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Determination of the Unit Cell for an Epitaxial Layer of $Hg_{1-x}Cd_xTe$ Deposited on GaAs

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Abstract

Stevenson *et al.* (1991) reported structural aspects of six metal organic chemical vapour deposition (MOCVD)-grown $Hg_{1-x}Cd_xTe$ epitaxial layers on novel GaAs substrates. Large layer miscuts (the angle between the surface and the Bragg planes of the nominal orientation) of 4·3° were reported for the samples of (311) and $(\bar{3}\bar{1}\bar{1})$ orientation, whereas the substrate miscuts were less than 1° (0·94° and 0·84° respectively). Double-crystal diffractometry has been used, employing the method described by Li Runshen and Zhu Nanchang (1990), to accurately determine the distorted unit cell of the $Hg_{1-x}Cd_xTe$ $(\bar{3}\bar{1}\bar{1})$ layer and its orientation relative to the unit cell of the GaAs $(\bar{3}\bar{1}\bar{1})$ substrate. The lattice parameters and angles for the layer have been determined to be $a = 6{\cdot}466(1)$ Å, $b = 6{\cdot}462(1)$ Å, $c = 6{\cdot}462(1)$ Å, $\alpha = 90{\cdot}00(1)°$, $\beta = 89{\cdot}99(1)°$ and $\gamma = 89{\cdot}94(1)°$. The tilt angle between the layer and the substrate is 4·66° (the direction of tilt of the layer being largely toward the substrate $[0\bar{1}\bar{1}]$ reciprocal-lattice direction). Four-circle diffractometry is used to relate the disposition of the unit cells to the sample surface.

1. Introduction

$Hg_{1-x}Cd_xTe$ (MCT) is a ternary alloy with the cubic zincblende structure. It is currently receiving much attention because of its applications in areas such as infrared detection, optoelectronic devices and solar cells. Stevenson, Gao, Pain and Wieluński (1991, hereafter SGPW) studied various structural aspects of six MCT samples, deposited as thin epitaxial layers (of order 1 to 2 μm thick) on novel GaAs substrates by metal organic chemical vapour deposition (MOCVD). The interest in GaAs, rather than say CdTe, as a substrate for MCT is due, at least in part, to its inexpensiveness, excellent structural quality and the availability of large-area material. The growth conditions and other details of these six samples were given by SGPW. These authors reported that large layer miscuts (the angle between the sample surface and the Bragg planes of the nominal orientation) of 4·3° existed for the samples of (311) and $(\bar{3}\bar{1}\bar{1})$ orientation; whereas the substrates (possessing the same orientation as the corresponding layer) have miscuts of only 0·94° and 0·84° respectively. We note that all six MCT/GaAs samples studied by SGPW had epitaxial layers whose orientation essentially followed that of the substrate [substrate-oriented (SO) layers rather than rotation-oriented (RO)* layers—see, for example, Cinader and Raizman (1992);

* The RO orientation is obtained by rotating the SO orientation by 180° about the $[\bar{1}11]$ direction and corresponds to the twin configuration.

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Smith *et al.* (1990)]. These results were obtained using a computer-controlled four-circle X-ray diffractometer.

The results presented in this paper were obtained using a computer-controlled high-resolution double-crystal X-ray diffractometer, and supplement the earlier four-circle diffractometer results. Double-crystal X-ray diffraction has been widely used to measure lattice constants of epitaxial layers, and so determine composition in systems such as $Ga_{1-x}Al_xAs/GaAs$ (e.g. Hornstra and Bartels 1978; Bartels and Nijman 1978; Pietsch and Borchard 1987). Our research on $Hg_{1-x}Cd_xTe/GaAs$ samples stems from the current interest in such systems for device applications. There is a very large lattice mismatch between MCT and GaAs (approximately 14·4%), the lattice constants of bulk CdTe, HgTe and GaAs being 6·481 Å (National Bureau of Standards 1964), 6·4604 Å (ASTM Card No. 32-665) and 5·6538 Å (ASTM Card No. 32-389) respectively. It is therefore of particular interest to accurately determine the unit cell, including any distortions, of MCT epitaxial layers on GaAs substrates.

