

Structural Aspects of MOCVD-Grown $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ Layers on Novel GaAs Substrates

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Abstract

X-ray diffraction studies of six samples of metal organic chemical vapour deposition (MOCVD)-grown $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ on novel GaAs substrates have been carried out. The six GaAs substrates have (311), ($\bar{3}\bar{1}\bar{1}$), (511), ($\bar{5}\bar{1}\bar{1}$), (711) and ($\bar{7}\bar{1}\bar{1}$) orientations. The absolute polarities of the six substrates, initially unknown, have been determined by X-ray anomalous scattering (after the layers were deposited). The orientations and absolute polarities of the six $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ layers have similarly been determined and follow the substrates. An extensive set of integrated-intensity data has been collected from the (311) $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ layer, which is of the order of 1 μm in thickness. Least-squares analysis of these data yields information about the thermal vibrations of the atomic species, extinction effects and the average composition of the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ layer. Some results of double-crystal rocking-curve measurements for each of the six samples are also reported. The Rutherford backscattering of 2 MeV He ions has been used to determine independently the absolute polarity, composition and quality of the (311) and ($\bar{3}\bar{1}\bar{1}$) $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ layers.

Introduction

The ternary alloy $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ (MCT) is an extremely important material with applications in areas such as infrared detection for military applications, optoelectronic devices, solar cells and charge-coupled devices. The direct band gap can be varied from -0.3 eV (for HgTe) to 1.6 eV (for CdTe) by changing x . There has recently been considerable interest in finding the optimum substrate material and orientation for growth of MCT. This choice can influence surface morphology, structural defects and impurity-atom incorporation and is an important consideration with regard to device fabrication.

The aim of the present study is to establish the orientation, absolute polarity and quality of six MCT

layers, grown by low-temperature metal organic chemical vapour deposition (MOCVD) on GaAs substrates of (311), ($\bar{3}\bar{1}\bar{1}$), (511), ($\bar{5}\bar{1}\bar{1}$), (711) and ($\bar{7}\bar{1}\bar{1}$) orientation. For one sample, a (311) MCT layer, an extensive set of Bragg intensity data is analysed to yield information about the thermal vibrations of the atomic species, extinction effects and the average composition of the layer. The authors are not aware of any such studies of a MCT layer having been carried out elsewhere. A knowledge of the values of thermal parameters such as Debye-Waller factors is particularly useful with regard to predicting band-gap temperature dependence and in studying diffusion, for example. The fact that such an experiment is possible is testimony to the power of extended-face crystal geometry for Bragg-reflection data collection (albeit, in the present case, the sample is not a true extended-face crystal in that it is not of effectively infinite thickness).

In addition to the X-ray diffraction techniques used, we have studied two of the MCT layers [(311) and ($\bar{3}\bar{1}\bar{1}$)] by the complementary technique of Rutherford backscattering (RBS) (Wieluński, Kwietniak, Pain & Rossouw, 1990). The RBS results are in agreement with the X-ray results with respect to the determination of polarity and quality for these two MCT layers. Some results on the depth dependence of the compositions for the two layers and layer thickness will also be presented.

Experimental

The MCT layers were grown in an MR Semicon Quantax 226 MOCVD reactor. The (2 in) GaAs substrates, supplied by Wacker-Chemitronic GMBH, Germany, were polished on both sides and of nominal (311), (511) and (711) orientations. The substrates were halved and one half was inverted in the reactor prior to deposition of the MCT layers, *i.e.* MCT layers were grown on ($n11$) and ($\bar{n}\bar{1}\bar{1}$) GaAs substrates placed side by side in the reactor, for $n = 3, 5$ and 7

(although the absolute polarity of the GaAs was not known initially). Each MCT layer was grown by depositing, alternately, CdTe and HgTe and each sample was capped by a very thin CdTe layer. In the case of the (511), ($\bar{5}\bar{1}\bar{1}$), (711) and ($\bar{7}\bar{1}\bar{1}$) GaAs substrates, the samples were annealed for one hour at the growth temperature (approximately 593 K). In the case of the (311) and ($\bar{3}\bar{1}\bar{1}$) GaAs substrates, the annealing was carried out at 50–60 K higher than the growth temperature (which was approximately 598 K), *i.e.* approximately 653 K. The degree of interdiffusion of the CdTe and HgTe ‘sublayers’, and thus the homogeneity of the MCT layer will, therefore, not be the same for all samples.

