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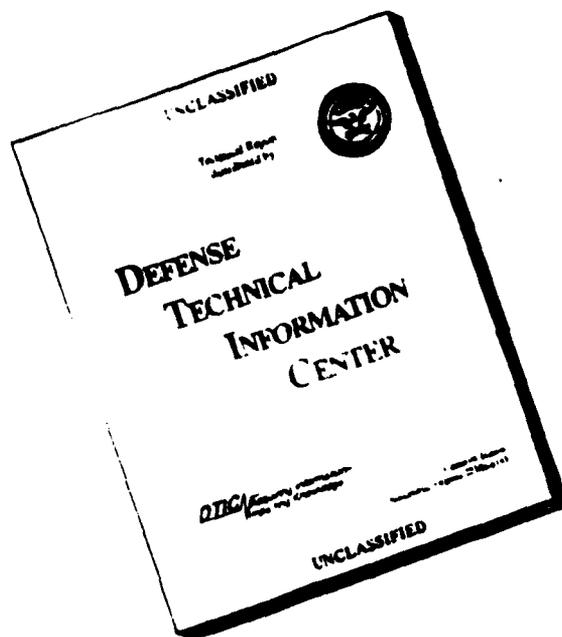
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The main objective of this contract was to improve the crystal quality of CdTe(111)B grown directly on silicon (100) substrate. At the starting date of this contract (Sept 1990) the best CdTe(111)B grown on Si(100) had double crystal x-ray rocking curves (DCRC) FWHM of 460 arcsec. These layers were exhibiting double domains and wer plagued by microtwins. At the end of this contact we are routinely growing single-domain twin-free CdTe(111)B epilayers on Si(100). The best DCRC FWHM are of 100 arcsec which is equivalent of better to th at of CdTe grown on Si with a buffer layer such as GaAs or (Ca,Ba)F<sub>2</sub>. The drastic improvement is due to a systematic investigation of the Si substrate tilt, an understanding of the driving forces for double-domain and microtwin suppression along with a precise control of the growth parameters.

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**MBE GROWTH, CHARACTERIZATION AND  
ELECTRONIC DEVICE PROCESSING OF Hg-BASED  
SEMICONDUCTING ALLOYS AND  
HETEROSTRUCTURES**

**DARPA CONTRACT MONITORED BY AFOSR**

**CONTRACT # F 49620-90-C-0090**

**SEPTEMBER 17, 1990 TO DECEMBER 16, 1993**

**FINAL TECHNICAL REPORT**

**JEAN-PIERRE FAURIE  
PRINCIPAL INVESTIGATOR**

**94-14337**  
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DARPA contract F49620-90-C-0090 entitled, "MBE growth characterization and electronic device processing of Hg-based semiconducting alloys and heterostructures" is monitored by the Air Force Office of Scientific Research (LT. Col. G. Pomrenke).

### **OBJECTIVE OF THE CONTRACT**

The main objective of this contract was to improve the crystal quality of CdTe(111)B grown directly on silicon (100) substrate. At the starting date of this contract (Sept 1990) the best CdTe(111)B grown on Si(100) had double crystal x-ray rocking curves (DCRC) FWHM of 460 arcsec. These layers were exhibiting double domains and were plagued by microtwins.

At the end of this contract we are routinely growing single-domain twin-free CdTe(111)B epilayers on Si(100). The best DCRC FWHM are of 100 arcsec which is equivalent of better to that of CdTe grown on Si with a buffer layer such as GaAs or (Ca,Ba)F<sub>2</sub>.

The drastic improvement is due to a systematic investigation of the Si substrate tilt, an understanding of the driving forces for double-domain and microtwin suppression along with a precise control of the growth parameters.

## I INTRODUCTION

Advanced IR focal plane applications require large HgCdTe arrays (256 x 256) or more elements operating at LWIR (8 to 12  $\mu\text{m}$ ). There is need for large (two to three-inches in diameter) and very large (four to five-inches in diameter) of high quality substrates to lower production cost by increasing throughput and yield.

The use of alternate substrates such as CdTe/Si and CdZnTe/Si for HgCdTe IR-based technology is extremely promising for the current hybrid approach as well as for a truly monolithic approach. Silicon is by far the most widely used semiconductor in modern electronics. It is available in large-area, it exhibits excellent crystalline quality and it is much less expensive, by a factor of 1000, than CdZnTe substrates. Si substrate is especially attractive in IR photodiode technology not only for these excellent reasons but also because in a FPA structure the coupling of the Si substrate with the Si readout will allow the fabrication of very large arrays exhibiting long-term thermal cycle reliability due to the absence of thermal expansion mismatch. The use of Si also allows the implementation of the concept of a truly monolithic approach which requires localized epitaxy of CdTe and HgCdTe homo- or heterojunction on a prepatterned Si readout already operational for signal processing.

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It has been recently reported that CdZnTe substrates can act as a source of impurities diffusing in HgCdTe epilayers during the growth and processes involving thermal treatment. This severe drawback is not expected to be experienced on Si based alternate substrates because of a much more mature bulk material technology.

The heteroepitaxy of CdTe on Si is very challenging due to the large mismatches existing in this system. The lattice mismatch of about 20% is one of the largest mismatches ever encountered in heteroepitaxy. In this system a semi-ionic compound CdTe is grown on covalent semiconductor Si. This valence mismatch can produce electrostatic charges at the interface. For many years the epitaxy of CdTe on silicon was considered virtually impossible despite considerable interest in this subject.

The very large lattice mismatch between CdTe and Si could lead to the idea that epitaxial growth of CdTe on Si is impossible. It is now well established that epitaxial growth does indeed occur, although the lattice mismatch is expected to create many dislocations at the CdTe/Si interface. Fortunately, this problem is reduced to some extent because the epitaxial relationship is CdTe(111)/Si(001), which brings the lattice mismatch down to 3.4% along the CdTe  $[\bar{2}11]$ . Also, it appears that the crystal quality of the CdTe layers has been improved tremendously during this three year program as it will be discussed later.

There is also a relatively large thermal mismatch between CdTe and Si. For practical device applications, one thus should be concerned about the risk of cracking or peeling of the films due to temperature changes either during the fabrication of the film or of the device or during its operation. Finally, as a result of the CdTe(111)/Si(001) epitaxial relationship, the CdTe  $[\bar{2}11]$  axis can be parallel to either the Si  $[1\bar{1}0]$  or the Si  $[110]$  direction. This can generate the formation of domains called antiphase domains (APD), rotated  $90^\circ$  apart, whose boundaries are defects which can lead to poor device performance. Therefore, it is important to develop a method to avoid the formation of such domains. This has been done during the second year of this contract.

As on other substrates, CdTe(111)B on Si(001) also suffers from the risk of twinning. This problem is not specific to the use of silicon substrates, but this is a severe drawback. Twinning will prevent the use of (111)B CdTe/(001)Si as a substrate for HgCdTe growth since twinning will propagate and the material will be useless for IR device fabrication. Therefore, it is imperative to investigate twin formation in CdTe(111)B epilayer. This has been done during the third year of this contract and more importantly we are understanding how to suppress twinning.

It should be pointed out that specific material issues have to be understood and controlled in order to grow HgCdTe which can be used to fabricate high

performance FPAs with a high yield at a low cost. It is also important to mention that up to now no one has been able to grow, by any growth technique, HgCdTe epitaxial material on GaAs, sapphire or Si with a crystal quality approaching that of HgCdTe grown on CdZnTe substrate.

Expressed in numbers, Double Crystal X-ray rocking Curve (DCRC) FWHM are for the best HgCdTe layers known to be of about 60 arcsec when grown on a composite substrate whereas FWHMs of about 15-20 arcsec have been reported by different groups, including EPIR Ltd., when HgCdTe is grown on CdZnTe substrate of high quality (which is not easy to find).

Such a difference must have an impact on detector performances. Even though IR photodiodes fabricated on HgCdTe grown on alternate substrates meet today's detector specifications, there is no doubt that a limitation exists for more demanding specifications, such as low background applications for which detector performances are limited by the heterogeneous properties of the HgCdTe material. Therefore, in depth work on material issues such as lattice, valence and thermal mismatch accommodations as well as interface engineering is required to insure success. This work must be primarily performed on the CdTe(CdZnTe) buffer layer since the quality of the HgCdTe epilayer mostly depends upon buffer layer quality. The MPLab has worked along those lines in this research program, with success as it will be shown hereafter.

## **II ACHIEVEMENTS**

### **II.1 GROWTH OF CdTe(111)B on Si(001)**

Figure 1 illustrates and summarizes the improvement on the crystallinity of the CdTe(111)B/Si(001) layers grown by MBE in the Microphysics Laboratory since 1989. The FWHM of the x-ray DCRCs is taken here as a measure of the structural quality of the layers. From about 1000 arcsec four years ago, the FWHM has been reduced to 100 arcsec for the best layers grown during the second quarter of 1992. Overall, this improvement correlates well with the decrease of the BE peak FWHM in the low-temperature photoluminescence spectra. At 12K, the FWHM is now as low as 1.4 meV, compared to 5.6 meV for some of the earlier samples.<sup>(1,2)</sup> The most recent data can be compared with values for CdTe/GaAs for which 60 arcsec and 0.7 meV are the best results reported so far for as-grown layers. Taking into account the fact that the growth for CdTe/GaAs is already much more mature, we consider the results on CdTe/Si as quite competitive. We have mentioned repeatedly that in order to grow CdTe layers for practical purposes, it is essential to develop a technique which consistently produces twin-free single-domain films. A first attempt to grow single-domain films involved the use of vicinal Si(100) surfaces, with a relatively large tilt ( $6-8^\circ$ ).<sup>(3)</sup>