Li Runshen and Zhu Nanchang (1990) described a method of accurately determining the unit cell of a single crystal and its orientation relative to a standard or reference crystal, e.g. a substrate. We employ this method for the MCT $(\bar{3}\bar{1}\bar{1})$/GaAs $(\bar{3}\bar{1}\bar{1})$ sample of SGPW. That is, the unit cell of the MCT $(\bar{3}\bar{1}\bar{1})$ epitaxial layer and its orientation relative to the GaAs $(\bar{3}\bar{1}\bar{1})$ substrate will be determined. Four-circle diffractometry is used to relate the disposition of the MCT and GaAs unit cells to the extended sample surface.

2. Experimental

The rocking curves collected in this paper were obtained with a computer-controlled high-resolution X-ray double-crystal diffractometer. The monochromator used was a symmetric Si (511) crystal and the asymmetric 311 Bragg planes (with maximum possible negative asymmetry)* were used to diffract Cu $K\alpha_1$ X-radiation from a normal focus Cu tube run at 35 kV, 20 mA in spot-focus mode. The angle between the incident X-ray beam and the Si surface was approximately 18·6° (asymmetry parameter $b = 0·52$). Three sample Bragg reflections were selected for measurement: $\bar{3}\bar{1}\bar{1}$, $\bar{4}00$ and $\bar{4}0\bar{4}$. The double-crystal diffractometer, arranged in the $(+,-)$ setting, will yield rocking curves with varying amounts of dispersion. In the current experiments this was not, however, thought to be a problem as we are primarily interested in peak positions.

The rocking curves were collected so that the accumulated X-ray count at each point reached a predetermined level and the results were then converted to counts per second (cps). The angular step size could be varied during the scan.

3. Results

The rocking-curve results are summarised in Table 1 for four azimuthal positions of the $\bar{3}\bar{1}\bar{1}$ reflection, four positions of the $\bar{4}00$ and three positions of the $\bar{4}0\bar{4}$. Various Bragg reflections were used as reference reflections to ensure the correct azimuthal orientation of the sample on the diffractometer. These reference

* Except for one rocking curve which was collected with the 511 (symmetric) Bragg planes (see Table 1).

reflections were selected so that quite different azimuthal positions of the $\bar{3}\bar{1}\bar{1}$, $\bar{4}00$ and $\bar{4}0\bar{4}$ reflections were achieved. The substrate peaks generally have quite small FWHMs, the $\bar{4}00$ #2 result is a little larger because of the negative asymmetry involved. The $\bar{4}0\bar{4}$ #1 and $\bar{4}0\bar{4}$ #2 substrate FWHMs are larger because of the considerable dispersion present, whereas there is little dispersion contributing to the $\bar{4}0\bar{4}$ #3 result (the Bragg angles involved are: Si 311 28·1°; Si 511 47·5°; GaAs $\bar{3}\bar{1}\bar{1}$ 26·9°; GaAs $\bar{4}00$ 33·0°; GaAs $\bar{4}0\bar{4}$ 50·4°; MCT $\bar{3}\bar{1}\bar{1}$ 23·3°; MCT $\bar{4}00$ 28·5°; MCT $\bar{4}0\bar{4}$ 42·4°). The layer peaks have FWHMs which display some anisotropy. For example, the four $\bar{3}\bar{1}\bar{1}$ results, which are all essentially symmetric reflections, have quite a range of FWHMs (the $\bar{3}\bar{1}\bar{1}$ #2 and $\bar{3}\bar{1}\bar{1}$ #4 results being quite consistent with the rocking-curve measurements of SGPW).

