 indicate a decreased density of extended defects with increasing epilayer thickness. Transmission electron microscopy (TEM) investigation of (100)- CdTe/(100)-GaAs has shown a region (~0.1μm) of very high dislocation density close to the CdTe/GaAs interface forming a regular dislocation network and a decreasing dislocation density with increasing distance

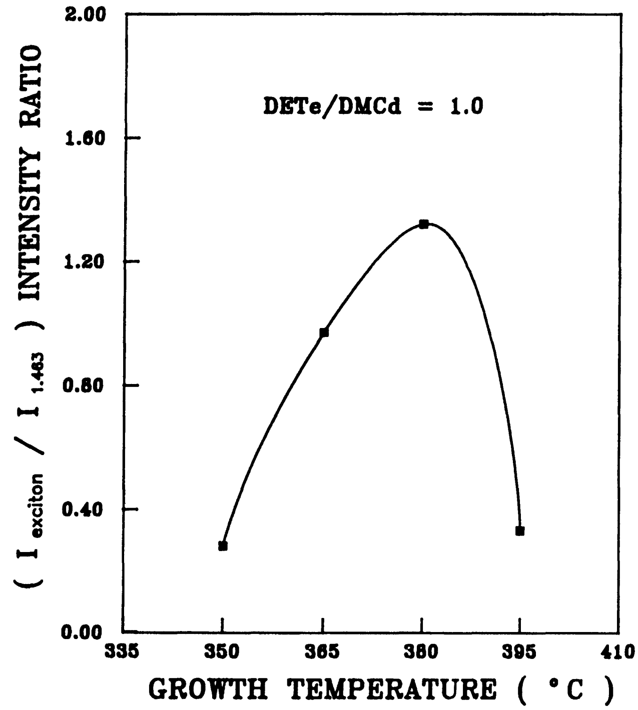

FIGURE 8 Intensity ratio of the bound-exciton emission line at 1.583 ev to the deep-level emission at 1.463 ev in CdTe prepared at different temperature, where the concentration of DMCd is $9.8*10^{-4}$ mole% and the DETe/DMCd ratio is equal to 1.0.

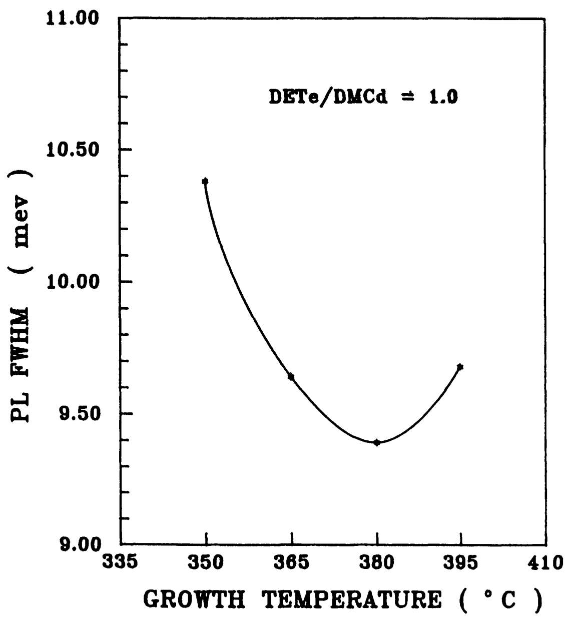

FIGURE 9 The FWHM of the bound-exciton emission line at 1.583 ev in CdTe samples prepared at different temperatures, where the concentration of DMCd is $9.8*10^{-4}$ mole% and the DETe/DMCd ratio is equal to 1.0.

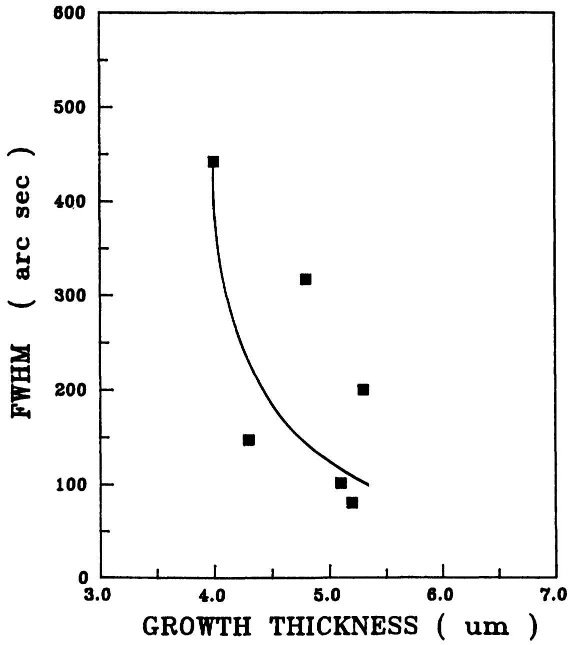

FIGURE 10 The width of (400) rocking curves, CdTe FWHM, versus the CdTe epilayer thickness, d, obtained from (100) oriented CdTe on (100) GaAs.

