

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 $270 \cdot 0 \text{ \AA}^3$. The lattice parameter for an undistorted (cubic) unit cell of this volume is $6 \cdot 463 \text{ \AA}$. 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:

$$\begin{aligned} \mathbf{a}^* &= 0 \cdot 1542 \mathbf{i} + 0 \cdot 0084 \mathbf{j} + 0 \cdot 0092 \mathbf{k} \text{ \AA}^{-1}, \\ \mathbf{b}^* &= -0 \cdot 0086 \mathbf{i} + 0 \cdot 1545 \mathbf{j} - 0 \cdot 0002 \mathbf{k} \text{ \AA}^{-1}, \\ \mathbf{c}^* &= -0 \cdot 0093 \mathbf{i} - 0 \cdot 0003 \mathbf{j} + 0 \cdot 1545 \mathbf{k} \text{ \AA}^{-1}, \end{aligned}$$

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

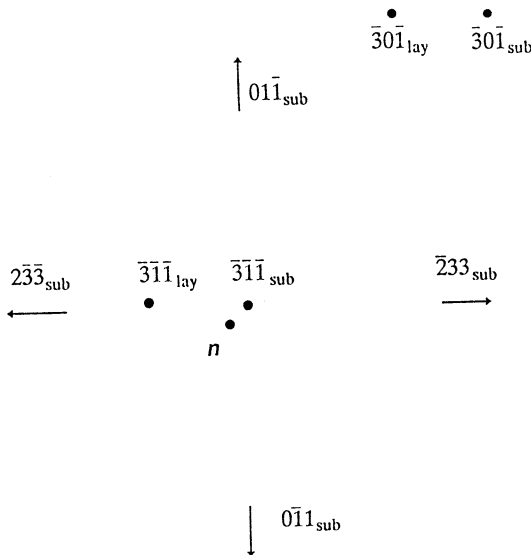


Fig. 3. Central part of a stereographic projection with various reciprocal-lattice directions, for both GaAs substrate and MCT layer as indicated. The surface-normal direction of the sample is also shown.

(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:

$$\mathbf{n}_{\text{sub}} = -3.00 \mathbf{a}_{\text{sub}}^* - 1.07 \mathbf{b}_{\text{sub}}^* - 1.01 \mathbf{c}_{\text{sub}}^* \text{ \AA}^{-1},$$

from which we get the unit vector

$$\hat{\mathbf{n}}_{\text{sub}} = -0.8982 \mathbf{i} - 0.3200 \mathbf{j} - 0.3015 \mathbf{k},$$

and from the MCT layer UB matrix:

$$\mathbf{n}_{\text{lay}} = -3.00 \mathbf{a}_{\text{lay}}^* - 0.866 \mathbf{b}_{\text{lay}}^* - 0.792 \mathbf{c}_{\text{lay}}^* \text{ \AA}^{-1},$$

from which we get the unit vector

$$\hat{\mathbf{n}}_{\text{lay}} = -0.8987 \mathbf{i} - 0.3189 \mathbf{j} - 0.3011 \mathbf{k}.$$

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 $\bar{3}\bar{1}\bar{1}$ reciprocal-lattice vectors and $\hat{\mathbf{n}}$) are 1.1° and 4.0° 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 $\text{Hg}_{1-x}\text{Cd}_x\text{Te}(\bar{3}\bar{1}\bar{1})$ epitaxial layer, deposited by MOCVD on a GaAs $(\bar{3}\bar{1}\bar{1})$ substrate. A large tilt angle between substrate and layer unit cells, consistent with the results of SGPW, has been accurately determined. The $\bar{3}\bar{1}\bar{1}$ 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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