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Citation: *Journal of Vacuum Science & Technology B* **28**, C3I1 (2010); doi: 10.1116/1.3414830

View online: <http://dx.doi.org/10.1116/1.3414830>

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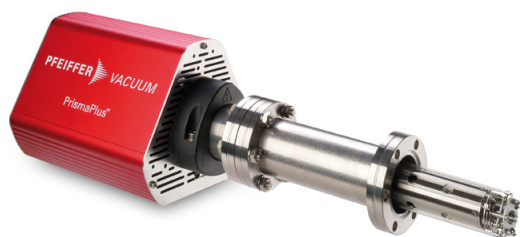
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Temperature dependent lattice constant of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$

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(Received 24 September 2009; accepted 5 April 2010; published 5 May 2010)

Using x-ray diffraction, the in-plane and out-of-plane lattice constants of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ epilayers grown on GaSb and GaAs substrates were determined between 30 and 398 °C for $y = 0.003\text{--}0.059$. The bulk lattice constant was then calculated from the in-plane and out-of-plane lattice constants. A polynomial function for the bulk lattice constant as a function of y and temperature was derived from a fit to the resulting data. Comparison to measured out-of-plane lattice constants of platinum-coated $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ indicates that the polynomial function is valid up to around 550 °C. The polynomial function can be used to determine the lattice matching of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ to, e.g., GaSb at typical growth temperatures used for growth of cladding layers in laser structures. A formula is given for calculating the As mole fraction for lattice matching to GaSb at a given temperature. © 2010 American Vacuum Society. [DOI: 10.1116/1.3414830]

I. INTRODUCTION

$\text{Al}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$ is a popular cladding material for GaSb-based laser structures due to its large band gap and low refractive index for high x and lattice matching to GaSb for low y . Using a high Al mole fraction also enables doping to a high electron carrier concentration.¹ From literature, e.g., Refs. 2–5, the chosen values for the As mole fraction y are typically 0.05–0.07. The As mole fraction is usually chosen to be close to the lattice matching value at room temperature, which depends on the Al mole fraction.

We have experimental results showing that lattice matching at the growth temperature is important in order to achieve dislocation-free layers. When comparing to $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ lattice-matched to GaSb at room temperature, x-ray diffraction (XRD) measurements show that a slight decrease in the As mole fraction results in a lower full width at half maximum (FWHM).⁶ We believe this to be due to a difference in the thermal expansion coefficients of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ and GaSb.⁶ The difference in strain at room temperature and at growth temperature, respectively, is called the “thermal misfit.” If large, the thermal misfit can significantly affect the critical thickness and the density of misfit dislocations. It is therefore important to take this into consideration when designing structures. To the authors’ knowledge, no systematic measurements have been performed on the temperature dependence of the lattice constant of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$. Additionally, no data for the thermal expansion coefficient (TEC) of AlSb above 340 K (Ref. 7) is reported in literature, making any interpolation of TEC data for the binary constituents uncertain above 340 K.

Using XRD measurements from several crystal lattice plane orientations, it is possible to measure the lattice constants accurately. The preferred method has been Bond’s method from the 1960s.⁸ For our measurements, we chose the Zone technique developed by Fatemi,^{9,10} as this method can be utilized in diffractometers with half circle geometry, i.e., $\theta, 2\theta \in [0^\circ, 180^\circ]$, while giving the same level of accuracy as Bond’s method.

In this work, we will present a polynomial fit for the temperature dependent lattice constant of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ valid from room temperature to around 550 °C, as determined from XRD measurements. The data are then used to determine the As mole fraction for lattice matching of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ to GaSb as a function of temperature.

II. THEORY

In order to calculate the bulk lattice constant of a zinc blende crystal from a strained epilayer, both the in-plane and out-of-plane lattice constants must be known, hereafter referred to as a_x and a_z , respectively. The relationship between the lattice constants of the strained layer and the bulk lattice constant can be calculated from the following equation:¹¹

$$a = \frac{a_z + (2C_{12}/C_{11})a_x}{1 + (2C_{12}/C_{11})}, \quad (1)$$

where a is the (unstrained) bulk lattice constant and C_{11} and C_{12} are the stiffness tensor elements. In this study, C_{11} and C_{12} were determined using interpolation of data for the binary constituents of (Al,Ga)(As,Sb).^{12,13} According to Ref. 14, C_{11} and C_{12} are temperature dependent for GaAs. However, the error induced in a by assuming that C_{11} and C_{12} are

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temperature *independent* is less than 1×10^{-4} Å from 0 to 550 °C. Since the error contribution is so small and since we have no corresponding data for the other binary constituents, the stiffness tensors were assumed to be temperature independent in our calculations.

The linear thermal expansion coefficient, $\alpha(T)$, is given by¹⁵

$$\alpha(T) = \frac{1}{a(T)} \frac{da(T)}{dT} \approx \frac{1}{a(T_0)} \frac{da(T)}{dT}, \quad (2)$$

where T is the temperature at which α is evaluated and T_0 is a reference temperature for which a is known, typically the room temperature. The above approximation, setting $a(T) \approx a(T_0)$, is a good approximation for all temperatures in this study since $[a(T)/a(T_0)] - 1$ is small.

