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X-RAY DETERMINATION OF THE GaSb(111)2 × 2 SURFACE STRUCTURE

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We have examined the GaSb(111)2×2 surface prepared by sputtering and annealing using grazing-incidence X-ray diffraction. Our structure factor analysis shows the similarity between this surface and the vacancy-buckling model for GaAs, GaP and InSb(111): it contains one Ga vacancy per unit cell and an adjustment of bond angles associated with valence change of the remaining surface atoms. Analysis of the integer-order intensities unambiguously determines the mode of attachment (registry) of the surface layer with the bulk crystal.

1. Introduction

The atomic geometry of the polar (111) surfaces of III–V semiconductors has recently been the subject of several studies [1–6]. On the basis of low energy electron diffraction (LEED) measurements [1] and total energy calculations [2] Tong et al. [1] and Chadi [2] have proposed a "vacancy-buckling" model for the GaAs(111)2 × 2 surface structure. In this model, a quarter of the surface Ga atoms are missing and the reconstructed bilayer is relaxed into an almost planar configuration. The resulting local bond geometry suggests an electronic rearrangement, whereby the bonding changes from sp^3 to sp^2 on the Group III elements and from sp^3 to s^2p^3 on the Group V elements. Our grazing-incidence X-ray diffraction measurements on the InSb(111)2 × 2 surface [3] directly confirmed the vacancy-buckling mechanism. Similar results were obtained from LEED measurements on GaP(111)2 × 2 [4].

Here we present a grazing-incidence X-ray diffraction analysis of the GaSb(111)2 × 2 surface and find that it has an analogous structure to GaAs, InSb and GaP. We have made significant improvements which allow us to address finer points of the structure. Firstly, the contrast in scattering power between Ga ($Z = 31$) and Sb ($Z = 51$) allows positive identification of atom types, only marginally possible for InSb because the atomic numbers are similar. This is a question not yet addressed in any of the LEED work [1,4]. Secondly, recent understanding of the bulk contributions to integer-order reflections [7] allows us to incorporate them in the surface crystallographic analysis. Since Fourier components from the surface and the bulk add coherently at these diffraction positions, they contain information about the relative position of the surface layer with respect to the bulk: in this way we directly determine the registry. Finally, we have made diffraction measurements out of the plane of the surface from which we can draw conclusions about atomic coordinates normal to the surface.

2. Experiment

The X-ray diffraction measurements were performed at the 32-pole wiggler beamline W1 at the Hamburg Synchrotron Radiation Laboratory (HASYLAB) under dedicated running conditions (3.7 GeV, 60 mA). A double crystal monochromator with flat Ge(111) crystals was used to select a wavelength of $\lambda = 1.242$ Å. The scattering took place in the horizontal plane on a two-circle diffractometer tilted slightly with respect to the synchrotron beam to control the angle of incidence to the sample surface. The optical surface of the sample was aligned normal to the axis of the instrument until the total reflected X-ray beam position was independent of azimuth. To profit from the intensity gain provided by the refraction effects [8] the angle of incidence was set equal to the critical angle of 0.257° and kept constant throughout. The data were collected with a detector subtending 0.5° in the scattering plane and 2° perpendicular to it. The in-plane collimation was provided by two 2 mm slits, one placed just before and the other one just after the sample.

The preparation of the surface was carried out at the FLIPPER II beamline. The surface was cleaned by 500 eV Ar^+ ion bombardment and subsequent annealing at 500°C. The sputter–anneal cycle was repeated until the surface had a sharp 2 × 2 LEED pattern and the photoemission spectra showed no trace of impurities. The sample was then transferred under UHV conditions to a small ion-pumped X-ray cell which could be detached from the preparation chamber and mounted on the X-ray diffractometer. The pressure in the X-ray cell was below 10^{-9} mbar and no change in the diffracted intensities was observed during the 14 h of data-collection.