Table 1. Summary of rocking-curve results for the eleven reflections studied from the MCT ($\bar{3}\bar{1}\bar{1}$)/GaAs ($\bar{3}\bar{1}\bar{1}$) sample

hkl and #	FWHM (arcsec)		Separation (deg.)	Asymmetry
	Substrate	Layer	(Layer–substrate)	(approx.)
$\bar{3}\bar{1}\bar{1}$ #1	10·2	81·5	−8·2491	zero
$\bar{3}\bar{1}\bar{1}$ #2	9·1	140·9	−5·0676	zero
$\bar{3}\bar{1}\bar{1}$ #3	10·4	87·7	1·0567	zero
$\bar{3}\bar{1}\bar{1}$ #4	8·7	133·3	−1·9746	zero
$\bar{4}00$ #1	10·0	97·4	−9·1956	pos.
$\bar{4}00$ #2	25·0	121·4	0·0678	neg.
$\bar{4}00$ #3	12·7	174·1	−4·2434	zero
$\bar{4}00$ #4	13·0	168·4	−4·6798	zero
$\bar{4}0\bar{4}$ #1	46·9	159·0	−9·5550	v. neg.
$\bar{4}0\bar{4}$ #2	47·3	154·6	−6·2925	v. pos.
$\bar{4}0\bar{4}$ #3*	17·9	114·0	−4·2713	zero

* All other rocking curves were collected with a Si (511) crystal, using the asymmetric 311 Bragg planes (with maximum possible negative asymmetry). This rocking curve was collected with the 511 (symmetric) Bragg planes.

The results in Table 1 show that the layer peak is generally on the low-angle side of the substrate peak. However, for the $\bar{3}\bar{1}\bar{1}$ #3 and $\bar{4}00$ #2 results this trend is reversed, due essentially to the large change in orientation of the MCT ($\bar{3}\bar{1}\bar{1}$) layer relative to the GaAs ($\bar{3}\bar{1}\bar{1}$) substrate. Fig. 1 shows the $\bar{4}00$ #2 result, both peaks being quite symmetric. Fig. 2 shows the four $\bar{3}\bar{1}\bar{1}$ results with the substrate peak positioned at 0° in each case. The results have been displaced along the vertical axis by 0, 10 000, 20 000 and 30 000 cps respectively for clarity of presentation.

The separations between the layer and substrate peaks for the eleven cases in Table 1 were analysed in the manner described by Li Runshen and Zhu Nanchang (1990) to yield the following results for the layer:

$$\boldsymbol{a} = 6{\cdot}444\,\boldsymbol{i} + 0{\cdot}358\,\boldsymbol{j} + 0{\cdot}387\,\boldsymbol{k}\ \text{Å},$$

$$\boldsymbol{b} = -0{\cdot}352\,\boldsymbol{i} + 6{\cdot}453\,\boldsymbol{j} - 0{\cdot}007\,\boldsymbol{k}\ \text{Å},$$

$$\boldsymbol{c} = -0{\cdot}386\,\boldsymbol{i} - 0{\cdot}015\,\boldsymbol{j} + 6{\cdot}451\,\boldsymbol{k}\ \text{Å}.$$

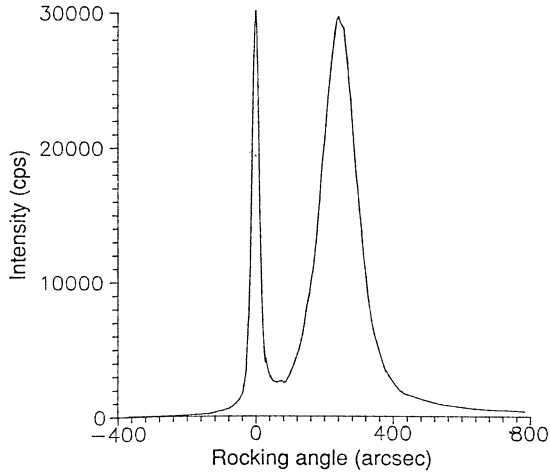

Fig. 1. Rocking curve ($\bar{4}00\#2$) for the $\bar{4}00$ Bragg reflection (negative asymmetry) of the MCT $(\bar{3}1\bar{1})$/GaAs $(\bar{3}1\bar{1})$ sample.