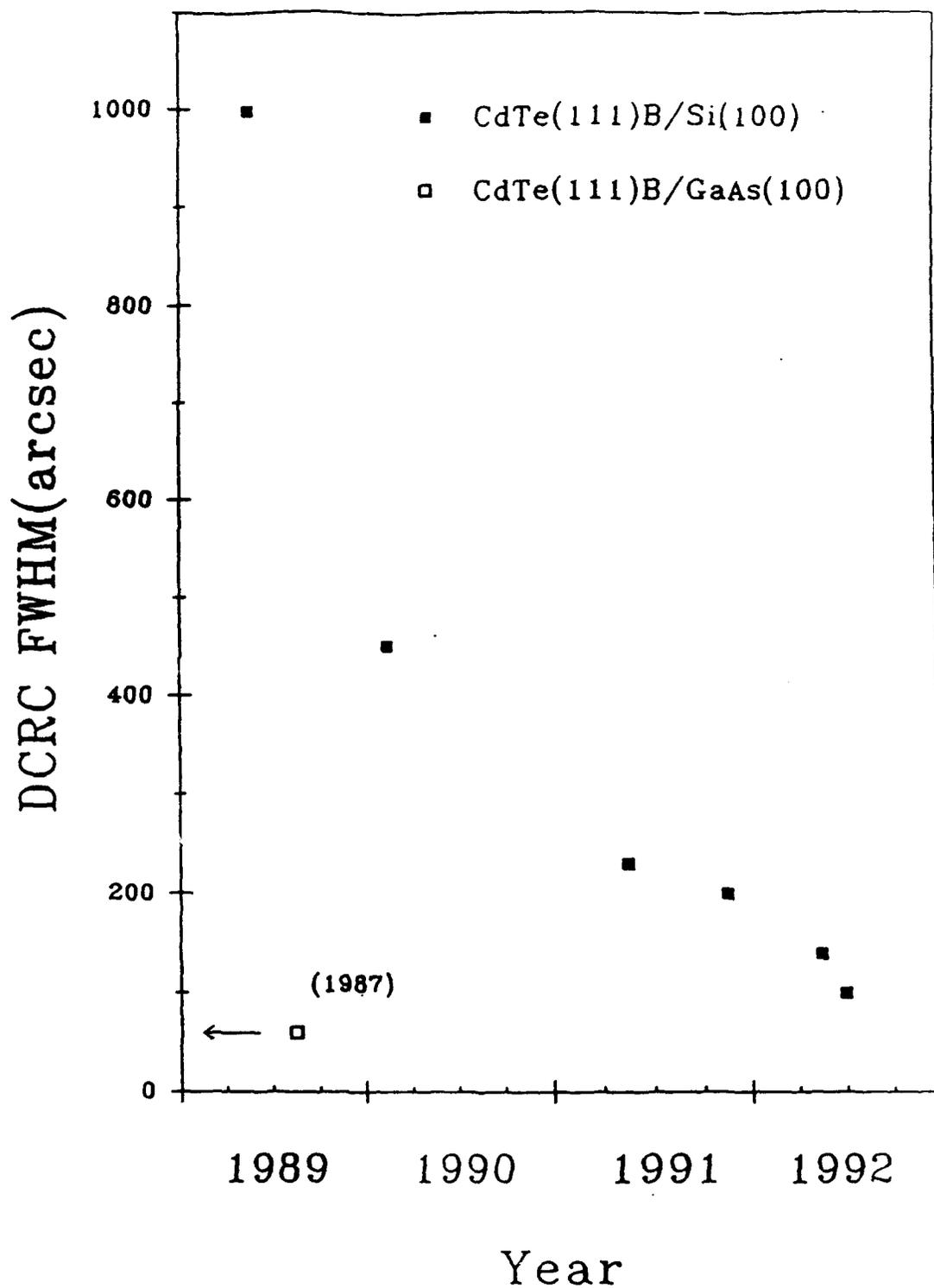


Fig. 1 Full width at half-maximum of the x-ray double-crystal rocking curves on CdTe(111)B/Si(100). Data are for some of the best samples grown in the Microphysics Laboratory since 1989. No distinction is made among substrates with different misorientations. The value for the best CdTe(111)B/GaAs(100) (60 arcsec obtained in 1987) is included for comparison.

On such substrates, the CdTe layers were always of the single-domain type, and the substrate tilt also seemed to help in avoiding the twinning, at least over large parts of the samples however, this last point has been ruled out later on. Concurrently with this obvious improvement the PL linewidth decreased to 3 MeV. Surprisingly however, the FWHM of the x-ray DCRCs was always larger than for layers grown on nominal Si(001), usually above 600 arcsec. Although we do not know the effect of these large FWHMs on the quality of subsequently grown  $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ , this fact prompted us to investigate the influence of other tilt angles.

The influence of the substrate tilt angle has been our main concern during the second year. The results obtained are presented in detail in the attached publication, "Structure of CdTe(111)B grown by MBE on misoriented Si(100)" published in the Journal of Electronic Materials [vol 22, 951 (1993)]. The results can be summarized as follows:

\* a small tilt (1-2° degrees) towards [110] is sufficient to grow single-domain CdTe(111)B film. However, at the initiation of the growth electron diffraction shows the existence of two domains, followed by the disappearance of one of the domains in less than 1  $\mu\text{m}$ .

\* The narrowest DCRC FWHMs are obtained on Si(001) substrates exhibiting a tilt of about  $1^\circ$ . In these experiments CdTe epitaxy has been carried out simultaneously on three 2-inch Si substrates of  $1^\circ$ ,  $2^\circ$ , and  $4^\circ$  respectively towards [110].

\* The model proposed by Nagai<sup>(4)</sup> does not account for the tilt angle value observed in the CdTe(111)B/Si(001) system. We have proposed a new model which involves a two-step reorientation of CdTe(111)B necessary to establish a coherent growth. This model takes into account photoemission experiments (reported during year I), which have clearly shown that the first step of the growth consists of the absorption of a submonolayer of tellurium. This model is consistent with the existence of two domains at the initiation of the growth, and the disappearance of one of them during the second reorientation.

\* Double domains can be effectively eliminated by using Si(001) tilted towards [110] which remove the  $90^\circ$ -rotations symmetry of the Si surface. However, when Si(001) is tilted towards [110] or [100] CdTe(111)B is always plagued by microtwins.

During the final year we have addressed simultaneously domain and twin issues. The results obtained are presented in detail in the attached paper

Fig. 3

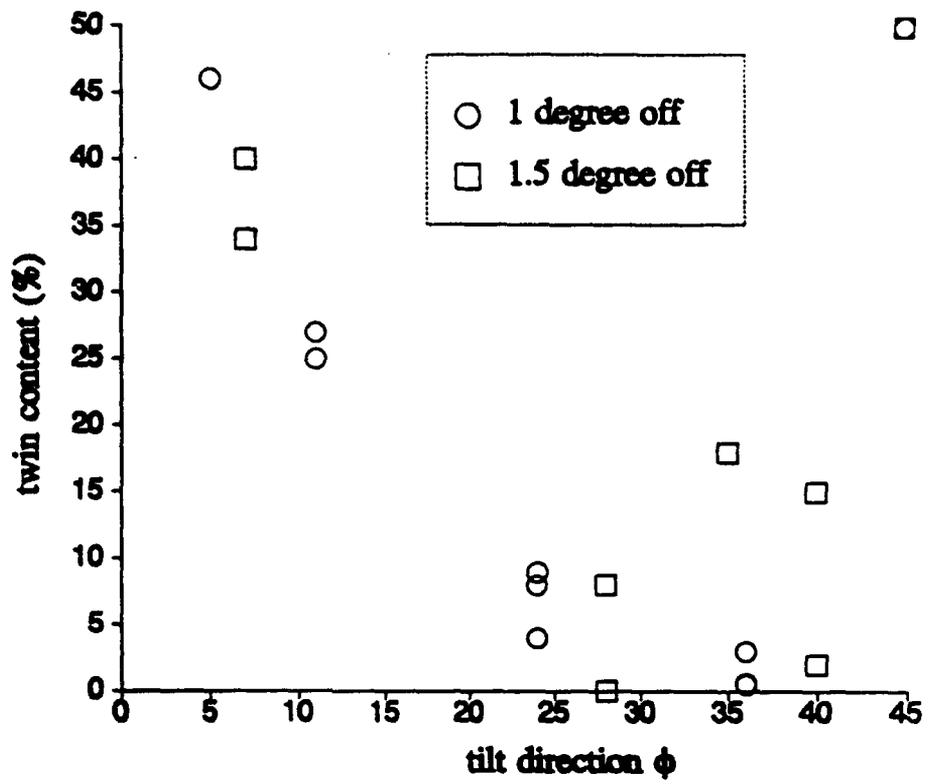
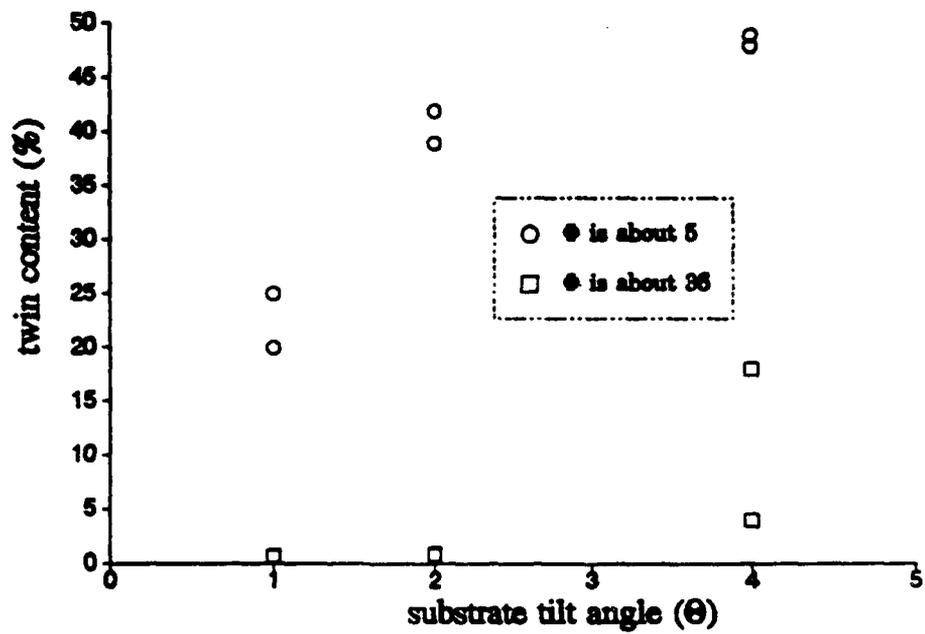


Fig. 4



"Suppression of twin formation in CdTe(111)B epilayers grown by MBE in misoriented Si(001)" which is accepted for publication in the Journal of Electronic Materials. The results can be summarized as follows:

\* CdTe(111)B epilayers have been grown on misoriented Si(001) with varying the tilt parameters ( $\theta, \Phi$ ) defined in Fig.2. The average domain and twin content of the as-grown layers were measured by x-ray diffraction. The crystalline quality was evaluated by the FWHM of x-ray rocking curves.

\* Fig.3 shows the twin contents of the as-grown layers vs. the substrate tilt direction ( $\Phi$ ) with two sets of tilt angle ( $\theta$ ). In the twin content definition (see attached paper) 50% stands for a fully twinned CdTe(111)B layer.

When CdTe(111)B is grown on Si(001) tilted towards [110] ( $\Phi=0$ ) twin content is almost 50%. The twin content reaches its minimum when  $\Phi$  values fall between  $30^\circ$  and  $36^\circ$  and it increases again when  $\Phi$  approaches  $45^\circ$  i.e Si(001) tilted towards [100]. These important results show that microtwin formation is very sensitive to the substrate tilt direction.

\* Fig.4 shows the twin contents vs. the substrate tilt angle ( $\theta$ ) with two sets of tilt direction. Twin contents tends to increase as  $\theta$  increases.

\* Cross section bright field TEM images of a CdTe(111)B layer grown on Si(001) with tilt parameters ( $\theta = 1^\circ$ ,  $\Phi = 35^\circ$ ) are displayed in Fig.5. These pictures show that heavy lamellar twinning is confined in a  $2\mu\text{m}$  thick interfacial region. Beyond  $3\mu\text{m}$  from the interface microtwins are completely absent and single domain is seen. The twin content measured by x-ray diffraction is 0.6% because of the large probing depth of the technique. The twin content of the upper part is actually 0%.

\* The major driving forces for suppressing double-positioning and lamellar twins are the preferential orientation of CdTe[11 $\bar{2}$ ] along Si[1 $\bar{1}$ 0] and lattice relaxation. Such a preferential orientation which has been confirmed by numerous x-ray diffraction experiments carried out during this program, is achieved when a tilt  $\Phi$  towards a direction between [110] and [100] is introduced. Such a tilt lifts the symmetry between [1 $\bar{1}$ 0] and [ $\bar{1}$ 10] axes by introducing dense kinks on Si(001) surface. Lattice relaxation occurs as the layer thickness increases.

## II.2 X-RAY DETECTORS

The x-ray detector activity developed in the MPLab has not been supported by this contract. However, since it is a related activity which benefit from the work performed in this program a summary of the current achievements is presented hereafter.