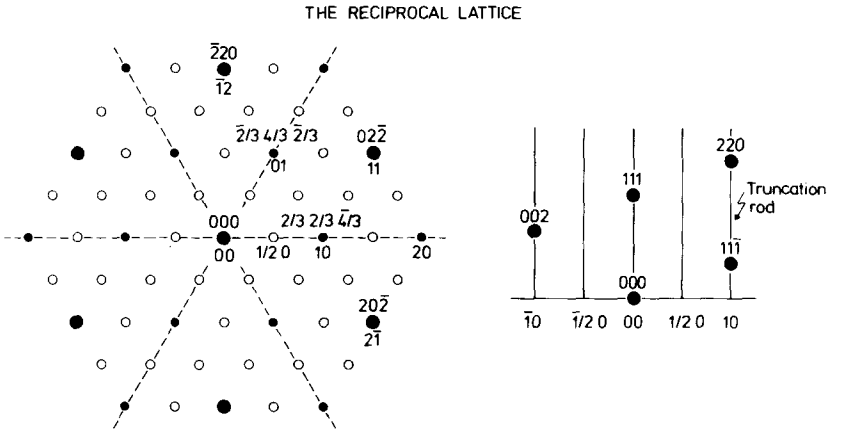

Fig. 1. Reciprocal lattice coordinate system. The left side shows the (111) plane. Large filled circles represents bulk Bragg points, small filled circles the interception of the integer-order truncation rods [7] with the plane and the open circles the Bragg rods induced by the surface reconstruction. The reflections are labelled by cubic notation above and hexagonal below the circles. The right side shows the (220) plane, which contains the surface normal and the $(10)_{hex}$ direction.

The crystallographic orientation of the (111) surface was determined by measuring the positions of the six in-plane [$2\bar{2}0$] reflections from the bulk. Because of the limited penetration of the X-ray beam into the surface, these were much weaker than out-of-plane bulk reflections, but still required attenuation to prevent detector saturation. We use the hexagonal coordinate frame described in fig. 1 to simplify indexing and to facilitate comparison with LEED. Thus the in-plane ($02\bar{2}$) reflection becomes $(11)_{hex}$, ($20\bar{2}$) becomes $(2\bar{1})_{hex}$, etc. The half-order reflections in the 2×2 pattern of the reconstruction were visited one-by-one, and a rocking curve (ω-scan) collected, of which fig. 2a is an example. As can be seen, the signal-to-background ratio was very good and not a serious limitation in the experiments. Every point on this scan contains X-rays received at *all* positions along the 2° vertical angle subtended by the position sensitive detector (PSD), the positional information not being used. Simultaneously, the same counts were binned in a multichannel analyser (MCA) resolving position and integrating angle. Because of the low background, this forms a faithful representation of the out-of-plane structure of a reflection. The 0.5° range of in-plane scattering angles accepted by the PSD is sufficient that no part of the peak is lost due to slight non-linearities of the Ewald sphere projection. Fig. 2b shows such a "rod scan" taken directly from the MCA; it has an onset due to refraction of the exit beam by the surface [12], but is otherwise flat, demonstrating the 2D nature of the diffraction. A special tiltable detector arm allowed us to piece together multiple slabs of PSD

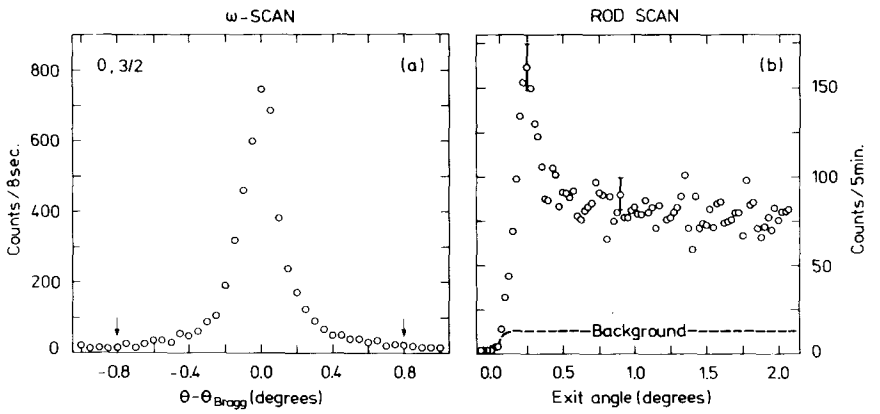

Fig. 2. (a) Rocking (ω) scan of $(0, \frac{3}{2})$ reflections. The arrows mark the background. (b) Rod scan collected simultaneously with the rocking scan. Each point therefore represents an integrated intensity (not background subtracted). The onset at an exit angle of 0.25° is due to refraction of the outgoing beam [12].

output to cover a total range of 6° out-of-plane, corresponding to a maximum out-of-plane momentum transfer of 0.5 Å^{-1}.