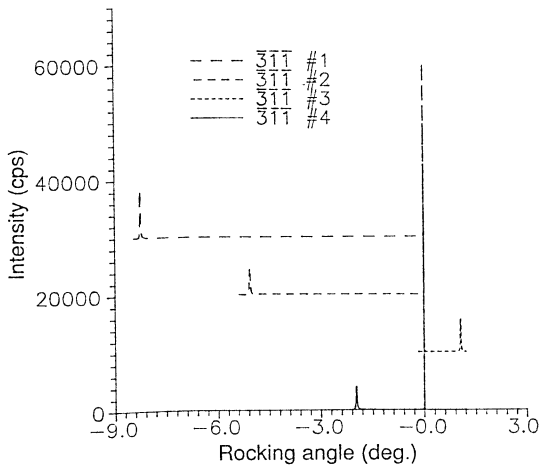

Fig. 2. Rocking curves for the $\bar{3}1\bar{1}$ Bragg reflection (all essentially symmetric) of the MCT $(\bar{3}1\bar{1})$/GaAs $(\bar{3}1\bar{1})$ sample. The curves have been displaced along the vertical axis by differing amounts for clarity. The substrate peaks are all at 0°.

These vectors can in turn be used to derive the values of the layer lattice parameters and angles: $a = 6{\cdot}466(1)$ Å, $b = 6{\cdot}462(1)$ Å, $c = 6{\cdot}462(1)$ Å, $\alpha = 90{\cdot}00(1)°$, $\beta = 89{\cdot}99(1)°$ and $\gamma = 89{\cdot}94(1)°$. We see that there is a significant distortion of the MCT layer from the bulk cubic unit cell. Since only three azimuthal positions of each of the three Bragg reflections are required for the calculation, there is some redundancy, which was used to estimate the standard deviations as given above. Li Runshen and Zhu Nanchang (1990) have provided a detailed discussion of the measurement errors involved in the technique and possible improvements

that can be made. We should also point out that we have implicitly assumed that the GaAs substrate is undistorted. In reality there will be some distortion of the near-surface region of the GaAs substrate, but the depth of penetration of the X-ray beam will be considerably larger than the thickness of the modified region.

The layer unit-cell volume derived from the three vectors given is 270·0 Å^3. The lattice parameter for an undistorted (cubic) unit cell of this volume is 6·463 Å. If we use Vegard's law we obtain a value $x = 0{\cdot}15$ for this lattice parameter. The results of Woolley and Ray (1960) yield $x = 0{\cdot}18$. These values are in good accord with the results of SGPW, where the Rutherford backscattering of 2 MeV He ions was used to determine an average value of $x = 0{\cdot}25$ with a variation with depth from 0·15 to 0·30.

The results obtained can also be used to ascertain the orientation of the MCT unit cell relative to the GaAs unit cell. The layer reciprocal-lattice vectors can be expressed as:

$$\boldsymbol{a}^* = 0{\cdot}1542\,\boldsymbol{i} + 0{\cdot}0084\,\boldsymbol{j} + 0{\cdot}0092\,\boldsymbol{k}\ \text{Å}^{-1},$$

$$\boldsymbol{b}^* = -0{\cdot}0086\,\boldsymbol{i} + 0{\cdot}1545\,\boldsymbol{j} - 0{\cdot}0002\,\boldsymbol{k}\ \text{Å}^{-1},$$

$$\boldsymbol{c}^* = -0{\cdot}0093\,\boldsymbol{i} - 0{\cdot}0003\,\boldsymbol{j} + 0{\cdot}1545\,\boldsymbol{k}\ \text{Å}^{-1},$$

from which we calculate the tilt angle between the layer and substrate (more specifically between the two $\bar{3}1\bar{1}$ reciprocal-lattice vectors) to be 4·66°. The direction of tilt of the layer is largely toward the substrate $[0\bar{1}\bar{1}]$ reciprocal-lattice direction, i.e. the $[01\bar{1}]$ in-plane reciprocal-lattice direction of the layer is parallel to that of the substrate [in agreement with the findings of Cinader and Raizman