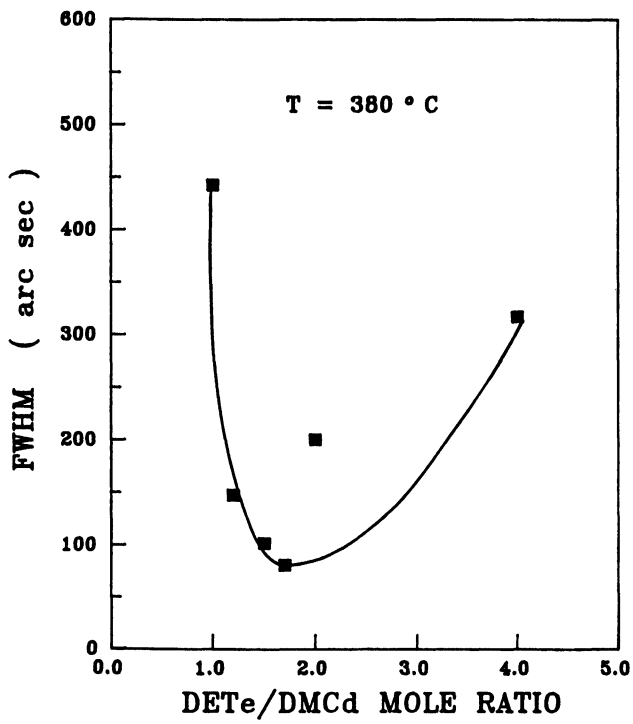

FIGURE 11 Variation of the FWHM of rocking curves at 380°C as a function of the DETe/DMCd ratio, where the concentration of DMCd is $9.8*10^{-4}$ mole%.

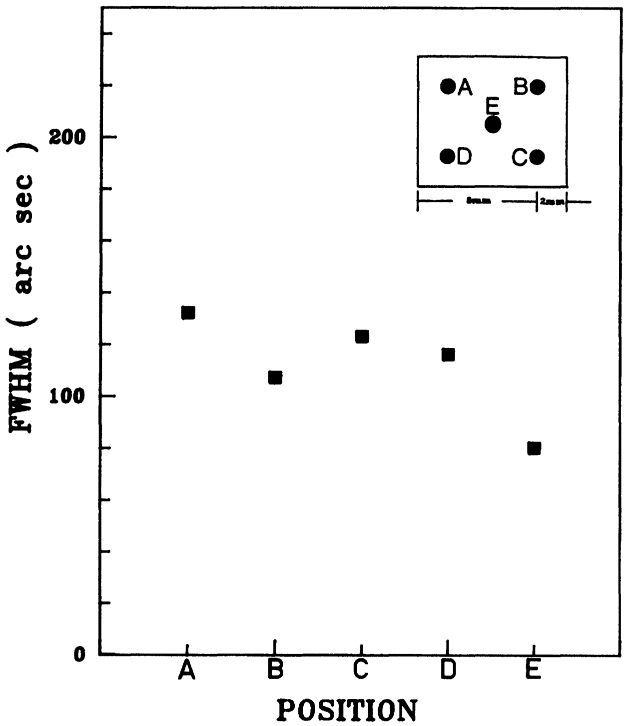

FIGURE 12 The experiment for examining the quality uniformity of CdTe epilayer grown at 380°C and DETe/DMCd ratio of 1.7.

from the interface. Fig. 11 shows the relation of FWHM with different DETe/DMCd concentration ratios in 380°C. It is found that the minimum value is up to 80 arc sec when the concentration ratio is 1.7.

For different positions in 10mm × 10mm CdTe epilayers, a rocking curve analysis is tested and the result is shown in Fig. 12. We find that the FWHMs of the rocking curves are changed from 80 to 130 arc sec when the tested positions are moved from the center to the outside GaAs substrate. It may have resulted from the non-uniform distribution MO gas through the surface of the GaAs substrate. By adding the flow of hydrogen, it will make the MO distribution much more flatter.