Forty-five fractional-order and twelve integer-order in-plane reflections were collected. The rocking curves were integrated numerically and background-subtracted to obtain integrated intensities. These were averaged for reflections related by symmetry to minimize any alignment errors. Typical agreement factors of the intensities between symmetry related reflections range between 14% ($(\frac{3}{2}, 1)$, 4 reflections, 6% statistical uncertainty) to 5% ($(\frac{5}{2}, 1)$, 4 reflections, 5% statistical uncertainty). In total, this gave fifteen fractional- and four integer-order intensities. Error bars were derived from counting statistics and reproducibility between equivalent reflections [13]. The lineshapes were not analysed further except to verify that their widths were consistent with a coherent domain size of ~ 600 Å on the surface. This size is not given by the resolution of the instrument since the bulk diffraction peaks were about ten times narrower.

3. Analysis

The integrated intensities were corrected for variations of the active surface area in the experiment ($\sin^{-1} 2\theta$) and for the polarization ($\cos^2 2\theta$) and Lorentz ($\sin^{-1} 2\theta$) factors to obtain the structure factor intensities listed in tables 1 and 2. A 2×2 surface unit cell of unreconstructed GaSb(111) is shown in fig. 3a. The 3m symmetry of the bulk crystal has been imposed on

Table 1
Observed and calculated fractional-order structure factor intensities

h	k	$\lvert F_{hk}^{\text{obs}} \rvert^2$	$\lvert F_{hk}^{\text{model}} \rvert^2$
$\frac{1}{2}$	0	0.04 ± 0.04	0.08
$\frac{1}{2}$	$\frac{1}{2}$	0.39 ± 0.10	0.52
1	$\frac{1}{2}$	10.2 ± 1.0	9.30
$\frac{3}{2}$	0	18.0 ± 0.8	18.25
$\frac{3}{2}$	$\frac{1}{2}$	1.6 ± 0.3	2.35
$\frac{3}{2}$	1	5.2 ± 0.5	3.53
2	$\frac{1}{2}$	7.7 ± 0.4	7.90
$\frac{5}{2}$	0	17.0 ± 2.9	15.52
$\frac{3}{2}$	$\frac{3}{2}$	3.9 ± 0.2	3.82
$\frac{5}{2}$	$\frac{1}{2}$	8.9 ± 0.8	9.08
2	$\frac{3}{2}$	10.9 ± 1.2	8.78
$\frac{5}{2}$	1	20.1 ± 1.1	20.67
3	$\frac{1}{2}$	1.5 ± 0.2	1.32
$\frac{7}{2}$	0	10.6 ± 3.2	4.77
$\frac{5}{2}$	$\frac{3}{2}$	8.9 ± 1.2	9.80

The indices (h, k) refer to the reciprocal lattice of the coordinate frame defined in fig. 1.

the surface unit cell giving the mirror planes indicated as dashed lines. A contour plot of the Patterson function

$$P(x, y) = \sum_{hk} |F_{hk}|^2 \cos[2\pi(hx + ky)] \quad (1)$$

gives a map of the interatomic vectors in the reconstructed unit cell [9]. Due to the inversion symmetry in $P(x, y)$ the asymmetric unit reduces to the triangle shown with thick lines in fig. 3a.