Fig. 5

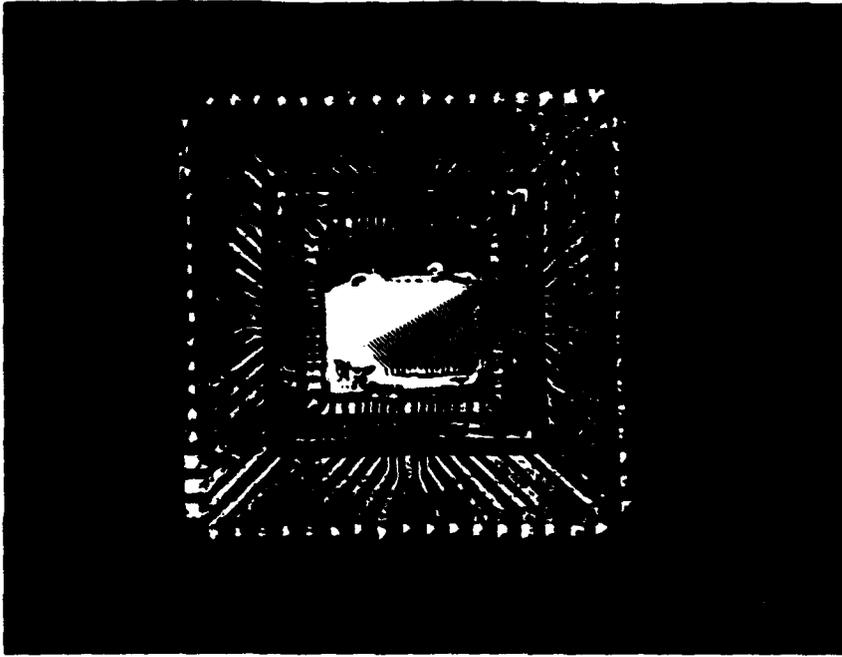


Fig. 6

# TEMPORAL RESPONSE TO Ti:Sapphire LASER PULSE

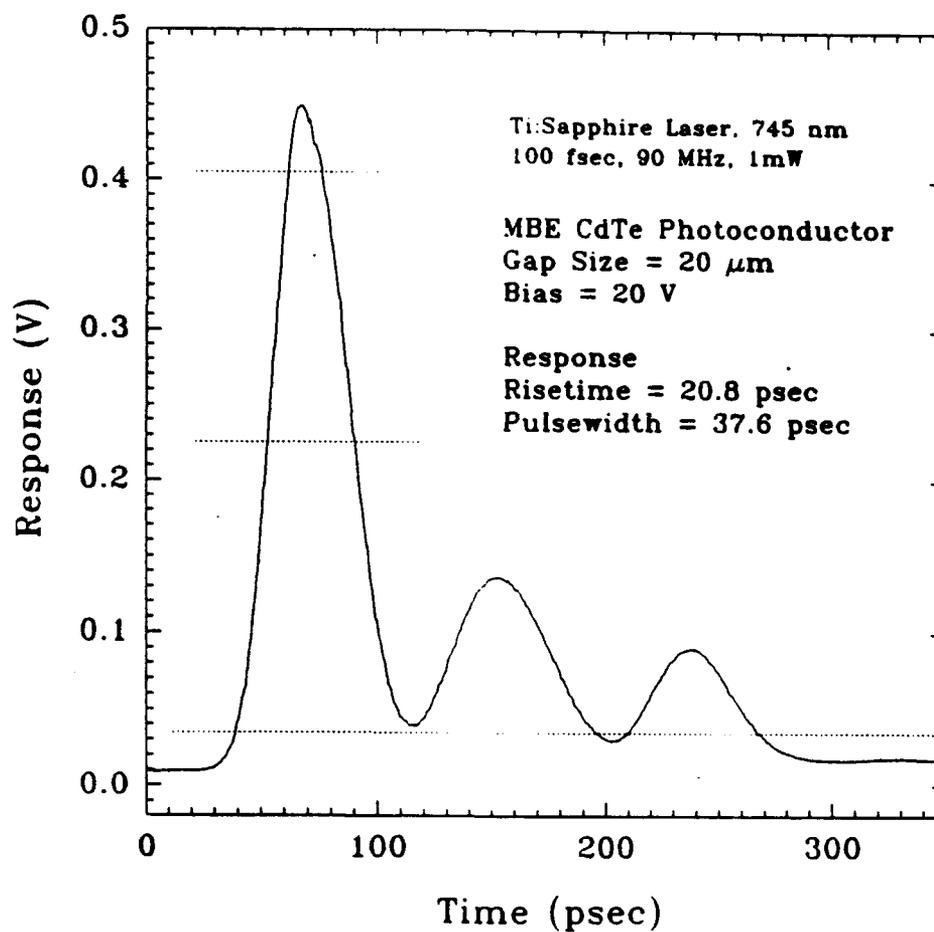


Fig. 7

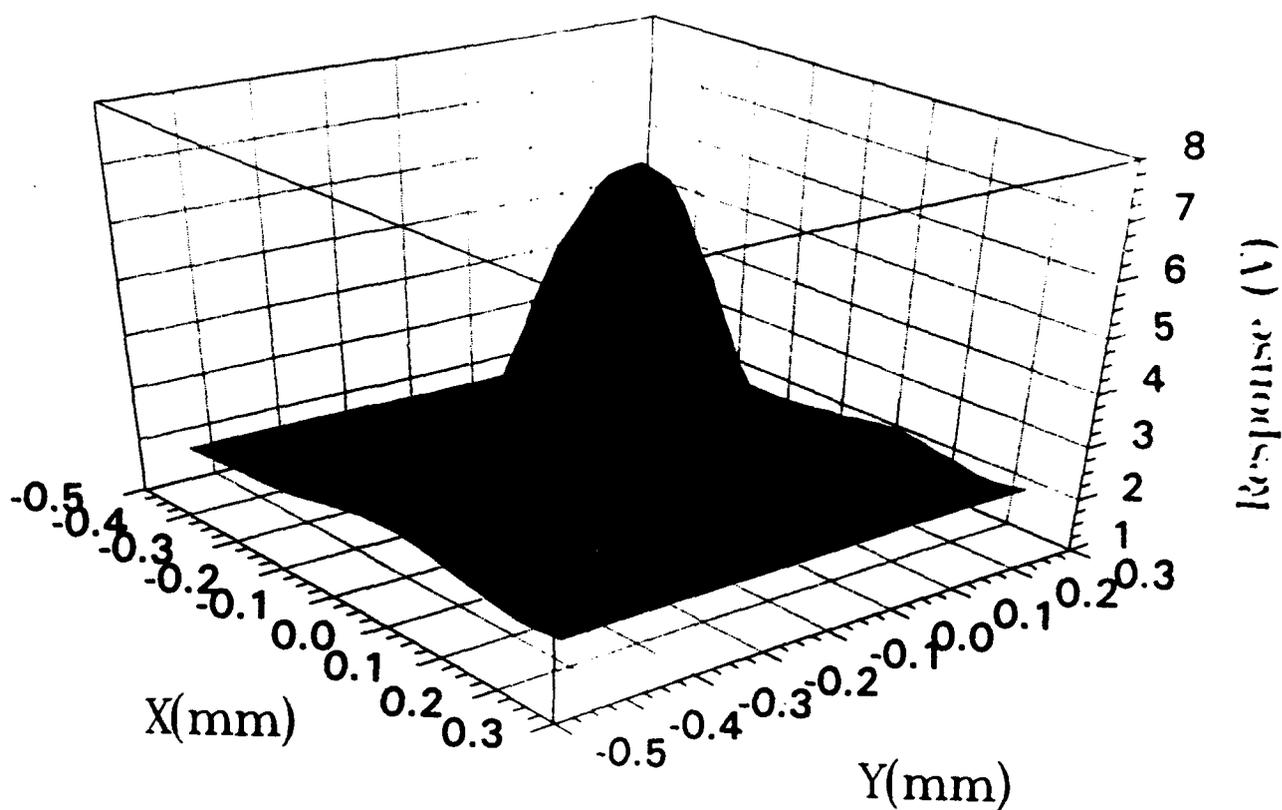
# Spatial Response of MBE CdTe Photoconductor

X-ray Energy = 8 KeV

CdTe Photoconductor

Slit Size = 300X200  $\mu\text{m}$

Gap Size = 15  $\mu\text{m}$ , Bias = 3 V



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Fig. 8

# Dynamic Range of MBE CdTe Photoconductor

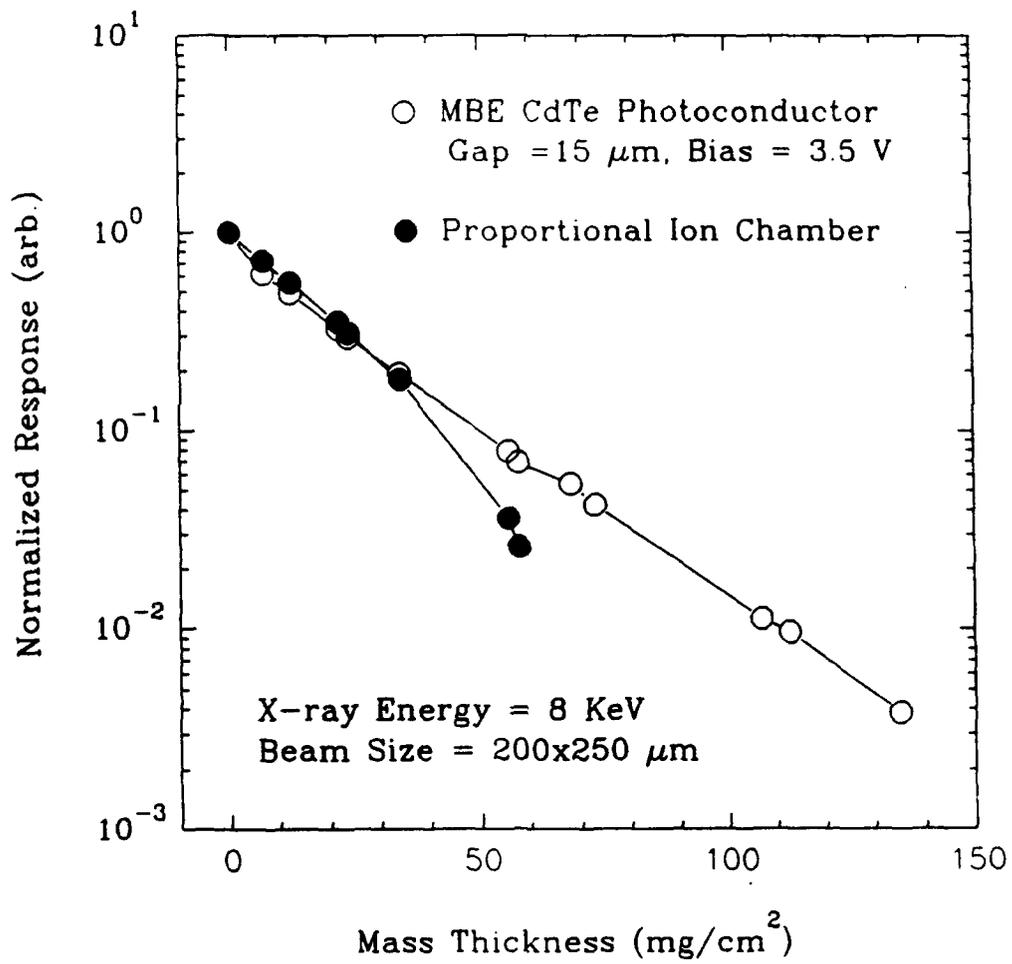


Fig. 9

\* CdTe photoconductor linear arrays of 32 elements have been fabricated and tested. Each PC has  $20\mu\text{m}$  gap and  $50\mu\text{m}$  width. Pitch size is  $100\mu\text{m}$ . (Fig. 6)

2. The response time of the photoconductor to 100 fsec Ti:Sapphire laser pulses is currently of 20-30 picoseconds. This was achieved by using a high bandwidth (20GHz) coaxial cable and a sample holder made of copper. (Fig. 7)

3. Spatial resolution measurement was made by rastering tube and synchrotron x-ray beams. Crosstalk was not found. This was achieved by etching the CdTe layer between photoconductors. The best resolution is currently  $80\mu\text{m}$  from bottom 10% to top 90% (Fig. 8). This is to our knowledge the best result achieved for solid state detector. It is promising for future digital medical imaging detectors.

4. The dynamic range of the photoconductor is nearly two and half decades (Fig.9). Considering the size of the photoconductor ( $15 \times 50\mu\text{m}$  area), the range is surprisingly large. For other detectors, such as Si APD for radiation detection, the dynamic range in current mode is 3 decades, but not with this small size (about  $1 \times 1\text{cm}^2$ )

5. The energy resolution was measured. The response of the photoconductor currently changes linearly to the x-ray energy.