The thickness of the MCT layer for a given sample can be estimated from the measured weights before and after deposition. The thicknesses of the MCT layers being studied in the present work are of order 1 to 2 μm .

The majority of the results presented in this paper were collected with a computer-controlled four-circle X-ray diffractometer. A high-resolution double-crystal diffractometer was used to collect rocking curves for each MCT layer. RBS with 2 MeV He ions was performed on the (311) and ($\bar{3}\bar{1}\bar{1}$) MCT samples in random and axial channelling directions ($\langle 411 \rangle$ and $\langle \bar{3}11 \rangle$) in order to estimate crystal quality and the composition profiles. We should point out that the X-ray and RBS results were determined from quite different sections of the samples.

Results – I

The four-circle diffractometer was used to collect several $\omega/2\theta$ scans (where different Bragg reflections were optimized initially) for each MCT layer. A slit, subtending an angle of approximately 0.02° at the crystal, in the diffraction plane, was placed in front of the scintillation detector. The results showed all six MCT layers to be single-crystal layers (at least at the sample positions studied) with orientations corresponding to those of the substrates (the absolute polarities, for substrates and epitaxial layers, still to be determined however).

The absolute polarities of all six substrates and epitaxial layers were determined by X-ray anomalous scattering, which involved the measurement of Bijvoet ratios using the four-circle diffractometer. The polarity determination for thin single-crystal layers has been discussed recently by Stevenson, Wilkins, Kwietniak & Pain (1989) and Stevenson & Pain (1990*a*). Stevenson & Pain (1990*b*) have discussed the extension of the technique to cases where the layer cannot be considered infinitely thick, as is the case in this work. In the case of polarity determinations for the GaAs substrates, measurements of integrated X-ray intensities were taken through the MCT layer and the results corrected for the absorp-

Table 1. *Observed Bijvoet ratios (%)*, with associated *e.s.d.’s*, for the six MCT/GaAs samples, assuming, initially, that all samples are of (*n*11) orientation

| Sample | Substrate | | Layer | |
|--------|---------------------------|---------------------------------|---------------------------------|---------------------------------|
| | $B_{971/\bar{9}7\bar{1}}$ | $B_{11,5,3/\bar{1}\bar{1},5,3}$ | $B_{311/\bar{3}\bar{1}\bar{1}}$ | $B_{331/\bar{3}\bar{3}\bar{1}}$ |
| S1 | -6.6 (21) | 9.5 (17) | -17.4 (10) | 20.5 (22) |
| S2 | 9.3 (26) | -14.2 (24) | 19.3 (11) | -22.1 (7) |
| S3 | 10.4 (67) | -6.4 (38) | 18.2 (15) | -20.3 (7) |
| S4 | -7.9 (15) | 8.9 (28) | -17.7 (19) | 21.3 (11) |
| S5 | -8.3 (20) | 6.7 (29) | -17.9 (26) | 22.0 (20) |
| S6 | 6.2 (20) | -7.2 (19) | 20.2 (13) | -22.8 (13) |

tion in the layer (Stevenson & Pain, 1990*b*). In all cases, integrated intensities were measured at several different azimuthal positions for a given Bragg reflection (to check for the presence of multiple diffraction effects) and for several equivalent reflections. The agreement between integrated intensities for equivalent Bragg reflections was generally significantly better after absorption effects in the layer were taken into account for substrate data and after the finite thickness of the layer was taken into account for layer data.

