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GaAs Substrates for the MOVPE Growth of (Hg,Cd)Te Layers

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After a review of the structural properties of (Hg,Cd)Te layers grown by MOVPE on GaAs substrates, topical questions such as out-diffusion of Ga and As from the substrate into the layers, monolithic integration of signal processing into the substrate and the presence of pyramidal defects in (100) layers will be discussed. In order to solve the last problem, a systematic study of the influence of the (*h*11) GaAs substrate orientation and polarity on the structural properties and surface morphology of CdTe layers grown by MOVPE has been carried out. Twin-free layers are obtained on (211)*A*, (311)*B* and (511)*B* GaAs surface orientations as explained by a model taking into account the type of dangling bonds at the interface. The performance of photoconductors fabricated on (Hg,Cd)Te layers of various orientations confirms these results. Particularly good results have been obtained for the (311)*B* orientation.

KEYWORDS Substrates MOVPE MCT Surface morphology Structural properties Photoconductors

INTRODUCTION

The lack of high-quality, large-area, low-price CdTe substrates has prompted extensive research in the area of alternative substrates for epitaxial growth of (Hg,Cd)Te (MCT). The capability of growing good-quality CdTe layers directly on GaAs substrates, in spite of a very large lattice mismatch of 13.6% was demonstrated by Mullin *et al.*[1] in 1981. Various questions associated with the use of GaAs substrates will be discussed: structural properties of the MCT epilayers, the orientation of the epitaxial layer on (100)-oriented GaAs surfaces, out-diffusion of Ga and As from the substrate into the layers, monolithic integration of electronic functions into the substrate and the presence of pyramid-shaped defects on (100) surfaces. In order to solve the last problem, a systematic investigation of the influence of the (*h*11) GaAs surface orientation and polarity on the structural properties and surface morphology of CdTe layers deposited by MOVPE has been carried out. The results are confirmed by the performance of photoconductors fabricated on MCT layers of various orientations.

STRUCTURAL PROPERTIES OF MCT LAYERS GROWN ON GaAs SUBSTRATES

The use of GaAs substrates is restricted to epitaxial growth techniques in the vapour phase such as MOVPE and MBE.

Table 1 displays typical results of double-crystal rocking curve (DCRC) widths of MCT layers grown on buffered GaAs substrates together with some values for growth on CdTe for comparison.

Despite the very large lattice mismatch between MCT and GaAs, similar DCRC widths have been measured on both GaAs and CdTe, and slightly better values by MBE than by MOVPE.

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Table 1. Structural properties of MCT layers grown by MOVPE and MBE on GaAs substrates

Technique of growth	GaGs orientation	MCT layer orientation	Layer thickness (μm)	DCRC-FWHM (arcsec)	Ref.
MOVPE	(311)*B*	311	Not stated	150–200	2
MOVPE	100	100 111	15–20	80–140 240–480	3
MOVPE	(100)2° → (110)	100	~12	< 84(8 × 8 mm^2) (best 55) 67–135(9 × 7.5 mm^2) on CdTe	4
MOVPE	(100)2° → (110)	100	~6	110 125 on CdTe	5
MOVPE			12	47–51 on Cd(Se,Te)	6
MBE	(211)*B*	211	~17.5	60	7

ORIENTATION OF CdTe EPITAXIAL LAYERS OF (100)-ORIENTED GaAs SURFACES

The growth of CdTe on (100) GaAs surfaces results in either (100)- or (111)-oriented layers depending on the structure of the GaAs surface, i.e. on the growth conditions and treatment of the surface prior to growth.