The lattice constant at a given temperature can then be calculated as

$$a(T) = a(T_0) \left(1 + \int_{T_0}^T \alpha(T) dT \right). \quad (3)$$

III. EXPERIMENT

All samples were grown in a Varian Gen II Modular molecular beam epitaxy system on (001)-oriented GaSb substrates, except sample As 510-2 that was grown on a (001)-oriented GaAs substrate. The group III composition was calibrated using reflection high-energy electron diffraction on dedicated GaAs samples.

High resolution XRD measurements were performed on a Bruker AXS D8 Discover XRD diffractometer with a half circle geometry. Incident beam optics include a Göbel mirror and a V-groove beam compressor giving $\text{Cu K}\alpha_1$ radiation and a FWHM for Si (111) of less than 0.01° .¹⁶ The diffractometer was equipped with an Anton-Paar DHS 900 temperature stage used to do measurements from 30 to 550 °C, as measured by a thermocouple (TC) inside the hot plate.¹⁷ A 5 min pause was used to allow the temperature to stabilize after each step in temperature. For temperatures above 150 °C, the temperature of the XRD-probed sample surface has been shifted by up to -4 °C (at 550 °C) relative to the TC reading to compensate for the temperature gradient through the sample, based on lattice constant measurements of a Si substrate on the DHS 900 temperature stage.¹⁸

Lattice constants were determined from symmetric and asymmetric reflections using a modified Zone technique.^{9,10} All XRD measurements were performed with an open detector and a 1 mm circular aperture on the source. Measurements were carried out on samples in a nitrogen atmosphere using at least four of the 115, 117, 226, 335, 444, 002, 004, and 006 reflections at each temperature. Asymmetric reflections were measured both in positive (“steep incidence”) and negative (“shallow incidence”) geometries. The 444 reflection was only used for sample As 510-2 due to an overlap of the substrate peak and the epilayer peak in positive geometry for all other samples at most temperatures. Reflections where the overlap of the substrate and epilayer peaks became too

TABLE I. Samples used for XRD study of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$. All samples were capped with 5–50 nm GaSb.

Sample ID	Thickness (μm)	y	Growth temperature (°C)
As 510-2	6	0.0027	530
Sb 54-3	2	0.0524	490
Sb 99-1	2	0.0670	490
Sb 122	2	0.0569	550
Sb 130-4	2	0.0589	550
Sb 141-2	0.5	0.0579	465

large for an accurate determination of the peak positions were not included in the calculations. The azimuthal (φ) and tilt (χ) angles of the samples were aligned to get a correct incidence angle on to the sample. This was done one to three times during a measurement series, at different temperatures.

Due to the large number of peaks (6–13 peaks each for epilayer and substrate for each calculated pair of lattice constants a_x and a_z), the peak positions were extracted automatically by taking the average angle between two points on opposite sides of the peak. The points were usually taken at 70% of the peak intensity but higher values were chosen when overlap of epilayer and substrate peaks became an issue.

The lattice constant was then determined by correcting for incident angle offsets and refractive index, in that order. Using a least-mean-square (LMS) approach, the extracted peak positions were shifted to account for an incident angle offset, followed by refractive index correction, minimizing for the residual error in a_x and a_z from different reflections. The refractive indices were taken to be $n = 1 - \delta$, with δ calculated using values from Ref. 19. The resulting LMS fit gave a good agreement between the lattice constants calculated from each reflection, as the standard deviation for a_x and a_z was between 5×10^{-5} and 3×10^{-4} Å. The bulk lattice constant a was then calculated using Eq. (1).

For each sample, the As mole fraction, y , was determined from the interpolation of lattice constants of the binaries at 30–32 °C to fit the found bulk lattice constant, assuming $x = 0.90$ and that Vegard’s law is valid. The lattice constant of GaSb (6.0970 Å) was taken from our own measurements.¹⁸ The lattice constant of GaAs (5.6538 Å) was taken from Ref. 14, while for AlAs (5.6610 Å) and AlSb (6.1359 Å), the lattice constants were taken from Refs. 7 and 20. The values given in parenthesis are at 32 °C.

XRD measurements were performed at TC temperatures from 100 to 400 °C in steps of 50 °C, as well as at 30–32 °C and at 65 °C. More than 50 values for a were calculated from the measurements of the samples. The important sample parameters are given in Table I. While the uncertainty in y is closer to $\pm 4 \times 10^{-4}$ ($\pm 2 \times 10^{-4}$ Å), it was determined down to 1×10^{-4} as this gave a smaller residual error between the measurements and the polynomial fit found in Sec. IV.

The As mole fraction was found to vary slightly (up to ± 0.001) across a 2 in. wafer. Smaller pieces (typically 8

$\times 8 \text{ mm}^2$) from the same sample in Table I would therefore often have slightly different As content. Typical values for y are listed in Table I.