The Patterson function is calculated from (1) using the fractional-order reflections listed in table 1 and a contour map is shown in fig. 4. For clarity,

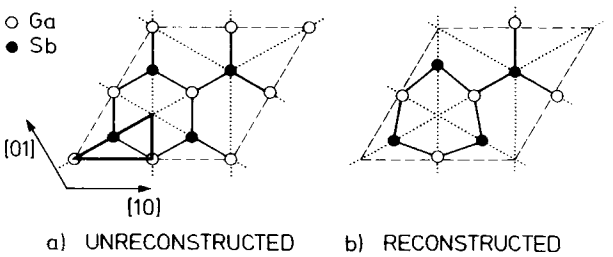

Fig. 3. (a) Undistorted 2×2 unit cell and (b) the reconstructed 2×2 unit cell for GaSb(111)2×2. Mirror planes from the 3m symmetry are indicated with dashed lines. The triangle with thick lines is the asymmetric unit for the Patterson function.

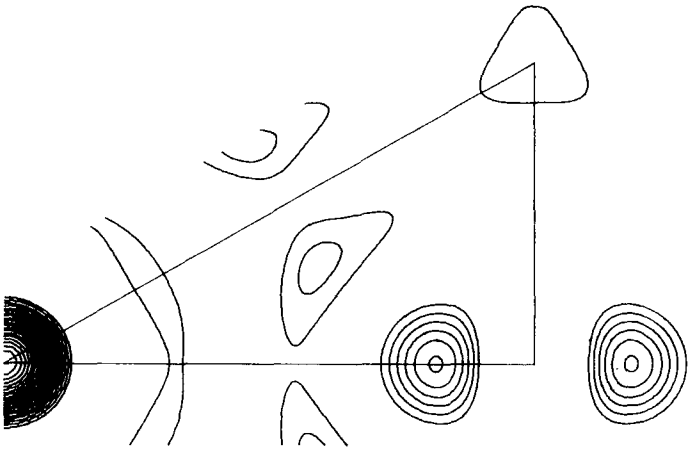

Fig. 4. Contour map of the Patterson function for GaSb(111)2×2 as calculated for the fractional-order structure intensities listed in table 1. Only positive contour levels above zero are shown, the peak at the origin rises twenty-one levels. The triangle correponds to the asymmetric unit shown in fig. 1.

only positive contours above zero are shown, however, negative peaks are present due to the omission of the integer-order reflections [10]. A full structural analysis could be performed but a shortcut is possible: the map resembles the Patterson map for InSb(111)2 × 2 [3] suggesting that the same seven-atom model should also apply for GaSb. The model is shown in fig. 3b. It consists of a distorted hexagon with three atoms displaced radially inwards and three atoms displaced radially outwards together with an atom sitting on one of the three-fold axes. Seven out of eight atoms in the 2 × 2 reconstructed unit cell implies that there is one vacancy.

In ref. [3] the assignment of atoms to In or Sb in 2 × 2 unit cell of InSb was supported by the fact that every Sb atom had only In nearest neighbours and vice versa. The data, however, were only marginally sensitive to other assignments. Following this, we start by building a model for GaSb with all atoms equal in size. Displacements of the atoms in the hexagon, 0.25 Å inwards and 0.42 Å outwards, are chosen to reproduce the peaks in the Patterson map by the interatomic vectors. Model structure factors

$$F_{hk}^{\text{model}} = \sum_j f_j(h, k)\, e^{i2\pi(hx_j + ky_j)}, \tag{2}$$

where f_j are the atomic form factors, are calculated and compared with the observed values by a chi-square test

$$\chi^2 = \frac{1}{N} \sum_{hk} \left(\frac{|F_{hk}^{\text{obs}}|^2 - |F_{hk}^{\text{model}}|^2}{\sigma_{hk}} \right)^2, \tag{3}$$

where N is the number of data points and σ_{hk} are the uncertainties in the structure factor intensities.

Only adjusting a scale-factor on the model structure factors, using the form factor for Nb ($Z = 41$) instead of Ga ($Z = 31$) and Sb ($Z = 51$), gives $\chi^2 = 17$. From the definiton of eq. (3) this means that the typical discrepancy is more than four times the measurement error. A least-squares fit on the atomic charges, denoted Z_1, Z_2 and Z_3 for the inequivalent atoms in the unit cell, keeping all other parameters fixed, gives $Z_1 = 29$ and $Z_2 = 50$ for the inwards and outwards displaced atoms, respectively, and $Z_3 = 41$ for the lone seventh atom. Clear assignments of $Z_1 = 31$ (Ga) and $Z_2 = 51$ (Sb) can be made. Releasing the scale and the displacements in a renewed fit with Z_1 and Z_2 fixed gives $Z_3 = 51$, therefore the lone seventh atom is Sb.