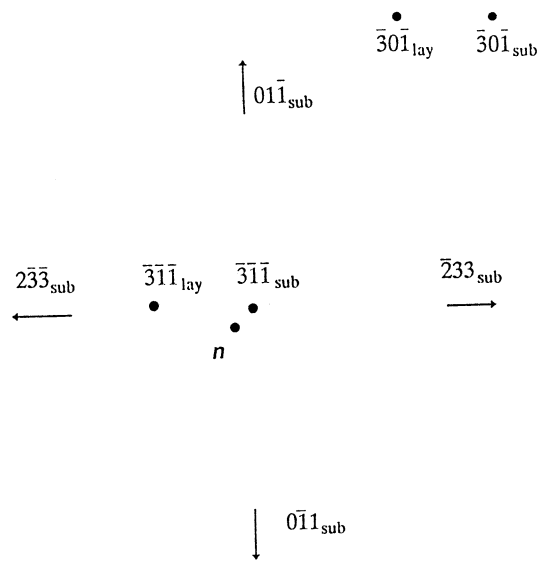

Fig. 3. Central part of a stereographic projection with various reciprocal-lattice directions, for both GaAs substrate and MCT layer as indicated. The surface-normal direction of the sample is also shown.

(1992) for various CdTe layers deposited on GaAs substrates with orientations belonging to the $\langle 01\bar{1} \rangle$ zone]. Fig. 3 shows the central part of a stereographic projection with various reciprocal-lattice directions marked.

Fig. 3 also shows the direction of the surface normal of the sample (the normals to the epitaxial-layer surface and substrate surface will be assumed to coincide). This was determined on a computer-controlled four-circle X-ray diffractometer, the surface normal having been accurately aligned along the diffractometer ϕ axis by using a laser (Moss and Barnea 1976; Stevenson *et al.* 1989). The surface-normal direction was determined from the GaAs substrate orientation (UB) matrix to be:

$$\boldsymbol{n}_{\text{sub}} = -3{\cdot}00\, \boldsymbol{a}^*_{\text{sub}} - 1{\cdot}07\, \boldsymbol{b}^*_{\text{sub}} - 1{\cdot}01\, \boldsymbol{c}^*_{\text{sub}}\ \text{Å}^{-1},$$

from which we get the unit vector

$$\hat{\boldsymbol{n}}_{\text{sub}} = -0{\cdot}8982\, \boldsymbol{i} - 0{\cdot}3200\, \boldsymbol{j} - 0{\cdot}3015\, \boldsymbol{k},$$

and from the MCT layer UB matrix:

$$\boldsymbol{n}_{\text{lay}} = -3{\cdot}00\, \boldsymbol{a}^*_{\text{lay}} - 0{\cdot}866\, \boldsymbol{b}^*_{\text{lay}} - 0{\cdot}792\, \boldsymbol{c}^*_{\text{lay}}\ \text{Å}^{-1},$$

from which we get the unit vector

$$\hat{\boldsymbol{n}}_{\text{lay}} = -0{\cdot}8987\, \boldsymbol{i} - 0{\cdot}3189\, \boldsymbol{j} - 0{\cdot}3011\, \boldsymbol{k}.$$

These two independent determinations are in excellent agreement. We thus know the way in which the substrate and layer unit cells are disposed relative to the surface. The miscut angles (that is, the angles between the two $\bar{3}1\bar{1}$ reciprocal-lattice vectors and $\hat{\boldsymbol{n}}$) are $1{\cdot}1°$ and $4{\cdot}0°$ for substrate and layer respectively, in very good agreement with the results of SGPW.

4. Conclusions

The double-crystal diffraction method of Li Runshen and Zhu Nanchang (1990) for accurately determining the unit cell of a single crystal and its orientation relative to a standard crystal has revealed a significant distortion of the unit cell for a $Hg_{1-x}Cd_xTe\,(\bar{3}1\bar{1})$ epitaxial layer, deposited by MOCVD on a GaAs $(\bar{3}1\bar{1})$ substrate. A large tilt angle between substrate and layer unit cells, consistent with the results of SGPW, has been accurately determined. The $\bar{3}1\bar{1}$ double-crystal rocking curves have revealed an anisotropy in the MCT layer, whose composition has also been determined. Four-circle diffractometry has been used to determine the disposition of the unit cells relative to the sample surface.

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