### III. SUMMARY

The main achievements obtained in this three year program can be summarized as follows:

- \* DCRC FWHM of 50 arcsec has been obtained for a CdTe(211) epilayer grown on GaAs (211) which is the best result ever reported for CdTe on GaAs.

- \* Dual epitaxy of CdTe [(211) or (133) orientations] on GaAs(211) has been found and the atomic structure of the (133) CdTe/(211)GaAs heterointerface has been analyzed by HRTEM. From this study we have proposed a general model for the accommodation of lattice mismatches in zinc-blend-type heteroepitaxial semiconductor systems.

- \* HgCdTe epilayers have been grown on both CdTe/GaAs and CdTe/Si composite substrates.

Diodes have been fabricated on HgCdTe(111)B layers grown on CdTe/GaAs substrates using the Low Energy Ion Etching (LEIE) technique. A RoA of 1.6 x

$10^4 \Omega \text{cm}^2$  at 77K has been obtained for a diode fabricated on a  $\text{Hg}_{0.72}\text{Cd}_{0.28}\text{Te}/\text{CdTe}/\text{GaAs}$  layer.

\* The LEIE technique developed in the MPLab turned out to be suitable for LWIR photodiodes and therefore it was not used after year I.

\* Mesa diodes have been fabricated on junctions obtained from an interdiffused arsenic-doped Multiple Quantum Well Structure deposited on a narrow gap indium-doped  $\text{HgCdTe}$  grown on GaAs substrate. A RoA of  $64 \Omega \text{cm}^2$  has been measured from a junction exhibiting a cadmium composition of 0.22. An excellent array distribution uniformity has been observed.

\* Single domain twin-free  $\text{CdTe}(111)\text{B}$  grown directly on  $\text{Si}(001)$  are routinely obtained in the Microphysics Laboratory. The best DCRC FWHM, which is a measure of the crystal quality, is currently 100 arcsec. Due to the large probing of x-ray analysis we believe that the top surface, which is of major importance for  $\text{HgCdTe}$  epitaxy, has FWHM lower than 100 arcsec. With DCRC FWHM of 100 arcsec  $\text{CdTe}$  grown directly on Si is equivalent or better to that of

CdTe grown on Si with a buffer layer such as GaAs or  $(\text{Ca}, \text{Ba})\text{F}_2$ . At the start of the contract the best result was 460 arcsec and CdTe(111)B exhibited double-domains and microtwins.

\* The drastic improvement in CdTe crystal quality obtained during year II and III is due to a systematic investigation of the Si(001) tilt parameters  $(\theta, \Phi)$ .

- A small tilt angle  $\theta$  of  $1^\circ$  has been found to help in double domain suppression while not introducing a too large step density on the surface.
- **Tilt direction  $\Phi$  has been found to be the most important parameter regarding microtwin formation.** Fully twinned layers are obtained when  $\Phi$  value is about  $0^\circ$  (tilt towards [110]) or  $45^\circ$  (tilt towards [100]). Twin-free layers are obtained when  $\Phi$  is around  $30^\circ$  to  $36^\circ$ . The substrate tilt angle ( $\theta$ ) plays a little role in suppressing microtwinning.
- A microscopic mechanism from double domain to single domain transition has been proposed. It has also been found that driving forces for twinning suppression are the preferential orientation of

CdTe[11 $\bar{2}$ ] axis along Si[1 $\bar{1}$ 0] and lattice relaxation. Preferential orientation can be enhanced when the substrate is tilted towards a tilted direction with  $\Phi$  significantly greater than zero. Lattice relaxation occurs as the layer thickness increases.

- These experiments and their analysis have determined with great precision which substrate tilt parameters have to be used in order to always get twin-free layers. The improvement in the growth conditions has produced the highest quality so far achieved for CdTe(111)B grown on Si(001).

\* HgCdTe epilayers have been grown by MBE on CdTe/Si substrate as large as 5-inch diameter; composition uniformity  $\sigma x/x$  of 0.6% has been achieved on 3-inch diameter wafer whereas  $\sigma x/x$  of 2.3% has been achieved on a 5-inch diameter wafer.

\* HgCdTe grown on CdTe(111)B/Si(001) alternate substrate with DCRC FWHM of 200 arcsec systematically exhibits lower FWHM (125 arcsec typically). After thermal anneal EPD of  $4 \times 10^6 \text{cm}^{-2}$  have been measured which compares very well

with EPD of HgCdTe grown on CdTe/GaAs alternate substrate but also of HgCdTe grown directly on CdTe. Very good electrical properties are also observed. HgCdTe growth has not been performed yet on the very best CdTe(111)B/Si(001) substrates obtained during year III.

\* CdTe(111)B/grown on Si(001) has been used for hard x-ray detection applications. CdTe x-ray detector is very fast and shows an excellent resolution and a large dynamic range.

**The work carried out on CdTe/Si in the Microphysics Laboratory is a remarkable example of dual use application in I.R technology and x-ray detection.**

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Y.P. Chen, J.P. Faurie and S. Sivananthan. J. Electron Mater ( In press)
14. Minority carrier lifetime in indium-doped HgCdTe(211)B epitaxial layers grown by MBE.  
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Y. P. Chen, J.P. Faurie and S. Sivananthan (submitted for publication).

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M.D. Lange (1993)

Y.P. Chen (summer 1994)

# Structure of CdTe(111)B Grown by MBE on Misoriented Si(001)

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Single domain CdTe (111)B has been grown on Si(001) substrates tilted  $1^\circ$ ,  $2^\circ$ , and  $4^\circ$  toward [110]. All the layers started with a double-domain structure, then a transition from a double- to a single-domain was observed by reflection high energy electron diffraction. A microscopic picture of this transition is presented. We also measured the tilt between CdTe (111)B and Si (001). The result does not follow the tilt predicted by the currently existing model. A new model of the microscopic mechanism of CdTe (111)B growth is presented. New evidence indicates that optimizing the tilt of the substrate surface is very crucial in improving the CdTe (111)B crystal quality.

**Key words:** CdTe epitaxial layers, MBE, RHEED analysis, Si substrates

## INTRODUCTION

CdTe has been viewed as an important semiconductor over the decades for both its almost ideal use as a substrate for HgCdTe and its potential applications in  $\gamma$ -ray and x-ray detection. However, it is also well recognized that it is technically difficult and costly to produce bulk CdTe single crystals with both high quality and large area. For this reason, epitaxial growth of CdTe on foreign substrates has received a great deal of attention for many years. The possible choices for substrates are InSb, sapphire, GaAs, and Si. Among them Si is the most promising since high quality and large size Si substrates are commercially available. Furthermore, advantage can be taken of the mature Si integrated circuit technology to fabricate monolithic integrated focal plane arrays, by combining the Si integrated circuit for signal processing with the detector fabricated on it. This promising future makes it very attractive for the direct growth of CdTe (111)B on Si (001), which has been an active research program in the Microphysics Laboratory for the last three years.

However, there are several obstacles which need to be overcome in order to produce high quality CdTe on

Si. One is the very large lattice mismatch (19%) between CdTe and Si, which will introduce large dislocation density along the interface. Second is the large thermal mismatch between the two materials, which will produce additional strain to the already strained CdTe layer. In the worse case, the thermal mismatch might cause some practical problems such as cracking or peeling of the CdTe layer for the system of CdTe/Si or HgCdTe/CdTe/Si when cycled from room temperature to low temperature. For the epitaxial relation of CdTe (111)B on Si(001) there is a third obstacle, which is the formation of double domains and twins. Since Si[110] is equivalent to Si[1 $\bar{1}$ 0], the CdTe[11 $\bar{2}$ ] can align with either the Si[110] or the Si[1 $\bar{1}$ 0]. This leads to the formation of double domains, in which one domain differs from the other by a  $90^\circ$  rotation. Furthermore, CdTe (111)B is known to be plagued by microtwin formation. Double-domain and microtwin in CdTe (111)B/Si(001) are structural defects which can significantly degrade the HgCdTe grown on such CdTe buffer layer. Therefore, ways to avoid the formation of the double domains and twins has always been a major concern to us.

We have previously reported<sup>1</sup> that CdTe (111)B grown on Si(001) tilted  $6^\circ$  or  $8^\circ$  toward [110], always exhibited single-domain structure, but the full width at half maximum (FWHM) of x-ray double crystal

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Fig. 3. Reflection high energy electron diffraction patterns of CdTe(111)B, grown on misoriented Si(001), taken at different growth stages while e-beam is along Si[110]: (a) about 360Å CdTe, (b) about 4000Å CdTe, (c) about 7500Å CdTe. The bright spots in (a) and the short light streaks in (b) between the regular streaks demonstrate the weak double-domain structure.

sample holder which allows for translation, tilt, and rotation adjustments. The set-up is illustrated in Fig. 1. The rotation angle of the sample varies from  $-102^\circ$  to  $102^\circ$  in  $12^\circ$  or  $30^\circ$  steps. For a misoriented sample, the position of the peak on the x-ray rocking curve ( $\gamma$ ) is a cosine function of the azimuthal angle ( $\phi$ ). When  $\phi$  is 0,  $\gamma$  reaches its minimum for a sample tilted toward [110], or its maximum for a sample tilted toward  $[\bar{1}\bar{1}0]$ . A typical curve of the peak position vs the azimuthal angle is shown in Fig. 2. A routine curve fitting can produce the tilt of a sample with respect to the surface normal.

### RESULTS

We have intensively studied the growth of CdTe(111)B on Si(001) substrates. For this epitaxial relationship, the lattice mismatch between CdTe(111)B and Si(001) can be reduced to 3.4% when CdTe [11 $\bar{2}$ ] is aligned with either one of the Si(110). Comparing with the overall mismatch of 19%, this epitaxial relation will, to some extent, reduce severeness of the lattice mismatch between the two materials. All our experiments show that CdTe(111)B grown on *exact* nominal Si(001) exhibits double domains. Here we mention the *exact* nominal Si(001), since some of the nominal Si(001) substrates have small accidental tilts. All CdTe(111)B layers grown on misoriented Si(001) are single domain. During the MBE growth, RHEED was performed in-situ on growing CdTe(111)B. From observation of RHEED patterns, we found that CdTe(111)B always started with double-domain structure on the misoriented Si(001), even on substrates with tilts up to four degrees. Then as the growth continues, the one domain gradually overwhelms the other until a single domain covers the whole layer. The size of the transition region from double domains to single domain depends on many parameters, such as substrate tilt, growth condition, the completeness of deoxidation of the substrate and vacuum condition of the growth chamber. Among them, the substrate tilt certainly plays the key role in suppressing double domain formation. A typical domain transition process can be revealed by the RHEED pattern sequence shown in Fig. 3. For a layer with double-domain structure, the RHEED pattern is the superposition of two sets of streaks corresponding to

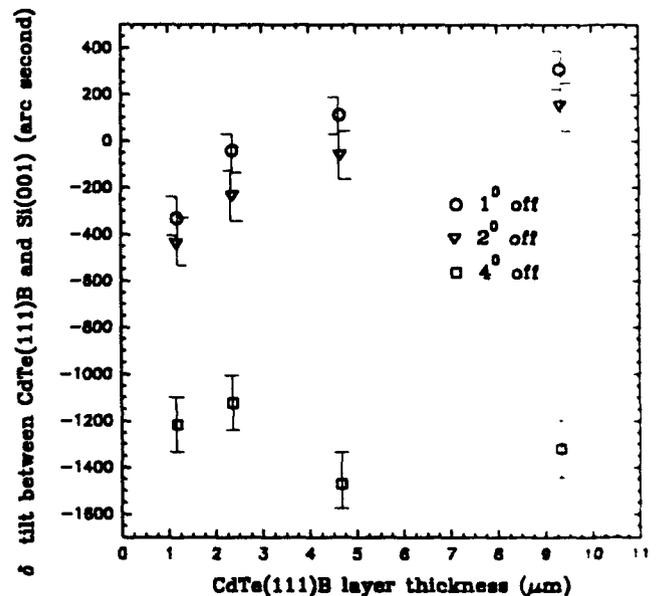


Fig. 4. The tilts between CdTe(111)B and Si(001) vs the layer thickness, obtained by the DCRC measurements. 1°, 2°, and 4° tilted Si(001) substrates were used in the experiment.

e-beam along both CdTe[11 $\bar{2}$ ] and CdTe[1 $\bar{1}0$ ] which is shown in Figs. 3a and 3b. For a layer with single-domain structure, however, RHEED only shows one set of the streaks as shown in Fig. 3c.