The final model is found in a four-parameter fit and is shown in fig. 3b. The three Sb atoms in the hexagon are displaced radially outwards by 0.38 ± 0.03 Å and the three Ga atoms radially inwards by 0.17 ± 0.06 Å. The thermal vibrations are described by a common Debye–Waller B-factor of $B = 0 \pm 1$ Å^2 and finally there is the arbitrary scale-factor. The model has $\chi^2 = 2.0$ and the structure factor intensities are listed in table 1. The low B-factor is probably due to errors in the polarization corrections, but is within the uncertainties of the bulk value of 0.91 Å^2 [11]. Changing the lone Sb atom to Ga gives $\chi^2 = 17$ after the four-parameter least-squares fit, which demonstrates the charge sensitivity.

4. The registry

The fractional-order reflections are not contributed to by the bulk crystal so they can only be used to determine the atomic positions inside the reconstructed surface region, but not to find the registry of the surface relative to the bulk. This registry can be found using the integer-order reflections, because they contain scattering both from the bulk and the surface added together coherently. Since we know the structure of the surface layer from the above analysis of fractional-order data, we can calculate its contribution to the integer-order positions on an absolute scale. This is done in table 2. The agreement, however, is not very good, with a χ^2 of 67.

Now we must consider the *bulk* contribution to these reciprocal space positions from a terminated (111) surface. The intensity here is due to the presence of a crystal truncation rod [7] joining bulk Bragg peaks above and below the surface, as shown in fig. 1. All the (111) bilayers of the bulk, which consist of one layer Ga and one layer Sb, have, except for a phase shift, the same in-plane structure factor

$$G_{hk} = 4f_{\mathrm{Ga}} + 4f_{\mathrm{Sb}} \exp\left[\mathrm{i}2\pi\left(\tfrac{2}{3}h + \tfrac{1}{3}k\right)\right]. \tag{4}$$

Table 2
Integer-order structure factor intensities

h	k	$\lvert F_{hk}^{obs}\rvert^2$	$\lvert F_{hk}^{surf}\rvert^2$	ψ_{hk}^{surf} (deg)	$\lvert F_{hk}^{bulk}\rvert^2$	ψ_{hk}^{bulk} (deg)	$\lvert F_{hk}^{tot}\rvert^2$		
							IABC	IABC [a]	IICAB
1	0	18.9±2.0	40.25	269	15.75	247	16.21	20.39	9.88
2	0	8.2±1.2	15.35	89	10.67	113	5.46	8.29	2.45
2	1	3.5±0.7	9.53	−72	8.32	247	0.97	3.18	0.12
3	1	5.4±0.7	0.67	88	5.77	115	3.16	4.69	2.82
			$\chi^2 = 67$				$\chi^2 = 7.6$	0.45	20

ψ_{hk}^{surf} and ψ_{hk}^{bulk} are the phases in degrees for F_{hk}^{surf} and F_{hk}^{bulk}, respectively, calculated with the origins of the unit cells as described in the text.

[a] Calculation where only 66% of the surface area is reconstructed.

The unit cell is chosen to be the same 2×2 cell so that no scale factor is needed between F_{hk} and G_{hk}. The factor 4 is due to the size of the 2×2 unit cell relative to the 1×1 cell. Due to their ABC stacking the bilayers are shifted by $(\frac{1}{2}, \frac{1}{2}, 0)_{\text{cub}} = (\frac{2}{3}, \frac{1}{3}, 1)_{\text{hex}}$ relative to each other which induces a phase difference ψ_{hk} between the structure factors of

$$\psi_{hk} = 2\pi\left(\tfrac{2}{3}h + \tfrac{1}{3}k\right). \tag{5}$$

Furthermore, because the X-ray beam is attenuated gradually as it passes below the surface each bilayer in the bulk contributes progressively less than those at the surface. Thus, the bulk in-plane structure factor is

$$F_{hk}^{\text{bulk}} = \sum_{n=0} G_{hk}\, \mathrm{e}^{\mathrm{i}n\psi_{hk}}\, \mathrm{e}^{-n\nu} = \frac{G_{hk}}{1 - \mathrm{e}^{-\nu + \mathrm{i}\psi_{hk}}}, \tag{6}$$

where ν is the damping amplitude per bilayer. ν is very small for the X-ray wavelength used and is only important when ψ_{hk} is close to 2π, that is if (h, k) is near a bulk Bragg point, and can be ignored elsewhere.