Throughout this paper we will assume that the MCT layers being investigated have the cubic zincblende structure, with space group $F\bar{4}3m$ (see, for example, Park, Jun, Kim & Park, 1989). The four *A* atoms present in the unit cell are assigned to the special positions 4(*a*), and the four *B* atoms to the special positions 4(*c*). The point symmetry is $\bar{4}3m$ for all atom positions. We assume that the distribution of Cd and Hg atoms on the *A* sites is random [evidence of structural ordering in MCT has been observed – see, for example, Compaan, Bowman & Cooper (1990)].

The substrate Bijvoet ratios were measured using Mo $K\alpha$ radiation (and a Zr filter). The layer Bijvoet ratios were measured using Cr $K\alpha$ radiation (and a V filter). We did not see any evidence of twinning in the MCT layers at the positions investigated. Table 1 shows the observed Bijvoet ratios for the six samples. We have assumed, initially, that all samples possess GaAs substrates and MCT epitaxial layers of (*n*11) orientation ($n=3$ for S1 and S2, $n=5$ for S3 and S4, $n=7$ for S5 and S6). It can be seen from Table 1 that the substrate Bijvoet ratios are less consistent (in magnitude) compared with the layer Bijvoet ratios. This reflects, to some extent, the greater importance of the layer thickness *t* for the substrate measurements, and the uncertainty in that quantity. We see that the *e.s.d.’s* for the sample S3 substrate Bijvoet ratios are significantly higher than those for the other values. We associate this with what was subsequently found to be poor surface condition at the position where the X-ray beam intercepted the sample. The sample S3 layer Bijvoet ratios were measured at a different sample position.

Table 2. Orientation and absolute polarity of the substrate and layer for each of the six samples; the experimentally determined 'miscut' for each substrate and layer is also included

| Sample | Substrate | Layer | Substrate miscut (°) | Layer miscut (°) |
|--------|-----------------------------|-----------------------------|----------------------|------------------|
| S1 | (311) | (311) | 0.94 | 4.3 |
| S2 | ($\bar{3}\bar{1}\bar{1}$) | ($\bar{3}\bar{1}\bar{1}$) | 0.84 | 4.3 |
| S3 | ($\bar{5}\bar{1}\bar{1}$) | ($\bar{5}\bar{1}\bar{1}$) | 0.71 | 2.5 |
| S4 | (511) | (511) | 0.66 | 2.2 |
| S5 | (711) | (711) | 0.73 | 1.1 |
| S6 | ($\bar{7}\bar{1}\bar{1}$) | ($\bar{7}\bar{1}\bar{1}$) | 0.69 | 1.2 |

The theoretical values of the Bijvoet ratios in Table 1 are, for the respective columns, -6.9 , 8.1 , -16.8 (-19.7) and 18.4 (23.6%), the first and second being for GaAs, the third and fourth for CdTe, and those values in brackets for HgTe. The atomic scattering factors of Doyle & Turner (1968) were used, as well as the anomalous-dispersion corrections of Cromer & Liberman (1970) and the Debye-Waller factors of Reid (1983) [shell model for GaAs, valence-shell model (I) for CdTe, deformation-dipole model for HgTe]. Anharmonic thermal vibrations and bonding effects were not included in the calculations. The lattice parameters used were $a = 5.6538 \text{ \AA}$ for GaAs (American Society for Testing Materials, ASTM Card no. 32-389), $a = 6.481 \text{ \AA}$ for CdTe (National Bureau of Standards, 1964) and $a = 6.4604 \text{ \AA}$ for HgTe (American Society for Testing Materials, ASTM Card no. 32-665). Table 2 shows the orientation and absolute polarity of the substrate and layer for each sample based on the results in Table 1. We see that the layer adopts the orientation and polarity of the substrate in each case. Table 2 also lists the 'miscut' [the angle between the surface and the respective ($n11$) and ($\bar{n}\bar{1}\bar{1}$) planes] for each substrate and layer, determined from certain Bragg-reflection peak positions for particular azimuthal angles, having ensured that the sample normal and diffractometer φ axis coincide (Moss & Barnea, 1976; Stevenson, Wilkins, Kwietniak & Pain, 1989). We see that the substrate miscuts are all less than 1° . The layer miscuts clearly show the expected consistency between ($n11$) and ($\bar{n}\bar{1}\bar{1}$) orientations, the values increasing as n decreases.