Various mechanisms have been suggested to explain these observations, based on considerations of interfacial phases of Te[8,9] or oxides[8,10] and on the influence of surface treatment prior to growth leading to micropits as nucleation sites[8,11,12] or to a variation in relative surface coverage of As and Ga.[8] In order to account for the heteroepitaxy of CdTe on (100) GaAs substrates, Cohen-Solal *et al.*[13] have proposed a model based on the formation, during the early stage of growth, of stable clusters of chemically bound tellurium atoms. According to this model, two types of cluster configurations are obtained depending on the atomic structure of the (100) GaAs surface: the first type, made up of tetrahedral unit cells is formed on an As-deficient surface and leads to a (111) orientation, whereas the second type, formed by twin tetrahedral structures developed on an As- or Ga-stabilised surface, gives rise to a (100) orientation.

OUT-DIFFUSION OF Ga AND As INTO THE LAYERS

The out-diffusion of Ga and As from the substrate into the layer has been stressed as a factor affecting the purity and electronic properties of the epitaxial layer. Ga migration into CdTe layers has been reported several times.[14–20] The presence of extended defects[17–21] and various substrate orientations[20] have been reported to enhance Ga diffusion. It has been found that growth on the (111)*B* orientation results in approximately 100 times more Ga incorporation than on the (111)*A* orientation, the (100) orientation falling between these other two.[20] These results were explained in terms of the chemical reactivity of each surface. The use of CdTe layers at least 0.5 μm thick[6] but less than 1μm thick[22] has been shown to significantly reduce the Ga penetration into the MCT layers. Ga can be reduced to background detection levels by growing a sufficiently thick buffer layer (8μm)[14] or by the use of CdTe/ZnTe superlattice buffer layers and nucleation on near-atomically planar GaAs surfaces.[17] It has also been suggested that the transport of Ga and As in the reactor through mechanisms involving chemical reactions of the organometallics at the rear surface of the GaAs substrates could be a source of Ga doping.[19,20,22]

MONOLITHIC INTEGRATION OF ELECTRONIC FUNCTIONS INTO THE SUBSTRATE

GaAs is still significantly less well developed than Si for the integration of signal processing. Nevertheless, in a preliminary study the possibility of integration of an interdigitated photoconductor (CdTe in a first step) with an AlGaAs FET has been demonstrated.[23] The authors showed that the intrinsic conduction properties of CdTe are not affected by the GaAs substrate. The realised photoconductors were reported to exhibit a maximum gain of 8, a response of 2 A W^{-1} and a gain-bandwidth product equal to 160 MHz at $V = 4$ V and $\lambda = 0.77$ μm. The FET contributed to an increase in the photoconductor response by a factor of 15. The authors stated that an integregation of the MCT/GaAs type capable of opening up new horizons in terms of optical fibre telecommunication (1.3–1.55 μm) and IR imagery (3–5 μm) could therefore be considered.

STRUCTURAL AND ELECTRONIC PROPERTIES OF MCT LAYERS VS. GaAs SUBSTRATE ORIENTATION AND POLARITY

A worrying problem, frequently stressed, is the presence of pyramid-type defects, so-called hillocks, that can develop on the surface of (100) MCT/(100) GaAs heterostructures and severely affect device fabrication.

Several solutions have been proposed to lower the hillock density:

(i) the use of alternative buffer layer strategies such as combinations of discrete CdTe and HgTe layers[24,25] or graded buffer layers, from ZnTe to CdTe, together with growth interruptions during IMP deposition[19]

(ii) a tilt of 3–4° of the (100) GaAs surface towards the (111)*B* plane;[26]

(iii) the use of various (*h*11)*A* or *B* GaAs orientations.

Pain *et al.*[2] have shown that MCT growth on (311), (511) and (711) GaAs substrates of both *A*- and *B*-polarity yields layers of superior morphology compared with layers grown on (100) or (100)2° → (110) GaAs substrates. The best results were obtained for the (311)*B* orientation with DCRC-FWHMs of 150–200 arcsec. Broader values (~700 arcsec) were obtained on the (511) and (711) orientations. Lange *et al.*[27] have reported on high-crystalline-quality CdTe layers of both (211) and especially (311) orientations grown by MBE on (211)*B* GaAs substrates. Arias *et al.*[7] have measured typical DCRC-FWHMs of 1.0 arcmin for MCT/CdTe layers on (211)*B* GaAs while Yuan *et al.*[28] have found good electrical properties on the same heterostructure with $x_{Cd} = 0.36$.