The total integer-order structure factor is

$$F_{hk}^{\text{tot}} = F_{hk}^{\text{surf}} + F_{hk}^{\text{bulk}}, \tag{7}$$

where F_{hk}^{surf} is the structure factor for the reconstructed bilayer defined above. The intensities and phases for F_{hk}^{bulk} and F_{hk}^{surf} are listed in table 2. The phases are calculated assuming that the bulk-terminated surface has a Ga atom at the origin and that the Ga vacancy in the reconstructed 2×2 cell is at the origin too. $|F_{hk}^{\text{tot}}|^2$ changes with the phase difference between F_{hk}^{surf} and F_{hk}^{bulk} and therefore changes with the registry of the 2×2 cell.

Due to the 3m symmetry there are six possibilities for the registry. Let I and II denote the two orientations of the surface unit cell as shown in fig. 5. The surface can now be completed by placing I or II on top of an ideal (unreconstructed) surface terminating either with an A, B or C bilayer, see fig. 5. This gives the possibilities IABCABC, IBCABCA, ICABCAB, IIABCABC, IIBCABCA or IICABCAB. Since I arises from a reconstructed C bilayer the "natural" choice would be IABCABC.

A change in the termination of the ideal surface changes the phase of F_{hk}^{bulk} by $\pm\psi_{hk}$ and rotating I to II changes the sign of the phase of F_{hk}^{surf}. A comparison between $|F_{hk}^{\text{tot}}|^2$ and the observed values can be made for the six possibilities. There are no adjustable parameters because the scale and the surface structure were determined by the fractional-order reflections.

IABCABC has the best agreement with $\chi^2 = 7.6$. The second-best case is IICABCAB with $\chi^2 = 20$, the other four have χ^2 in excess of 250. Hence a clear assignment of the registry can be made. The agreement can be improved by allowing only a part of the surface to be reconstructed and assuming the rest to be terminated-bulk like. Adding the intensities of the two parts gives

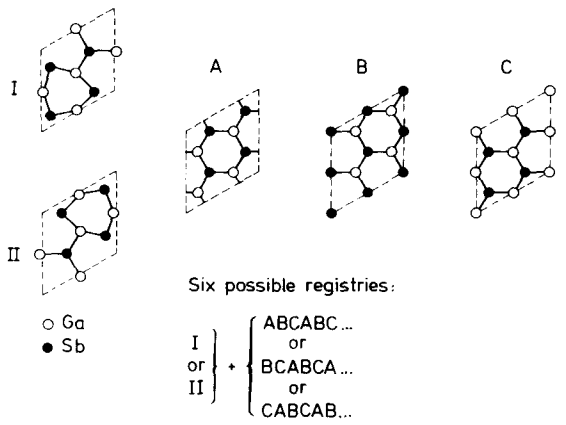

Fig. 5. Possible registries for the reconstructed surface unit cell. I and II denote two possible orientations of the 2×2 cell while A, B and C decribe the three possible terminations of the underlying bulk crystal.

$\chi^2 = 0.5$ with $66\% \pm 10\%$ of the surface area reconstructed. The structure factor intensities are listed in table 2.

5. Out-of-plane structure

From in-plane measurements alone it is not possible to obtain information about atomic displacements in the direction normal to the surface; out-of-plane measurements, the so-called rod scans, are necessary. These were performed as described in section 2 by moving the detector out of the surface plane, keeping the angle of incidence fixed. Due to mechanical restrictions the maximal obtainable momentum transfer in the direction normal to the surface was ~ 0.5 Å^{-1}, which is not sufficient to give the same accuracy as LEED [1,4].