CONCLUSIONS

High quality (100)-CdTe epilayers have been successfully grown on (100)-GaAs by the MOCVD method with DETe and DMCd as source materials. The activation growth energy in the reaction-limited growth region is 21.3Kcal/mole and the DETe is the key element in controlling growth rate. Basically, the growth temperature controls the volume of pyramids by supplying enough surface kinetics. The modulation of DETe/DMCd concentration ratio also can decrease the density of defects. From the low temperature PL measurement, it is found that 380°C is the most suitable temperature for CdTe growth. Besides, the DCRC experimental results also show that the FWHM of CdTe films even at higher growth rate (above 5.1μm/hr) is low to 80 arc sec, which is the best value ever reported.

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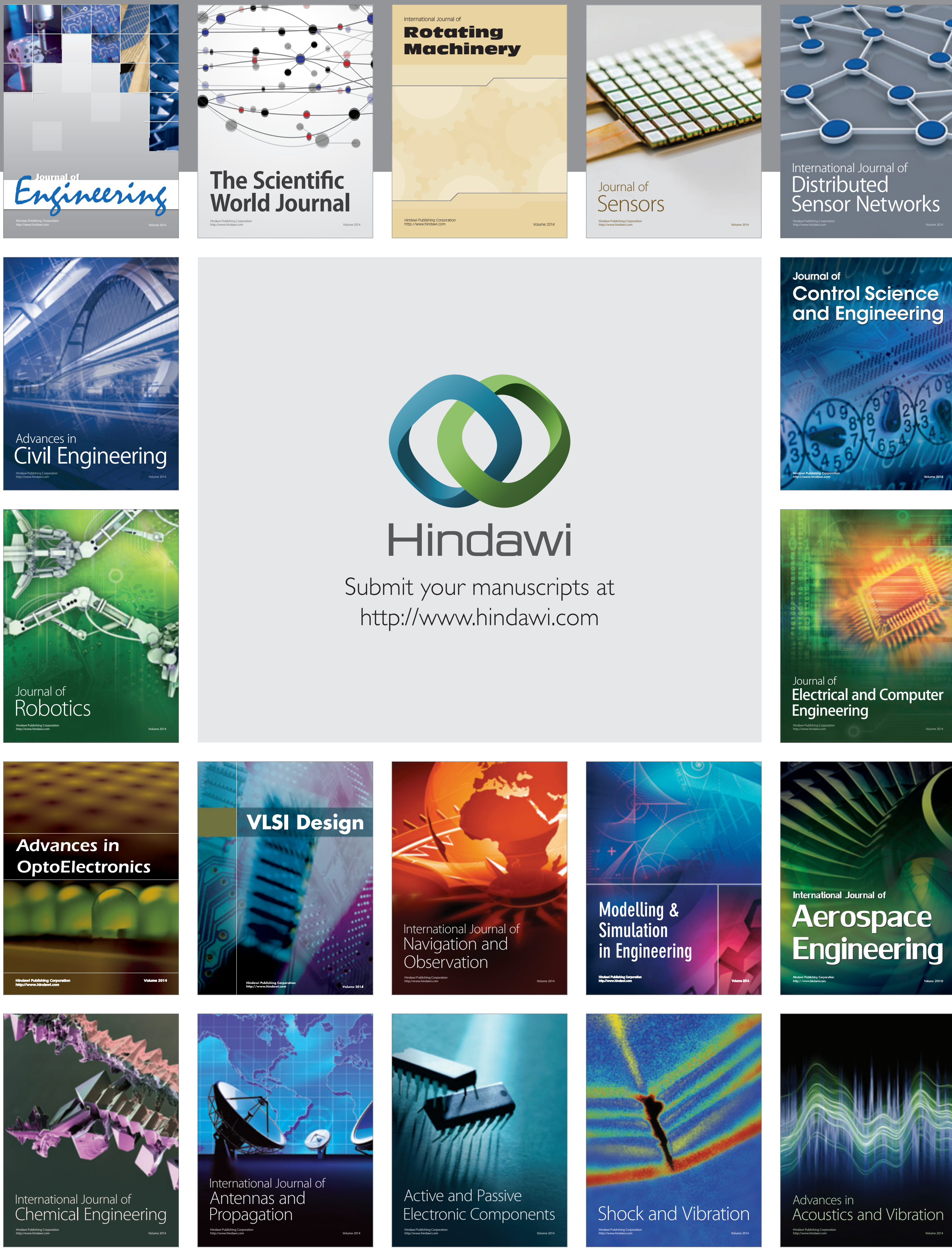
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