In an attempt to solve this problem of hillocks, we have carried out a systematic investigation of the influence of the (*h*11) GaAs substrate orientation and polarity on the structural and electronic properties and surface morphology of CdTe and MCT/CdTe layers grown by MOVPE. The polarity of the (*h*11)GaAs surface was determined without ambiguity by electron microscopy.[29] The experimental techniques that have been used in this study are double-crystal X-ray diffraction (DCXRD) to assess the structural quality of the CdTe and MCT layers, electron-channelling patterning (ECP) to determine the tilt of the layers and cross-sectional transmission electron microscopy (TEM) to observe the atomic planes at the CdTe/GaAs interface.

Two different growth orientations of the CdTe layers are found on (211)*B* and (311)*A* GaAs from TEM experiments.[30] (311) and (011) CdTe coexist on (311) GaAs, while (211) and (133) CdTe coexist on (211)*B* GaAs as already pointed out by Faurie *et al.*[31] (311) CdTe on (311)*A* GaAs and (211) CdTe on (211)*B* GaAs can be explained by a rule, found experimentally, governing the growth of CdTe on GaAs by MOVPE at a growth temperature of about 350 °C: there is a continuity of the most inclined (111) atomic planes (lowest 'interface/(111) plane' angle) through the GaAs/CdTe interface. For (311) CdTe/(311)*A* GaAs and (211) CdTe/(211)*B* GaAs the alignment of the (111) planes necessitates a tilt of 5° and 3° respectively to account for the lattice parameter difference between GaAs and CdTe, as found experimentally. For an interface at an angle θ to the substrate (111) planes, the layer is tilted by an angle ϕ, the two being related by the classical equation[32]

$$d_{GaAs}/\sin\theta = d_{CdTe}/\sin(\theta + \phi)$$

Here d_{GaAs} and d_{CdTe} are the interplanar distances for the planes in continuity through the interface. (011) CdTe/(311)*A* GaAs and (133) CdTe/(211)*B* GaAs correspond to a rotation of 109° of the (111) CdTe planes around $[0\bar{1}1]$ associated with twining, leading to an alignment of (111) GaAs planes with (200) CdTe. The transition between two orientations, (311) and (011) on (311)*A* GaAs and (133) and (211) on (211)*B* GaAs, constitutes a twining (111) CdTe plane, both orientations having a common ⟨111⟩ direction. This is expressed by the high density of twins found in

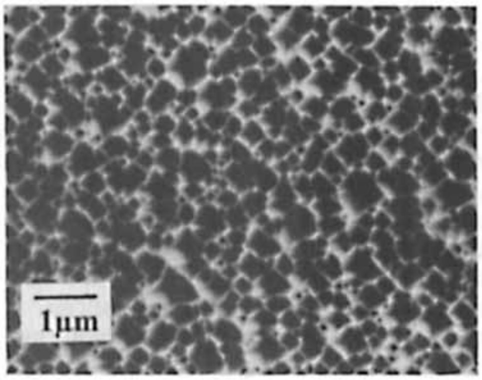

Fig. 1. Surface morphology of CdTe layers grown on (211)*A* GaAs substrates

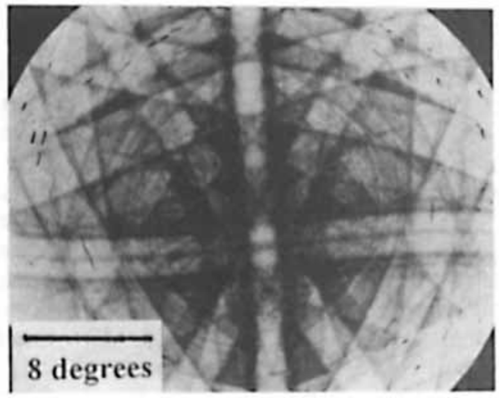

Fig. 3. Electron-channelling pattern of a CdTe layer grown on a (211)*A* GaAs substrate

the layers grown on (211)*B*, (311)*A* and likely on (511)*A* GaAs.