The rod scans for the $(\frac{3}{2}, 0)$, $(1, \frac{1}{2})$ and $(\frac{3}{2}, \frac{1}{2})$ are shown in fig. 6. The momentum transfer normal to the surface is described in units of $(111)_{cub}$. Due to Friedel's inversion law, $|F_{-h-k-l}| = |F_{hkl}|$, and the 3-fold symmetry, a rod scan of $(hk\bar{l})$ is equivalent to a rod scan of (khl). Therefore, the $(1, \frac{1}{2})$ scan is a juxtaposition of two pieces, one for $(1, \frac{1}{2})$, $l \geqslant 0$ and one for $(\frac{1}{2}, 1)$, $l \leqslant 0$. The rod scans consist of background subtracted integrated intensities and are normalized to 1 close to $l = 0$.

Rod scans calculated for three model structures with different vertical but identical lateral atomic displacements (as derived in section 3) are shown in fig. 6:

(i) The full curve. No vertical displacements are included and thus the distance between the Ga layer and the Sb layer in the surface unit cell is equal to the bulk value of $\sqrt{3}\, a_0/12 = 0.88$ Å.

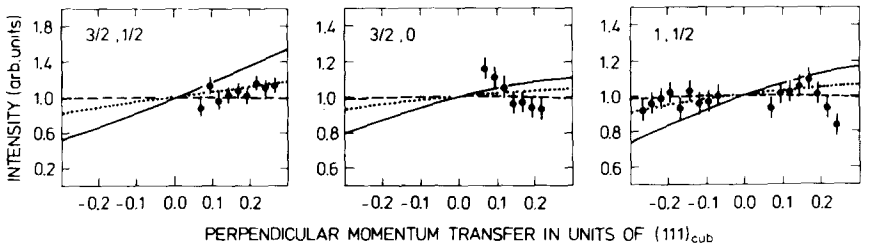

Fig. 6. Rod scans for the $(\frac{3}{2}, 0)$, $(1, \frac{1}{2})$ and $(\frac{3}{2}, \frac{1}{2})$ reflections. Data points affected by refraction effects are omitted. The full, dashed and broken curves represent calculations with an intralayer distance in the surface bilayer of 0.88 , 0.3 and 0.0 Å, respectively.

(ii) The dashed curve. The distance is reduced to 0.3 Å.
(iii) The broken curve. All atoms in the surface unit cell are in the same layer.

It can be concluded from fig. 6 that the reconstructed surface bilayer is flat to within ~ 0.3 Å. Similar measurements have been performed for InSb(111)-2 × 2 [12]. This surface was flat to within ~ 0.2 Å. To obtain a more detailed picture of the vertical displacements more extensive measurements would have to be performed.

6. Discussion and conclusion

The flatness of the reconstructed surface bilayer compares very well with the picture obtained from LEED intensity measurements: GaAs [1] and GaP(111)2 × 2 [4] are flat to within 0.2 and 0.1 Å, respectively. The projected bond distances of 2.64 ± 0.04 Å between the Ga and Sb atoms in the hexagon and 2.66 ± 0.06 Å between Ga and the lone Sb atoms are within the uncertainties equal to the bulk value of 2.639 Å. The projected bond angles at the three equivalent Sb atoms are 98° ± 3° and 142° ± 3° and 109° ± 2° for the Ga atoms. This confirms that the reconstruction is driven by rehybridization at the surface: the electronic configurations are s^2p^3 (5 electrons) on the three Sb in the hexagon, sp^2 for the three Ga and sp^3 for the seventh Sb.

In conclusion we have shown that the "vacancy-buckling" mechanism applies to GaSb(111)2 × 2 and we have determined the projected coordinates and types of the atoms in the reconstructed surface unit cell. We have explained the intensities of the integer-order reflections and used them to find the registry of the 2 × 2 surface unit cell. The interpretation opens up new possibilities for surface X-ray diffraction: The sites of chemisorbed atoms can be determined [14], studies of 1 × 1 surface structures can be made and the integer-order reflections can perhaps even be used to get phase information on the surface structure factors.

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