Table 3 shows the average FWHM, using two or more positions on each of the six MCT layers, for double-crystal rocking curves collected with a high-resolution diffractometer. It is not possible to draw any definite conclusions about the quality of the ($n11$) versus ($\bar{n}\bar{1}\bar{1}$) MCT layers from these data. However, examination of the six samples by Nomarski interference contrast microscopy shows that each ($\bar{n}\bar{1}\bar{1}$) MCT layer is smoother than the associated ($n11$) layer, for $n = 3, 5$ and 7 (Pain, Sandford, Smith, Stevenson, Gao, Wieluński, Russo, Reeves & Elliman, 1990).

Table 3. Average FWHM for double-crystal rocking curves collected from each epitaxial layer

| Sample | Layer reflection | Rocking-curve FWHM (") |
|--------|-------------------------|------------------------|
| S1 | 311 | 212 (11) |
| S2 | $\bar{3}\bar{1}\bar{1}$ | 167 (33) |
| S3 | $\bar{5}\bar{1}\bar{1}$ | 787 (155) |
| S4 | 511 | 713 (71) |
| S5 | 711 | 736 (121) |
| S6 | $\bar{7}\bar{1}\bar{1}$ | 575 (21) |

Results - II

Sample S1 was chosen to carry out an extensive integrated-intensity data collection for the MCT layer. S1 was felt to be an appropriate sample because there is an appreciable angle between the 'surface' Bragg planes [(311) planes for S1] for the substrate and layer, and so we can expect less interference from substrate reflections during data collection. Also, the annealing conditions for S1 ensure a greater degree of interdiffusion of the CdTe and HgTe sublayers and therefore a more homogeneous MCT layer. The four-circle diffractometer was used to collect integrated intensities [$\omega/2\theta$ scan mode; scan range $1.6^\circ + 3.2^\circ \tan \theta$ in ω ; Mo $K\alpha$ (Zr filter) radiation from a standard X-ray tube; detector aperture $1.4 \times 1.4^\circ$; temperature 293 K]. Reference reflections were measured at regular intervals during the data collection and each reflection was measured at four azimuthal positions to check for multiple-diffraction effects. After averaging over different azimuthal positions (and making Lorentz-polarization corrections) there were 231 reflections, which reduced to 70 independent reflections.

In order to carry out the absorption corrections required we must know μt , where μ is the linear absorption coefficient. Initially, we had no accurate value for t or x , the Cd fraction (which is needed in calculating μ for the MCT layer). Fig. 1 shows two quantities, the average deviation of the integrated

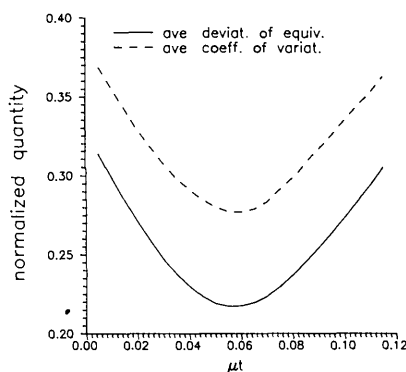


Fig. 1. Average deviation of the integrated intensity for a Bragg reflection from the mean value for its equivalent-reflection group, and the average coefficient of variation, as a function of μt , for the sample S1 data set.