We propose an explanation based on the type of dangling bonds present on the GaAs surface after chemical etching to account for the presence or absence of twining.

Let us consider as an example the results obtained on (211) surfaces. On the *A*-face the surface morphology is not very smooth, but is regularly faceted without polycrystalline defects (Fig. 1). No twining is seen on TEM cross-section micrographs; however, numerous dislocations, about 10^8 cm^{-2}, rise from the interface through the buffer layer (Fig. 2). The ECP picture displays a tilt of $\sim 4°$ (Fig. 3) and the orientation of the surface lies between (211)*A* and (311)*A* owing to some rotation around [011]. This asymmetry is verified using DCXRD measurements in two orthogonal directions. The narrowest DCRC-FWHM (180 arcsec) occurs when the measurement axis is parallel to the cleavage plane. On the *B*-face the surface is rough (Fig. 4) as confirmed by the poorly defined pseudo-Kikuchi lines of Fig. 5, which gives a disorientation of $\sim 4°$ around the $[0\bar{1}1]$ axis, as for the *A*-face. The rocking curve widths are larger than those measured on the (211)*A* layer. The TEM cross-section micrograph indicates that twining occurs at the interface (Fig. 6).

The atomic structures of ideal *A* and *B* (211) surfaces projected on the $(0\bar{1}1)$ plane, as presented in Figs. 7(a) and 7(b), show that these surfaces

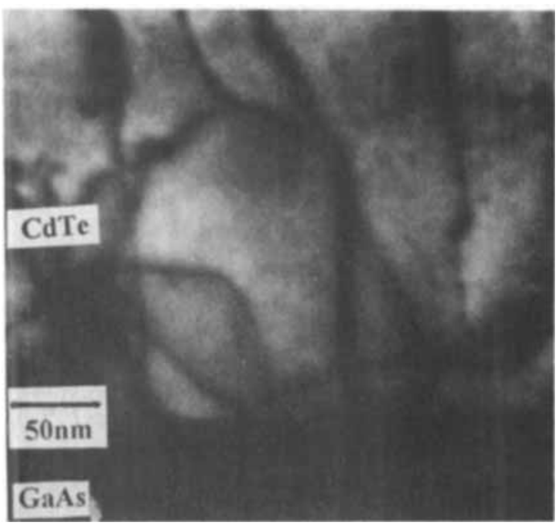

Fig. 2. TEM cross-section micrograph of a CdTe layer grown on a (211)*A* GaAs substrate

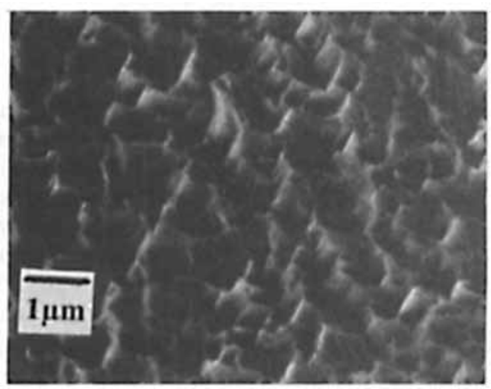

Fig. 4. Surface morphology of CdTe layers grown on (211)*B* substrates

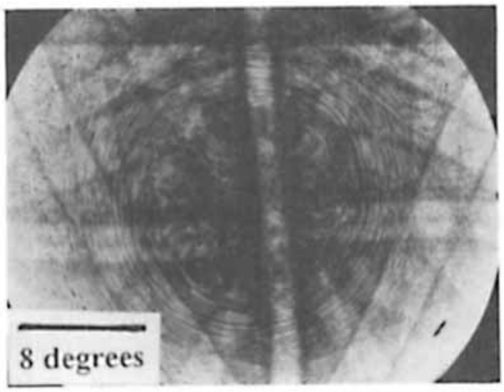

Fig. 5. Electron-channelling pattern of a CdTe layer grown on a (211)*B* GaAs substrate