For a heteroepitaxial system where a tilted substrate is used, it has been proposed by Nagai<sup>7</sup> that a tilt between the epilayer and the substrate must be introduced in order to eliminate an incoherent growth, caused by the vertical lattice mismatch between the two materials. The tilt relationship is described by

$$\tan \delta = \frac{\Delta d}{d} \tan \theta$$

where  $\delta$  is the tilt between the epilayer and substrate lattice,  $\Delta d$  is the vertical lattice difference between the two materials,  $d$  is the atomic step height of the substrate and  $\theta$  is the tilt angle of the substrate.

A similar tilt relationship has been observed by E. Ligeon and coworkers<sup>8</sup> for the heterostructure of CdTe(111) on GaAs(001), except that the tilts they observed are always larger than or equal to the values

steps will completely cover, or at least dominate, the Si(001) surface with a tilt less than four degrees toward [110]. Indeed a  $(2 \times 2)$  surface reconstruction was observed by RHEED on such Si(001) substrates after an oxide layer was removed in vacuum. That means a double-domain structure does exist on a Si(001) surface with a tilt as large as four degrees.

In a previous paper<sup>1</sup>, we presented a microscopic model for the interface formation between CdTe(111)B and Si(001). In this model, a Te atom forms tetrahedral bonds with three Si atoms by kicking out one of the two Si atoms which form the dimer on the surface, leaving single dangling bond upward, as shown in Fig. 6. Then an arriving Cd atom can attach to the dangling bond and initialize the CdTe(111)B growth. In such a CdTe(111)B layer, CdTe[11 $\bar{2}$ ] always aligns with either Si[110] or Si[1 $\bar{1}$ 0]. This has been confirmed by our experiments. We have performed DCRC measurements on many CdTe(111)B/Si(001) samples and have found without exception that CdTe[11 $\bar{2}$ ] always aligns with both the Si[110] and the Si[1 $\bar{1}$ 0] for double-domain samples, and the CdTe[11 $\bar{2}$ ] aligns with one of the Si(110) for single domain samples.

With all this concept and fact in mind, it is easy to understand why on exact nominal Si(001) a double-domain and twined layer of CdTe(111)B was always obtained, since the same number of  $S_A$  and  $S_B$  steps with same terrace widths coexist on the Si(001) surface. As for the Si(001) surface, Te atoms have an equal opportunity to form tetrahedral unit cells on both terraces, which leads to the formation of double domains. Even on the same domain, the Te atom can replace either one of the two Si atoms which form the dimer. Therefore, some of the Te atoms form the tetrahedral unit cells with [11 $\bar{2}$ ] aligned with Si[110], and the others form the tetrahedral unit cells with [11 $\bar{2}$ ] aligned with Si[1 $\bar{1}$ 0], which can lead to the formation of laminar twin.

Now when a Si(001) substrate is slightly tilted toward [110], the surface structure changes drastically. First, the steps run down steadily from one side to the other, instead of running up and down as on the nominal Si(001). Second, the size of  $S_B$  and  $S_A$  terraces are no longer equal. Actually, the S-steps on the surface become paired, with a wider  $S_B$  terrace and narrower  $S_A$  terrace. For example, on Si(001) tilted toward [110] by one degree, the average terrace width is about 80Å. Because of the pairing, the average width of an  $S_A$  terrace might shrink down to 50Å or below. Furthermore, the high-temperature annealing of the substrate at over 850°, and the interaction of Si atoms with Te atoms, will enhance the pairing, as we discussed in previous paper<sup>1</sup>.

When CdTe(111)B is deposited on Si(001) with paired S-steps, we believe the initiation of CdTe(111)B happens on both terraces, which produces an initial layer with double-domain structure. This agrees with our experimental observations by RHEED, as shown in Fig. 3. However, since the  $S_B$  terrace is much wider than the  $S_A$  terrace, the consequences of the initiation of the tetrahedral unit cells on the two

terraces are not equivalent. The tetrahedral unit cells formed on  $S_B$  terraces have their [11 $\bar{2}$ ] axes parallel with the step edge, or Si[1 $\bar{1}$ 0]. Along this direction, the lattice mismatch between the two materials is 3.4%. The small mismatch makes it easy to form long chains of the tetrahedral unit cells. However, the tetrahedral unit cells formed on  $S_A$  terraces have their [11 $\bar{2}$ ] axes perpendicular to the step edge. Since the width of an  $S_A$  terrace is very narrow (about tens of angstroms), and along the step edge the relationship of CdTe [1 $\bar{1}$ 0]/Si[1 $\bar{1}$ 0] leads to a 19% lattice mismatch, it is very difficult to form long chains of the tetrahedral unit cells on  $S_A$  terraces. The difference will make the coverage of the tetrahedral unit cells on  $S_B$  terraces much faster than that on  $S_A$  terraces. As a consequence, the CdTe(111)B unit cells on  $S_B$  terraces will grow faster than those on  $S_A$  terraces, which will enhance the spread of the domain on an  $S_B$  terrace over that on a nearby  $S_A$  terrace. This was also observed in our experiments by RHEED, where the RHEED streaks are much brighter and smoother when the e-beam is along Si[110] than the same set of the streaks when e-beam is along Si[1 $\bar{1}$ 0].

Our experimental results show that the tilt between CdTe(111)B and Si(001) is negative at the early growth stage of CdTe(111)B. One possible explanation is that the tetrahedral unit cells were initiated both on the terrace and at the step edge. The tetrahedral unit cells started at the edge will lead to CdTe(111)B tilted away from Si(001) toward the surface normal. This tilt tends to direct the growth of CdTe(111)B toward nearby  $S_A$  terraces until it meets the domain on the next  $S_B$  terrace. This process completes the conversion of the initial double domain to single domain, and produces a negative tilt between CdTe(111)B and Si(001) at the early stage of CdTe(111)B growth. Such a tilt was indeed observed on all the samples in our experiment, as shown in Fig. 4. In this process, we also expect large distortions along the step edges where two domains meet, which will in turn result in a large dislocation density. The dislocation density seems to be proportional to the step density. The DCRC performed on the samples with 1  $\mu$ m thickness indicated that the x-ray FWHM does increase as substrate tilt increases, as shown in Fig. 5.

In our experiments, we did not observe the tilt suggested in Nagai's model at the beginning of CdTe(111)B growth. For the epitaxial relationship of CdTe(111)B/Si(001), the atomic-step-height difference between the two materials is as large as 2.38Å, which is almost twice of the Si atomic step height. It seems, therefore, that incoherent growth is inevitable at the beginning of CdTe growth in order to reduce the vertical lattice distortion to a minimum. We have already mentioned that the initiation of CdTe tetrahedral unit cells at the step edge will produce a negative tilt between CdTe(111)B and Si(001), after which the double domains merges into single domain. We call this process the first reorientation of the CdTe(111)B. The tilt ( $\delta'$ ) introduced in this process is

ning of the growth. A transition of domain structure from double to single domain is observed for all layers. The tilt between CdTe (111)B and Si(001) was measured for these layers. The results are completely different from what we expected by applying Nagai's model. We present a new model for the growth of single-domain CdTe (111)B on misoriented Si(001), and the microscopic mechanism for domain transition from double to single, in which the tilt of the substrate toward [110] plays the key role.

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SUPPRESSION OF TWIN FORMATION IN CdTe(111)B EPILAYERS  
GROWN BY MBE ON MISORIENTED Si(001)

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ABSTRACT

CdTe(111)B layers have been grown on misoriented Si(001). Twin formation inside CdTe(111)B layer is very sensitive to the substrate tilt direction. When Si(001) is tilted towards [110] or [100], a fully twinned layer is obtained. When Si(001) is tilted towards a direction significantly away from [110], a twin-free layer is obtained. Microtwins inside the CdTe(111)B layers are overwhelmingly dominated by the lamellar twins. CdTe(111)B layers always start with heavily lamellar twinning. For twin-free layers the lamellar twins are gradually suppressed and give way to twin-free CdTe(111)B layer. The major driving forces for suppressing the lamellar twinning are the preferential orientation of CdTe[11 $\bar{2}$ ] along Si[1 $\bar{1}$ 0] and lattice relaxation. Such preferential orientation is found to exist for the CdTe(111)B layers grown on Si(001) tilted towards a direction between [110] and [100].

## INTRODUCTION

Before CdTe(111)B grown on Si(001) can be considered as an alternative substrate for the growth of HgCdTe, there are several obstacles to be eliminated. Foremost of those is formation of double-domain and twin in CdTe(111)B layers grown on Si(001), since CdTe[1 $\bar{1}$ 2] can align with any one of Si  $\langle$ 001 $\rangle$  axes<sup>1</sup>. Such structural defects are nicely revealed by Transmission Electron Microscopy (TEM) pictures<sup>2</sup>. In our previous publication<sup>1</sup> we have also shown that the double-domain defect can be effectively eliminated by using the misoriented Si(001) tilted towards [110], which lifts the 90<sup>0</sup>-rotation symmetry of the Si(001) surface. In this paper we present our investigation towards understanding and suppressing the formation of twin.

Microtwins are known to be the common defects in CdTe(111) layers. Along the [111] orientation the crystal with zinc-blende structure, like the CdTe, can be visualized as being continuously piled up close packed planes. Each plane contains two sheets of atoms. There are two possible packing sequences, which are almost energetically identical. One is ABCABC ... The other is ACBACB ... The twin is presented when both types of sequences coexist inside the crystal. Basically there are two types of twins, as shown in Fig. 1. The lamellar twin is formed with a coherent twin boundary parallel to the (111) plane, when layers in different sequences are packed on top of each other. The double-positioning twin is formed with an incoherent boundary perpendicular to the (111) plane, when layers in different sequences are packed side by side. Both twin configurations possess 180<sup>0</sup>-rotation symmetry.

In order to prevent the formation of twin in CdTe(111)B layer grown on Si(001) substrate we have to avoid at least the 180<sup>0</sup>-rotation symmetry of the Si(001) surface. This can be achieved by using the misoriented Si(001) with tilt parameters ( $\theta$ ,  $\phi$ ), as defined in Fig. 2. In

this paper we present our experimental results on the growth of CdTe(111)B on misoriented Si(001) with varying tilt parameters ( $\theta$ ,  $\phi$ ). The the microtwin structure is revealed by TEM. The microtwin content is detected by x-ray Double Crystal Diffractometer (DCD).

## EXPERIMENT

The substrates used for this research are 2-in diam misoriented Si(001) wafers with varying tilt parameters ( $\theta$ ,  $\phi$ ). All the CdTe(111)B layers are grown in OPUS 45 which is a multiwafer MBE system manufactured by ISA-Riber. This system can handle up to three 2-in diam or one 5-in diam wafer. In each run CdTe(111)B layers are grown simultaneously on three 2-in diam Si(001) substrates with same  $\theta$  and different  $\phi$  values, or vice versa. From run to run we also use the same growth conditions, so that the experimental results are compatible.

The substrates used for the MBE growth of CdTe(111)B first go through routine chemical cleaning procedure just before they are loaded into the MBE chamber. This chemical cleaning procedure is developed from both the RCA method,<sup>3</sup> and the method described by Ishizaka and Shiraki.<sup>4</sup> The procedure includes a degreasing step, a wet chemical etching and an oxidation step. Between each step the wafer is thoroughly rinsed with de-ionized water. As a result, at the end of the process the wafer is covered by a protective thin oxide film. Immediately before deposition of CdTe, the oxide film is removed in-situ by heating up the wafer over 850°C.