Table 4. Description and results of layer-thickness determinations for sample S1

| <i>hkl</i> | ψ_{\min} (°) | ψ_{\max} (°) | ψ_{step} (°) | <i>t</i> (μm) |
|------------|-------------------|-------------------|--------------------------|---------------|
| 555 | -40 | 40 | 1 | 1.25 (13) |
| 642 | -90 | 90 | 2 | 1.34 (6) |
| 731 | -50 | 50 | 1 | 1.95 (14) |
| 531 | -50 | 50 | 1 | 1.49 (6) |
| Average | | | | 1.51 (31) |

intensity for a Bragg reflection from the mean value for its equivalent-reflection group and the average coefficient of variation (σ_{pop}/I , where σ_{pop} is the standard deviation for the integrated intensity *I*, from population statistics), plotted against μt . The two quantities plotted in Fig. 1 have been normalized by their values in the absence of any absorption correction, namely 10.19% for the average deviation of an equivalent reflection and 0.106 for the average coefficient of variation. We see quite clearly that there is an optimum value of μt (0.0573). We also know the mass of the deposited MCT layer (9.0 mg). Using these two pieces of information we can calculate *x* and then get values for μ and *t*. The results are $x = 0.44$, $\mu = 455.9 \text{ cm}^{-1}$ and $t = 1.25 \text{ μm}$.

In order to check the value obtained for *x* (and thereby μ), we carried out a least-squares refinement with the 70 2θ values for the data set, varying the lattice parameter, *a*, to obtain a fit. The result was $a = 6.4674(5) \text{ Å}$, and Hamilton's *R* factor was 0.068%. This lattice-parameter value yields a value of $x = 0.42$ from the data of Woolley & Ray (1960) (*cf.* 0.34 if we use Vegard's law), in excellent agreement with the earlier value. The change in μ , associated with a change in *x* from 0.44 to 0.42, is approximately 2%. In order to (further) check the value obtained for *t*, integrated-intensity data were collected, from the MCT layer, for four Bragg reflections (same data-collection conditions as already described) as a function of azimuthal angle ψ . The data were analysed as described by Stevenson & Pain (1990*b*) and the results are given in Table 4. We are unable to account for the obvious disparity between the third value of *t* and the others, the average value being 1.36 (12) μm if we neglect the third value. In any event, we have quite reasonable agreement with the earlier value of *t*.

The data (70 independent reflections) were corrected for the contributions from anisotropic first-order thermal diffuse scattering (TDS) by acoustic lattice vibrations. The program used is that described by Sakata, Stevenson & Harada (1983). The elastic constants used were those of McSkimin & Thomas (1962) and Cottam & Saunders (1975) for CdTe and HgTe, respectively, and an average of the two sets was taken (the differences being only 0.2, 0.6 and 6.3% for C_{11} , C_{12} and C_{44} , respectively). The largest TDS correction (α) was 0.166 for the 10,4,2 and 10,4,2 reflections.

Table 5. Refined parameter values and Hamilton's *R*-factor values for the least-squares analysis of data collected from the sample S1 MCT layer - model I (harmonic); model II (anharmonic)

| | I | II |
|---------------------------------|----------|---------------------------|
| $B_{\text{Cd/Hg}} (\text{Å}^2)$ | 2.8 (1) | 2.8 (1) |
| $B_{\text{Te}} (\text{Å}^2)$ | 2.1 (1) | 2.0 (1) |
| <i>x</i> | 0.28 (4) | 0.27 (4) |
| <i>s</i> | 3.57 (7) | 3.58 (6) |
| r^* (nm) | 3 (10) | 4 (10) |
| β' (J Å^{-3}) | — | $-1.5(7) \times 10^{-19}$ |
| R_H (%) | 3.88 | 3.71 |

The weighting scheme used for the least-squares refinement of data was that of Hughes (1941). The quantity minimized in the least-squares refinement was

$$M = \sum_{i=1}^{70} w_i (|F_{oi}| - |F_{ci}|)^2, \quad (1)$$

where F_{oi} and F_{ci} are the observed and calculated structure factors for the *i*th observation, respectively, and w_i is the weight given to $(|F_{oi}| - |F_{ci}|)$. The parameters that could be refined were: the Debye-Waller factors, $B_{\text{Cd/Hg}}$ and B_{Te} ; *x*; a scale factor *s*; an extinction parameter r^* [effective domain radius (Zachariasen, 1967)]; anharmonic thermal parameters $\beta_{\text{Cd/Hg}}$ and β_{Te} [or the effective anharmonic thermal parameter β' (Cooper, Rouse & Fues, 1973)]; bonding parameters α_0 , α_3 , C_0 and C_3 (Moss, 1977). In addition to the sources of atomic scattering factors and anomalous-dispersion corrections already mentioned, we included the corrections to the anomalous-dispersion corrections given by Kissel & Pratt (1990).