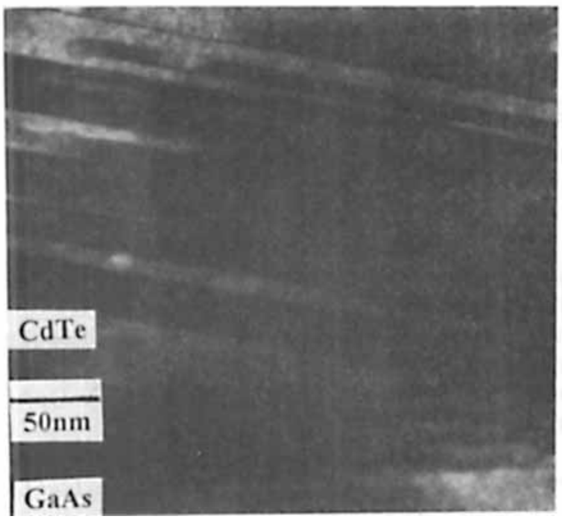

Fig. 6. TEM cross-section micrograph of a CdTe layer grown on a (211)*B* GaAs substrate

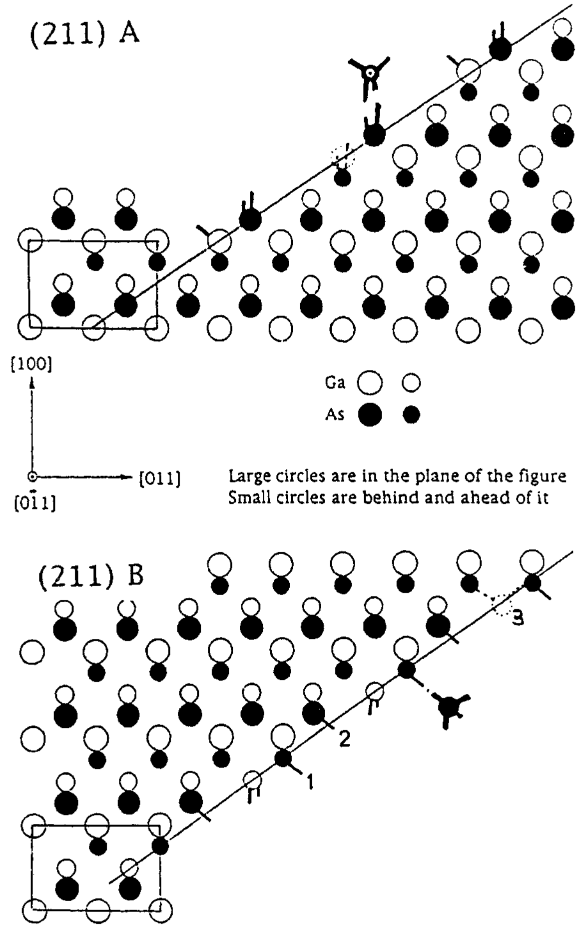

Fig. 7. Atomic structure of ideal (a) (211)*A* and (b) (211)*B* GaAs surfaces

expose an equal number of Ga and As atoms but the bonds are not identical. Ga atoms, as shown by several authors,[33–35] are preferentially removed by chemical etching from the GaAs surface, leaving it As-rich. On the (211)*A* surface the remaining As atoms, with double dangling bonds, are able to induce epitaxy without twining, while the remaining As atoms on the *B*-face present single dangling bonds that may induce twins, visible in the TEM micrograph (Fig. 6)

The same kind of consideration holds for the (311) and (511) orientations. The presence of single dangling bonds on the (311)*A* and (511)*A* faces after chemical etching is at the origin of twining, while the double dangling bonds on the (311) and (511)*B* faces prevent twining, as verified experimentally and analysed in detail in Ref. 36.