CdTe(111)B layers are grown on Si(001) by using a two-step method which is similar to the method used routinely for the growth of GaAs on Si. CdTe is first grown at about 220°C for several minutes, then grown at about 260°C for about 10 minutes. The as-grown layer is then annealed at about 360°C under Te flux for 10 minutes. The remainder of the CdTe layer

is grown at about 310 °C. At the end of the growth, the layer is annealed in-situ at 360 °C under Te flux for about 30 minutes. During the annealing no surface reevaporation is observed by reflection high energy electron diffraction (RHEED). The typical growth rate is about 2 Å/S.

The as-grown layers are then evaluated by x-ray DCD for the layer quality and twin content. The layer quality is indicated by the line width which is defined as the full width at half maximum (FWHM) of the x-ray rocking curves. The twin content of the layers can be detected by x-ray diffraction. For a CdTe single crystal (111) orientation possesses a three-fold symmetry, which can be identified by a set of planes such as {224}, {335} etc. For a twinned CdTe layer the twin counterpart is rotated around [111] axis by 180°. These are illustrated in Fig. 3. In present work we use the symmetry of {224} diffraction to study the twin content of the CdTe(111)B layers. The experimental set-up for detecting the twin content in CdTe layers is demonstrated in Fig. 4a. When a sample is rotated around its surface normal we expect to obtain 3 peaks of the rocking curves corresponding to {224} reflection for a twin-free layer. Additional minor peaks, however, are recorded in between the two principal peaks. These are shown in Fig. 4b. The twin content is defined as following:

$$\text{twin content} = \frac{I_m}{I_m + I_p} \times 100\%,$$

where  $I_m$  and  $I_p$  are the intensities of minor peak and principal peak respectively. In such a definition the 50% twin content stands for a fully twinned CdTe(111)B layer.

Some CdTe(111)B layers are also examined by TEM. A cross-section bright field image can clearly reveal the microtwin structure inside the CdTe(111)B layers. This work is done in Purdue University.

## RESULTS AND DISCUSSIONS

CdTe(111)B layers have been grown on Si(001) substrates with different tilt parameters ( $\theta$ ,  $\phi$ ). The twin contents of the layers are assessed by x-ray diffraction. Figure 5 shows the twin contents of the as-grown layers vs the substrate tilt directions ( $\phi$ ) with two sets of tilt angle ( $\theta$ ). When CdTe(111)B was grown on Si(001) tilted towards [110] ( $\phi = 0$ ), the as-grown layers are plagued by heavy twinning. As the substrate tilt direction turns away from [110] or  $\phi$  value increases the twin content of the epilayers decreases. The twin content reaches its minimum when  $\phi$  values fall between  $30^\circ$  and  $36^\circ$ . Then the twin content increases again as the  $\phi$  value approaches  $45^\circ$ . These results indicate that the twin content is very sensitive to the substrate tilt direction.

In order to find out the contribution of the substrate tilt angle to the formation of the twin we also grow CdTe(111)B on Si(001) with similar tilt direction and different tilt angle. In fig. 6 we show the twin contents of the epilayers vs the substrate tilt angle with two sets of tilt directions. The results exhibit that the twin content tends to increase as the tilt angle increases. In other words the increase of the tilt angle does not enhance suppression of the twin formation at all.

Since the x-ray diffraction can only provide the average twin content of the epilayer, the results give us no hint about the microtwin structure and its evolution as the layer thickness increases. Therefore we also examine the epilayers by the TEM. Figure 7 shows the cross-section bright field TEM images taken from different parts of the CdTe(111)B layer at increasing distance from the CdTe/Si interface. The layer are grown on Si(001) tilted  $1^\circ$  towards [170] which is about  $35^\circ$  rotated from [110]. The twin content measured by x-ray diffraction is 0.6%.

The pictures clearly indicate that the microtwins of the CdTe(111)B grown on Si(001) are overwhelmingly dominated by the lamellar twins, which is quite similar to the microtwin structures of the CdTe(111)B grown on GaAs(001), GaAs(111)B and CdTe(111)B<sup>5,6</sup>. But, in our case, the lamellar twin does not extend throughout the whole layer. The heavy twinning is confined in a region within 2  $\mu\text{m}$  from the interface. Then a few scattering twins present in the next 3  $\mu\text{m}$  region. Beyond that the twins completely die out and give way to twin-free region of the CdTe(111)B layer. Similar microtwinning evolution is also observed by A. Hobbs *et al.* on the CdTe(111)B grown by hot wall epitaxy (HWE) on GaAs(111)B<sup>7</sup>. In that case the lamellar twins stop at about 6  $\mu\text{m}$  from the interface and give way to a six-fold symmetric pattern of twinned sectors found at the layer surface. They attribute such a microtwinning evolution to the curvature growth front which produces a series of surface steps in the radiant direction. In the case of CdTe(111)B on Si(001), however, we do not observe such a symmetric twinned sector on the layer surface. The twin content on the CdTe(111)B surface is uniformly distributed over the whole wafer. The thickness of the layer is also very uniform over the whole wafer. Therefore the diminishing of the lamellar twins in CdTe(111)B layer grown on Si(001) can not be explained by the argument which seems to explain the development of microtwinning in the CdTe(111)B grown by HWE on GaAs(111)B.

Based on our experimental results we may come out with a picture which may explain the development of the microtwinning in CdTe(111)B grown on Si(001) by MBE. Since the twin content is very sensitive to the substrate tilt direction which in turn determines the Si(001) surface step structure, The surface structure of the substrate must play some role in suppressing the microtwinning in CdTe(111)B layers. Figure 8a and 8b show schematic surface structure of misoriented Si(001) with  $\phi = 0$  and  $\phi > 0$  respectively. The only difference is the dense

kinks which are introduced when Si(001) is tilted towards a direction away from  $[110]$ .

In Fig. 8a Si(001) is tilted towards  $[110]$ . The step edge is rather flat, except for some thermally excited random kinks. Still the symmetry relative to  $(110)$  plane remains on such a surface. therefore CdTe(111)B layer has equal probability to be grown with its  $[11\bar{2}]$  aligned with either one of Si  $\langle 1\bar{1}0 \rangle$  axes, which leads to the formation of twins.

In Fig. 8b the Si(001) is tilted towards a direction with  $\phi$  value significantly greater than zero. The same kind of dense kinks is introduced at the step edges, which, as a consequence, destroys the symmetry of the Si(001) surface structure relative to  $(110)$  plane. Therefore CdTe(111)B layer has an unequal probability to be grown with its  $[11\bar{2}]$  aligned with Si  $[1\bar{1}0]$  or Si  $[\bar{1}10]$ . In fact there is a preferential orientation of the CdTe  $[11\bar{2}]$  along Si  $[1\bar{1}0]$  axis. Such a preferential orientation of the CdTe  $[11\bar{2}]$  has been confirmed by our experimental observation. We have measured numerous CdTe(111)B layers with x-ray diffraction. With no exception the CdTe  $[11\bar{2}]$  axis is always aligned with Si  $[1\bar{1}0]$ , as shown in Fig. 8b. Even for a twinned CdTe(111)B layer the domain of the CdTe(111)B with its  $[11\bar{2}] \parallel$  Si  $[1\bar{1}0]$  always gives large (422) x-ray diffraction intensity. In other words the CdTe(111)B layers tend to be grown with its  $[11\bar{2}]$  aligned with Si  $[1\bar{1}0]$  or upwards direction of the steps running along the Si  $[1\bar{1}0]$ . When the substrate tilt direction is reversed, the CdTe  $[11\bar{2}]$  is also reversed. Therefore, the kinks on the Si(001) surface do induce the preferential growth of CdTe(111)B, which can effectively prevent the formation of massive double-positioning twins at the interface as well as inside the CdTe layer. However, the microtwinning can happen in the other type of twin, namely lamellar twins. Since the lamellar twin boundary preserves the bonding between Cd and Te as shown in Fig. 1, we can expect the formation energy for a lamellar twin is very small. After the CdTe(111)B is initiated on the Si(001) substrate there is still a finite probability to

form the lamellar twins. For the CdTe/Si system the huge lattice mismatches both in horizontal and vertical directions make the initial growth of CdTe(111)B especially turbulent. In other words the system is in a very energetic state. Therefore, it is not surprising to see the dense lamellar twins crowded in the region close to the interface. As the layer thickness increases the strain caused by the lattice mismatches is being relaxed. The growth of CdTe(111)B is approaching the equilibrium state. The tendency to form lamellar twins is diminishing. This was also observed by our experiments. We have measured by x-ray diffraction the twin content of CdTe(111)B layers, grown on misoriented Si(001), with different layer thicknesses. We found that twin content decreases steadily as the layer thickness increases, when the layers are grown on the Si(001) with  $\phi$  greater than zero. On the other hand the twin content virtually remains constant as the layer thickness increases, when the layers are grown on Si(001) tilted towards [110]. The results are shown in Fig. 9. Another important fact is the preferential orientation of CdTe[11 $\bar{2}$ ] axis. Experimentally we have found the CdTe(111)B preserves the tilt of Si(001) substrate. That means that the CdTe(111)B has the similar step structure to that of the misoriented Si(001). Therefore, one domain of the CdTe(111)B, with its [11 $\bar{2}$ ] aligned with Si[1 $\bar{1}$ 0] has higher probability to be grown than its twin counterpart. Above are mentioned two factors which will enhance the suppression of the formation of the lamellar twins. At a certain point the domain with its [11 $\bar{2}$ ] aligned with Si[1 $\bar{1}$ 0] completely dominates the CdTe(111)B growth, and the twin-free layer is established.

Under such a model a twin-free CdTe(111)B layer can be divided into three regions, as shown in Fig. 10. In region I heavily lamellar twinning is presented due to turbulent initial growth of CdTe(111)B on Si(001). In region II only a few scattering lamellar twins are presented. The suppression of twin is attributed to the preferential orientation of CdTe[11 $\bar{2}$ ] axis

and relaxation of crystal lattice. Finally, in region III, twin-free layer is obtained as the domain of CdTe(111)B layer with its  $[11\bar{2}]$  axis aligned with Si $[1\bar{1}0]$  completely dominates the growth.

It is also interesting to note that a fully twinned layer is obtained when substrate tilt direction is approaching  $[100]$  ( $\phi=45^\circ$ ). This is understandable when we notice that Si(001) surface regains its  $90^\circ$ -rotation symmetry. Then the as-grown CdTe(111)B layer is plagued by double-domain defect as well as twins. Therefore substrate tilt direction must be carefully chosen so that a twin-free layer can be obtained.

For CdTe(111)B layers grown on misoriented Si(001) with  $\phi = 0$ , the results are quite different. Although the system is being relaxed as the layer thickness increases, the lamellar twins are still likely to happen since there is no preferential orientation of the CdTe $[11\bar{2}]$  axis. That is what we observed in our experiments. When Si(001) substrate is tilted towards  $[110]$ , even with tilt angle as large as  $4^\circ$ , a twinned CdTe(111)B layer is always obtained. It is also interesting to note that the substrate tilt angle plays little role in suppressing the microtwinning. It is so even for the substrate with  $\phi$  greater than zero. As we pointed out in our previous publication<sup>1</sup>, the step density on the surface is large for large tilt angle. Since at the step edge CdTe(111)B lattice suffers from huge distortion due to the large vertical lattice mismatch between the two materials, it is, in general, more difficult for the system to recover from such large distortion. As a result it is easier to stimulate the formation of the lamellar twins.

There are also some other factors which might affect the formation of twins, such as substrate preparation and growth conditions. Since the tendency to form twin-free layer is weak, any disturbance might stimulate the twin formation. Therefore it is suggested that extra care must be taken for the growth of CdTe(111)B on Si(001).