The values of the refined parameters for model I (harmonic) and model II (anharmonic) are given in Table 5, together with the values of Hamilton's *R* factor, R_H . The largest correlation coefficient was 0.84, between B_{Te} and *x* (for both models). We found, as expected, that the inclusion of bonding effects in the refinements did not significantly improve the overall fit. The same can be said for extinction effects, the value(s) of r^* in Table 5 being very small [the smallest extinction factors (*y*'s) being 0.983 and 0.978 for models I and II, respectively]. The e.s.d. for r^* in Table 5 precludes further discussion, except to say that although the value is very small, such values of r^* have been reported in the literature [*e.g.* 22 nm for an LiF sphere with Mo $K\alpha$ radiation (Zachariasen, 1968)]. Correlations between $\beta_{\text{Cd/Hg}}$ and β_{Te} , and apparent multiple minima, precluded us from making a meaningful simultaneous refinement of both cubic anharmonic thermal parameters [a similar situation was encountered, for example, with ZnS (Moss, McMullan & Koetzle, 1980)]. Consequently, in model II, we refined the effective anharmonic thermal parameter introduced by Cooper, Rouse &

Fuess (1973):

$$\beta' = \beta_{\text{Te}} - \beta_{\text{Cd/Hg}} (B_{\text{Cd/Hg}}/B_{\text{Te}})^3. \quad (2)$$

The ratio of the values of R_H for models I and II corresponds to a significance level of less than 2.5%, which means that the improved agreement resulting from the inclusion of anharmonic effects is very significant (Hamilton, 1964, 1965).

The refined values of x in Table 5 are significantly different from the earlier determinations (0.44 and 0.42). This discrepancy may be due to subtle differences in the techniques used and may also be attributable to certain aspects of the MCT layer which we have not taken into account, e.g. ordering of Cd and Hg atoms on the A sites and inhomogeneity of the layer with depth (due to incomplete interdiffusion).

In regard to the refined values of the Debye-Waller factors, the fact that the larger value corresponds to the heavier of the two 'species' (a hybrid Cd/Hg atom) may at first seem surprising. However, given that we are operating above the Debye temperature* and that the unit cell is reasonably large this result is not very unusual (Huiszoon & Groenewegen, 1972; Scheringer, 1973).

The authors are not aware of any theoretical or experimental values for the Debye-Waller factors of MCT. Guenzer & Bienenstock (1971) provide experimentally determined relationships between the mean square displacements for Hg and Te in HgTe and temperature which yield, at 293 K, $B_{\text{Hg}} = 2.8$ and $B_{\text{Te}} = 2.0 \text{ \AA}^2$. Skelton, Radoff, Bolsaitis & Verbalis (1972) have determined the Debye-Waller factors (actually converted from their mean square displacements) at 296 K to be $B_{\text{Hg}} = 2.3 (+0.9, -0.2)$ and $B_{\text{Te}} = 1.7 (+0.4, -0.2) \text{ \AA}^2$. Reid (1983) has presented lattice-dynamical calculations (using various models) of Debye-Waller factors for various materials with the zincblende structure, including CdTe and HgTe. The values obtained are very model dependent and for the purposes of comparison we have averaged the values from the different models for CdTe and HgTe, and then taken an 'x-weighted' average. This rather simplistic approach yields $B_{\text{Cd/Hg}} = 4.0$ and $B_{\text{Te}} = 1.7 \text{ \AA}^2$. Finally, Madhavan, Ramachandran & Haridasan (1989) have calculated, using a modified rigid-ion model, that $B_{\text{Hg}} = 2.2$ and $B_{\text{Te}} = 1.8 \text{ \AA}^2$ for HgTe at 300 K. Clearly there is a fair degree of variability between Debye-Waller-factor values (both theoretical and experimental). It can be said, however, that the values given in Table 5, for our MCT sample, are quite reasonable.