It is thus demonstrated that the (211)*A*, (311)*B* and (511)*B* faces present structures that avoid twining.

MCT layers 10 μm thick ($x = 0.3$) have been deposited on these CdTe/GaAs hybrid substrates by MOVPE according to the interdiffused multilayer process.[19]

The DCRC-FWHMs measured on these layers are given in Table 2.

Photoconductors have been fabricated on these layers in Société Anonyme de Télécommunications. Their detectivity at 300 K as a function of their cut-off wavelength is presented in Fig. 8.

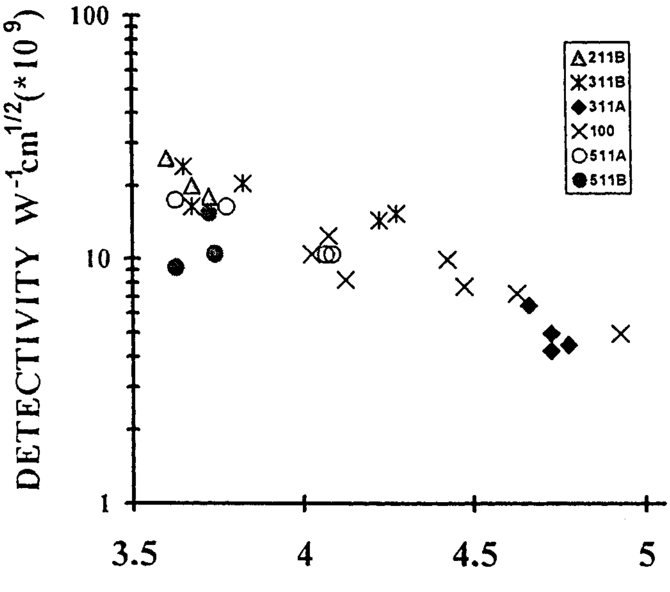

Fig. 8. Detectivity at 300 K and 10 kHz of photoconductors fabricated on MCT layers grown on GaAs substrates of various orientations and polarities

Table 2. DCRC-FWHMs of MCT layers grown by IMP on GaAs substrates of various (*h*11) orientations and polarities

Orientation	DCRC-FWHM (arcsec)
⟨100⟩	150
⟨211⟩*A*	320
⟨211⟩*B*	320
⟨311⟩*A*	200
⟨311⟩*B*	220
⟨511⟩*A*	250
⟨511⟩*B*	380

Particularly good results are obtained on (311)*B* orientations, demonstrating the importance of twin-free layers, as confirmed by lifetimes greater than 600 ns at 150 K measured by transient wave reflectance (TWR) at LTV Aerospace and Defence Co. on our (311)*B* samples.[37]

CONCLUSIONS

MCT layers of excellent structural and electronic properties can be deposited on GaAs substrates by MOVPE or MBE. The presence of extended defects and specific orientations enhance Ga diffusion. Ga doping can also occur through mechanisms involving chemical reactions of the organometallics at the rear surface of the GaAs substrates.

Two modes of growth leading to two different orientations have been shown to coexist on (211)*B* and (311)*A* GaAs faces and to be at the origin of twining. A model taking into account the type of dangling bonds on the GaAs surface after chemical etching has been suggested to explain the presence of twins on (211)*B*, (311)*A* and (511)*A* faces and their absence on (211)*A*, (311)*B* and (511)*B* faces. High-performance MCT photo conductors have been obtained on these non-standard orientations, mainly on (311)*B*.

All these results show that CdTe-buffered GaAs is a viable alternative to CdTe substrates for (Hg,Cd)Te for some applications. Nevertheless, luminescence experiments have shown that CdTe layers deposited on CdTe substrates by MOVPE present better optical properties than those deposited on GaAs,[38] while devices with higher performance have been obtained on MCT layers deposited on CdZnTe substrates than on GaAs.[39]

These results stress the prime importance of lattice-matched substrates.

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