## CONCLUSIONS

We have reported that twin-free CdTe(111)B layers can be grown on misoriented Si(001). Suppression of twin formation is very sensitive to the substrate tilt direction ( $\phi$ ). Twinned layers are obtained when  $\phi$  value is about 0 or 45°. Twin-free layers are obtained when  $\phi$  is around 30° to 36°. The microtwins inside the CdTe(111)B layer are overwhelmingly dominated by the lamellar twins. Dense lamellar twins are always found in the region close to CdTe/Si interface. For a twin-free layer density of lamellar twin diminishes very fast as the layer thickness increases. Then a twin-free layer is established on such a twinned region. The major motive forces for suppression of twins are the preferential orientation of the CdTe  $[11\bar{2}]$  axis, which is introduced when substrate is tilted towards a direction with  $\phi$  significantly greater than zero, and the lattice relaxation as the layer thickness increases.

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FIGURE CAPTIONS:

Fig. 1 Two types of microtwin structures in CdTe(111) layer.

Fig. 2 Schematic illustration of substrate tilt and its tilt parameters.

Fig. 3 Schematic illustration of part of stereographic (111) projection, the projection in dash line shows presentation of twin as a result of  $180^\circ$ -rotation around [111] axis.

Fig. 4 a) Experimental set-up for measuring twin content in CdTe(111)B layers by x-ray diffraction, where  $\theta$  is Bragg angle for (422) reflection and  $\phi$  is rotation angle of the sample around its surface normal. b) Schematic illustration of x-ray rocking curves of CdTe(111)B layer measured by the set-up shown in a). Presentation of minor peaks indicates a twinned layer.

Fig. 5 Twin content of CdTe(111)B layers vs substrate tilt direction ( $\phi$ ) for two sets of tilt angles ( $\theta$ ).

Fig. 6 Twin content of CdTe(111)B layers vs substrate tilt angle ( $\theta$ ) for two sets of tilt directions ( $\phi$ ).

Fig. 7 Cross-section bright field TEM images of CdTe(111)B layer taken from different regions inside the layer, bright and dark contrast in the picture shows presentation of twins.

Fig. 8 Schematic step structure of Si(001) surface, a) Si(001) is tilted towards [110], b) Si(001) is tilted towards a direction rotated from [110] by an angle  $\phi$ , and orientation of CdTe(111)B grown on such Si(001) substrate is also shown in up-right corner.

Fig. 9 Twin content of CdTe(111)B layers vs the layer thickness with three sets of tilt parameters.

Fig. 10 Schematic cross-section illustration of evolution of twin structure in CdTe(111)B layers.