Table 6 shows the only room-temperature determinations of β' for zincblende materials known to the authors (they are all experimental values). [Tibballs,

Table 6. Room-temperature determinations of β' for zincblende materials

| Material | β' ($10^{-19} \text{ J \AA}^{-3}$) | Reference |
|----------|--|---------------------------------|
| CuCl | -7.1 (44) | Sakata, Hoshino & Harada (1974) |
| CuCl | -5.7 (11) | Valvoda & Ječný (1978) |
| CuBr | -4.9 (13) | Harada, Suzuki & Hoshino (1976) |
| ZnS | -4.8 (13) | Moss, McMullan & Koetzle (1980) |
| ZnS | -4.2 (11) | Cooper, Rouse & Fuess (1973) |
| ZnTe | -3.8 (10) | Cooper, Rouse & Fuess (1973) |
| ZnSe | -5.6 (9) | McIntyre, Moss & Barnea (1980) |
| InAs | -3.1 (22) | Stevenson (1983) |
| MCT | -1.5 (7) | Present study |

Feteris & Barnea (1981) have determined room-temperature values of an effective cubic anharmonic parameter by neutron diffraction for InAs and GaSb. We are not, however, completely certain of the definition of this parameter and so have not included the results in Table 6.] We see that the value for MCT determined in this study is comparable to those listed, if a little lower. There is no reason to expect any better agreement and, indeed, we might well be surprised if there was, given the masses of the atomic species involved.

Results - III

The 2 MeV He channelling analysis of samples S1 and S2 showed good crystal quality of the MCT layers. The composition of these MCT layers has been estimated as a function of depth using a comparison of random and computer-simulated spectra for different values of x . The average x value for S1 is approximately 0.20 (a variation with depth from 0.14 to 0.27), and approximately 0.25 for S2 (a variation with depth from 0.15 to 0.30). The precision in the x -value determinations is better than 0.05.

The strong enhancement and decrease observed in Hg and Te signals in RBS spectra near the (111) planar channelling direction confirms the X-ray polarity determinations for both MCT layers (S1 and S2), as well as the absence of twins.

Concluding remarks

The power of the X-ray diffraction technique for (nondestructive) absolute polarity determination of crystalline substrates and layers has been clearly demonstrated. We have found that the six MOCVD-grown MCT layers, deposited on GaAs substrates of (311), ($\bar{3}\bar{1}\bar{1}$), (511), ($\bar{5}\bar{1}\bar{1}$), (711) and ($\bar{7}\bar{1}\bar{1}$) orientations, follow the substrate orientation and polarity. The quality of the six MCT layers varies, but is generally quite good. No evidence of twinning was observed and all observed Bragg reflections could be indexed in terms of the GaAs substrate or single-crystal MCT with the zincblende structure.

The harmonic thermal vibration effects observed from the sample S1 MCT layer are consistent with

* We can estimate the Debye temperature using the refined parameter values ($B_{\text{Cd/Hg}}$, B_{Te} and x) in Table 5 (model II), the result being 95 K.

the few experimental and theoretical studies in the literature for CdTe and HgTe. A significant cubic anharmonic thermal vibration component has also been found. The present study has revealed the possibility of investigating atomic thermal vibrations in crystalline layers of order 1 μm thick, at room temperature and with a conventional X-ray tube source.

The use of RBS techniques to investigate two of the MCT layers has produced results which confirm the X-ray findings on layer quality and polarity. The average value of x for sample S1 is in quite good agreement with the X-ray result in Table 5 (remembering, however, that there may be some variation from point to point on the sample). [The S1 MCT layer thickness was determined to be 1.5 (1) μm by RBS, in good agreement with the X-ray value.]

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