Fig. 1

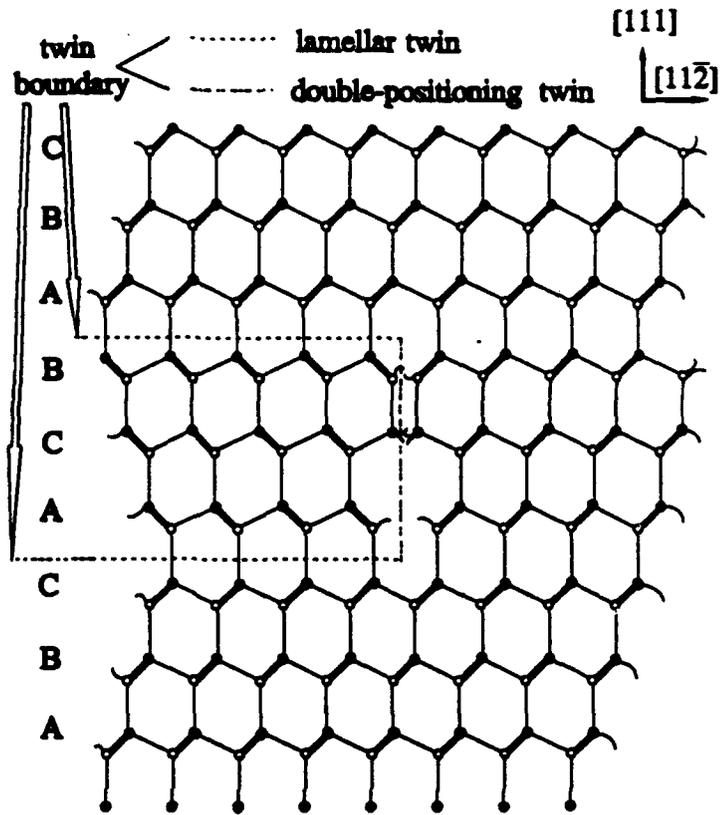


Fig. 2

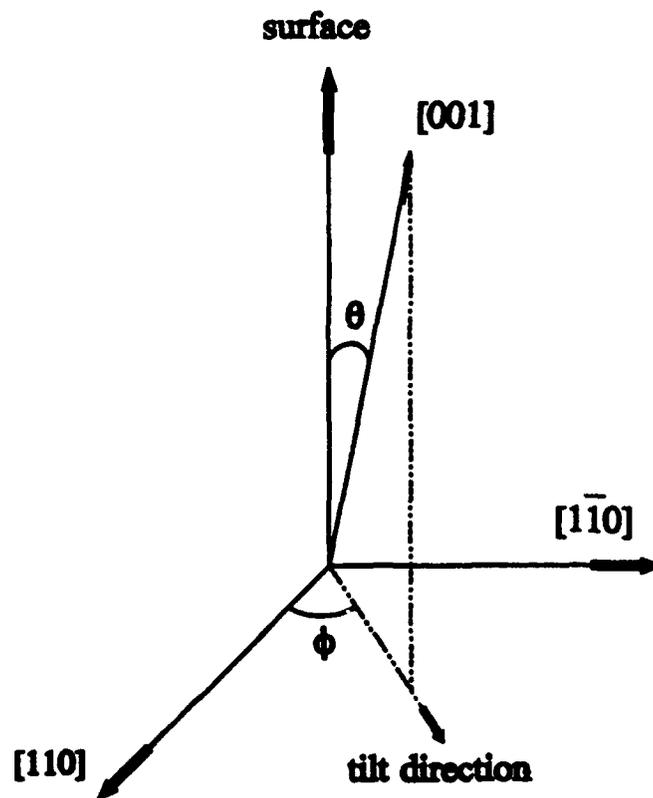


Fig. 3

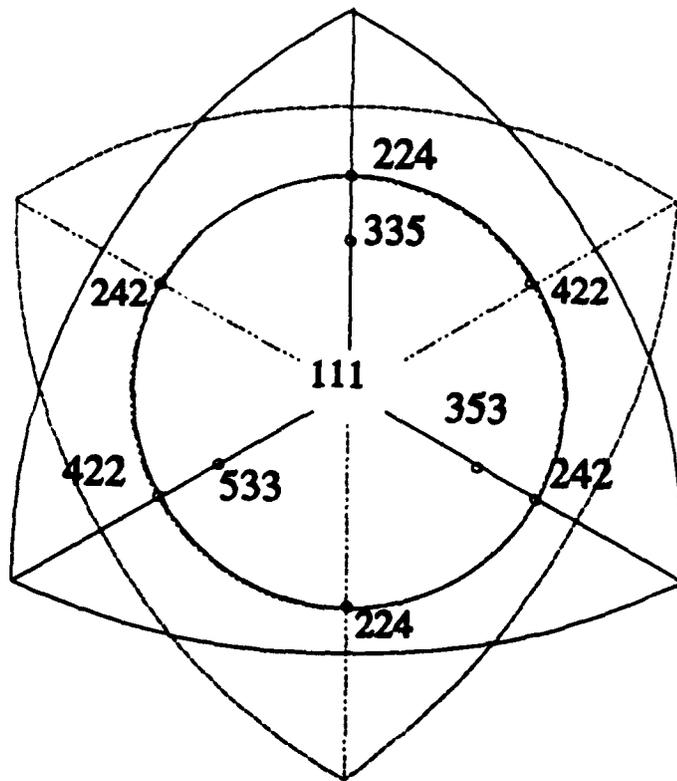


Fig. 4a

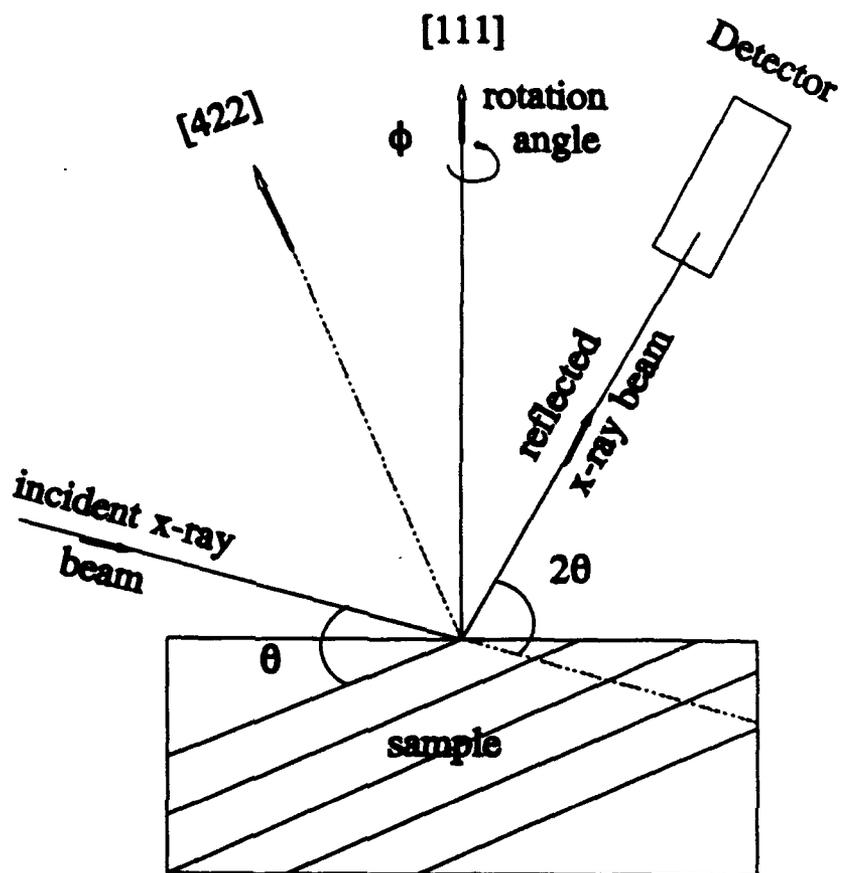


Fig. 4b

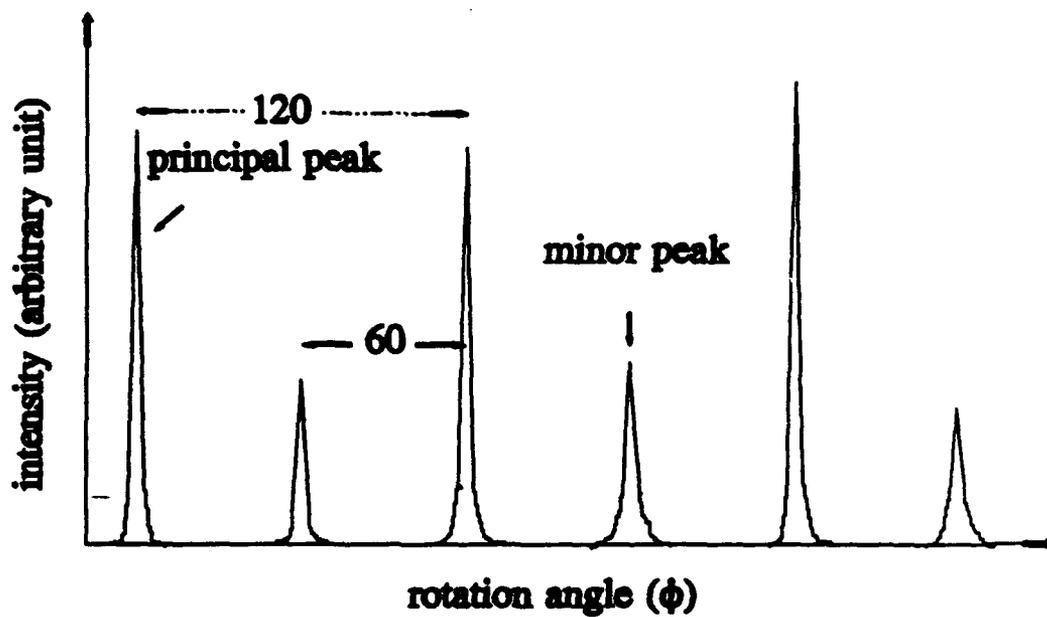


Fig. 5

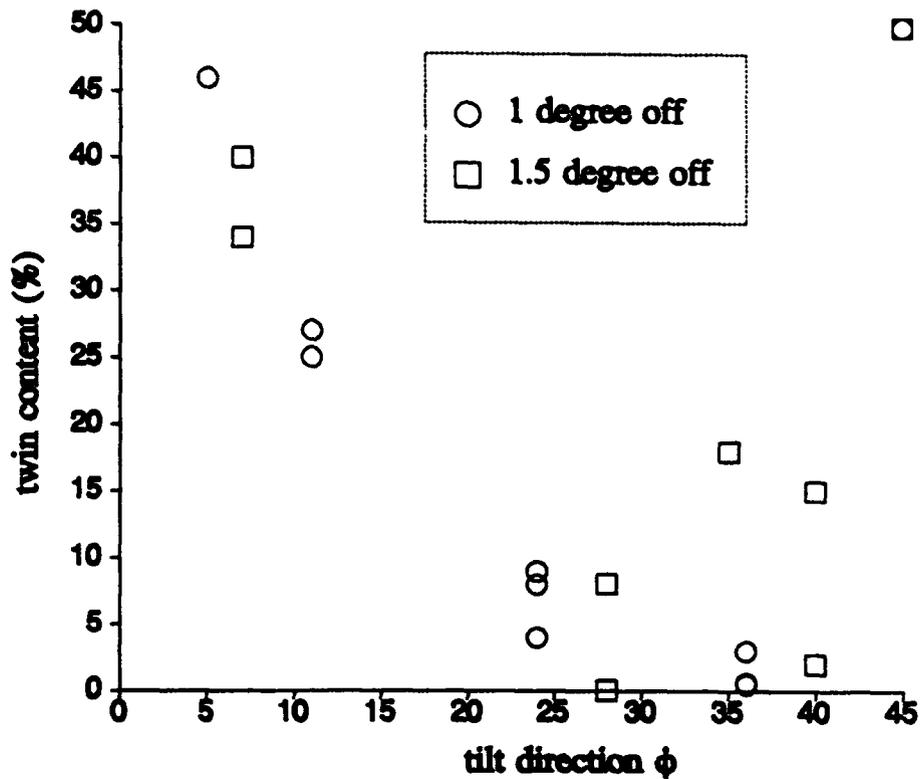
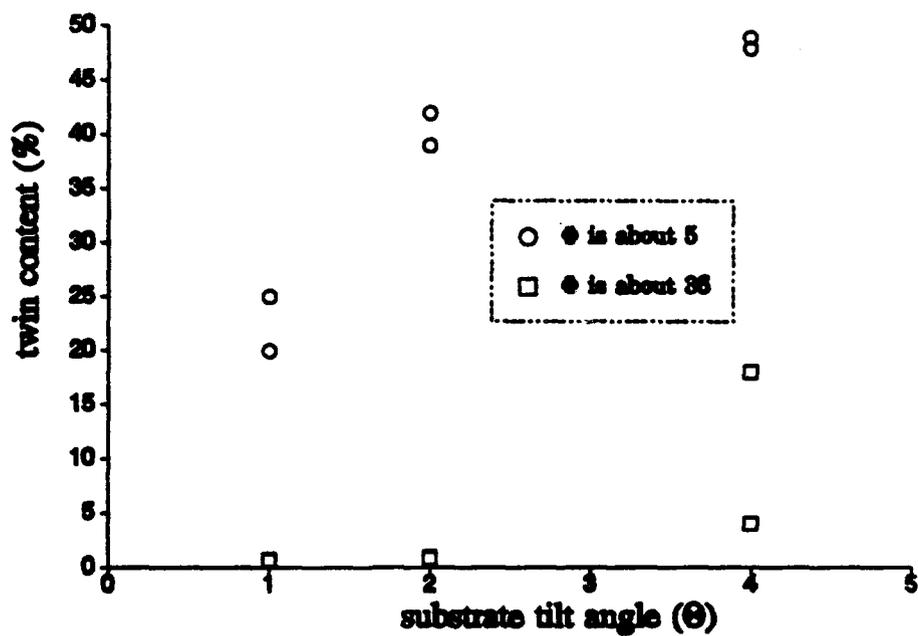


Fig. 6



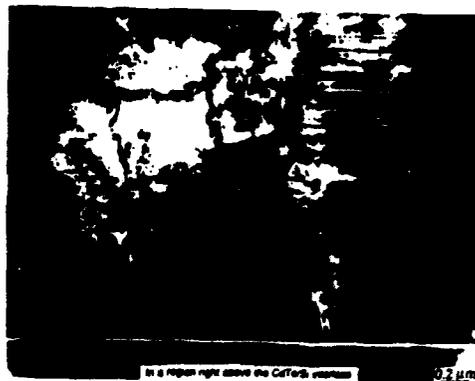
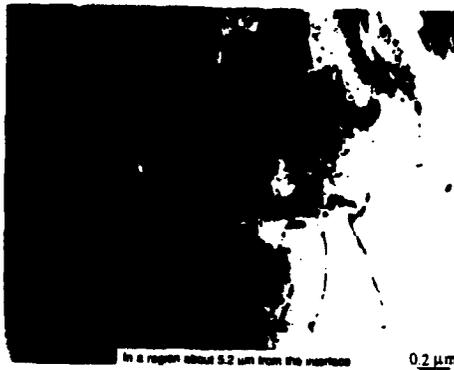


Fig. 7

Fig. 8a

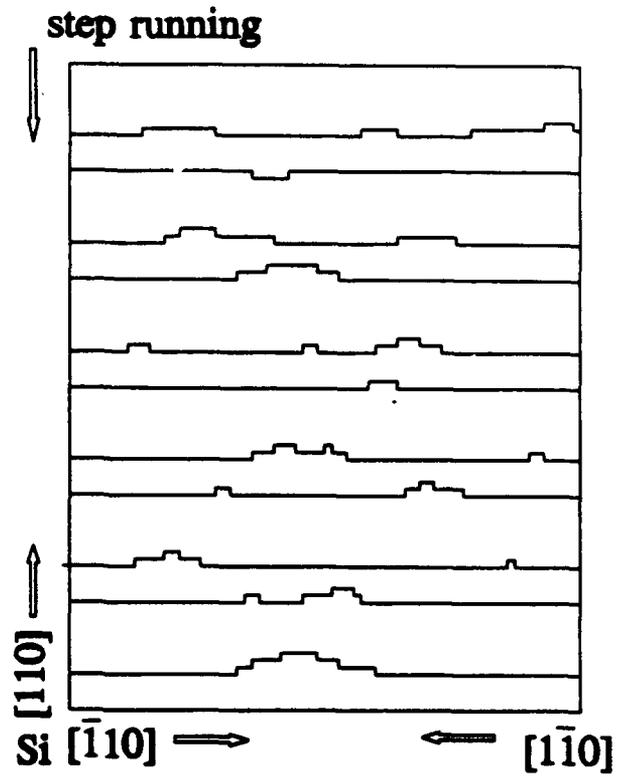
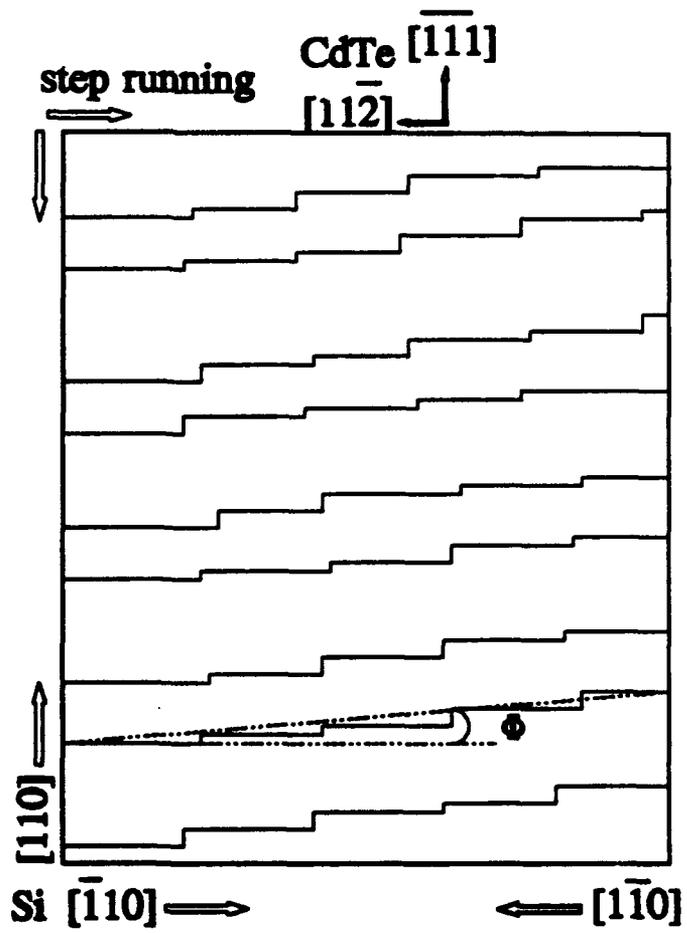


Fig. 8b



(ORNA) 11-11-11

at 1000°C  
Si(100) substrate

Fig. 9

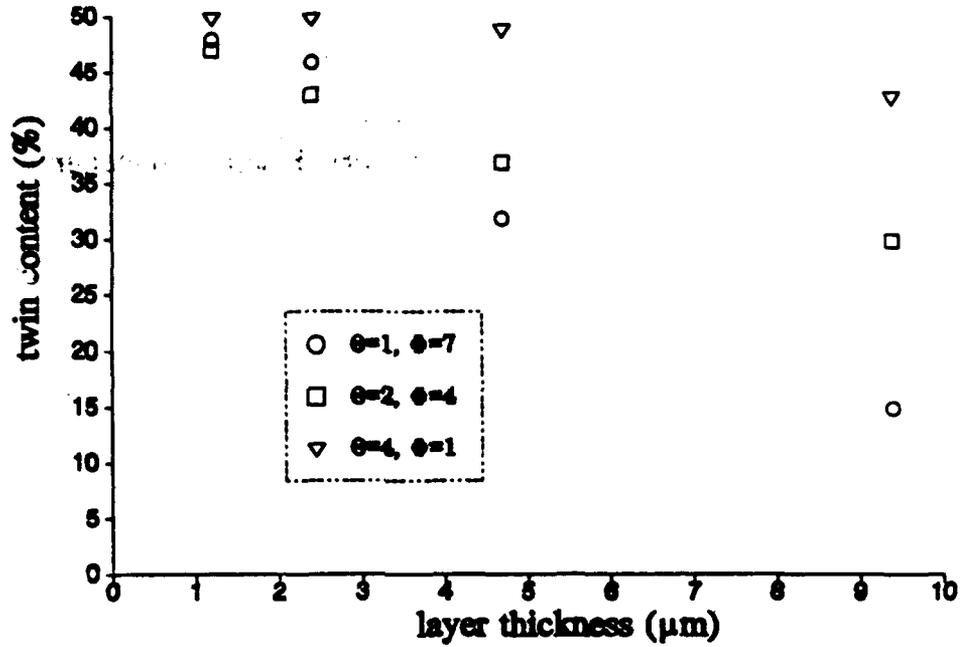


Fig. 10