Due to a degradation of the epilayer at temperatures above 350–400 °C, believed to be due to outdiffusion of the group V constituents, the measurements have mainly been performed up to 400 °C. The samples measured above 400 °C were prepared by evaporating Pt layers of varying thicknesses on to the sample in an e-beam evaporator. A minimum thickness of 100 nm was found to be necessary to stop the degradation of the epilayer.

IV. RESULTS AND DISCUSSION

The calculated lattice constants from all samples except Sb 99-1 and Sb 122 resulted in 52 values for a in the temperature range of 30–398 °C. These values were used to make the polynomial fit

$$a(y, T) = b_0 + b_1 \times y + b_2 \times T + b_3 \times T^2 \text{ (\AA)}. \quad (4)$$

Sb 99-1 was not included due to an overlap of the peaks in the measured temperature range (lattice matching). For Sb 122, temperature dependent XRD measurements were only performed on Pt-coated pieces due to time constraints. To avoid any potential Pt influence on Eq. (4), these results were not used in the polynomial fit.

The best fit was with $b_0 = 6.1310 \text{ \AA}$, $b_1 = -0.4702 \text{ \AA}$, $b_2 = 2.856 \times 10^{-5} \text{ \AA/}^\circ\text{C}$, and $b_3 = 5.03 \times 10^{-9} \text{ \AA/}^\circ\text{C}^2$, when T is given in °C. yT and y^2 were not included, as the contributions were found to be less than the measurement uncertainty in the measured ranges for y and T . The standard error of the fit was $1.5 \times 10^{-4} \text{ \AA}$.

Equations (2) and (4) then give the following linear TEC:

$$\begin{aligned} \alpha(T) &\approx \frac{b_2 + 2b_3T}{b_0 + b_1y} \\ &\approx 4.68 \times 10^{-6} + 1.65 \times 10^{-9} \times T \text{ (}^\circ\text{C}^{-1}) \end{aligned} \quad (5)$$

for $y \approx 0.06$, where T is given in °C and $a(T_0)$ is evaluated at 0 °C.

The As mole fraction y required for lattice matching to GaSb as a function of T has been calculated from Eq. (4) and our measurements for GaSb (Ref. 18) and is presented in Fig. 1.

A linear fit to the curve in Fig. 1 gives the following criterion for lattice matching to GaSb:

$$y = 0.0751 - 2.59 \times 10^{-5} \times T, \quad (6)$$

where T is given in °C. For a fully strained $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ epilayer on GaSb, y can quickly be determined from a 004 XRD scan at room temperature (25 °C) using $y = 0.0744 - 0.1971 \times \Delta\theta$, where $\Delta\theta$ is the angular separation (in degrees) between the $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ peak and the GaSb peak.

A topographical representation of the temperature shift of the $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_{0.0671}\text{Sb}_{0.9329}$ and GaSb 004 XRD peaks for a piece of sample Sb 99-1 is shown in Fig. 2. The substrate and epilayer peak positions merge close to 305 °C. This is

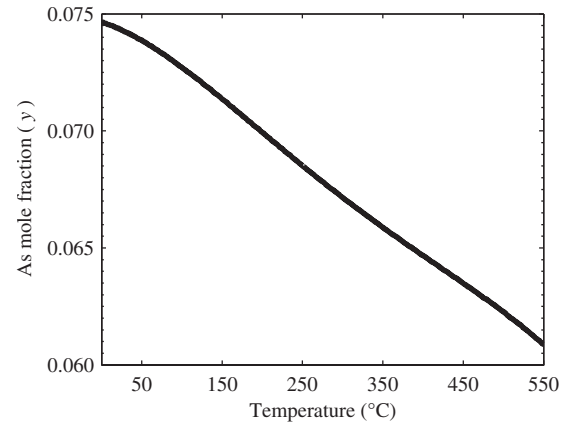


FIG. 1. Lattice matching criteria for $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ on GaSb.

close to the value of 309 °C found from Eq. (6) and the As mole fraction calculated from asymmetric XRD measurements at 32 °C. Note that for all topographical plots (Figs. 2–4), each constituent scan has been shifted so that the GaSb peak is at its theoretical position, given by the polynomial in Ref. 18. The shift is necessary due to an inhomogeneous expansion of the DHS 900 hot plate, leading to a temperature dependent angular offset of the sample.¹⁷

In order to measure the lattice misfit at higher temperatures and examine the validity of Eq. (4) above 400 °C, $8 \times 8 \text{ mm}^2$ pieces of sample Sb 122 were capped with either a 100 nm thick or a 200 nm thick Pt layer on the epise. A topographical representation of the temperature shift of 004 peaks up to 546 °C for the piece coated with 100 nm is shown in Fig. 3.

The resulting bulk lattice constants a of (unstrained) $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_{0.0566}\text{Sb}_{0.9434}$ at different temperatures are listed in Table II. The bulk lattice constant was calculated from Eq. (1), where a_x was assumed to be equal to the GaSb lattice constant¹⁸ (i.e., fully strained epilayers) and a_z was derived

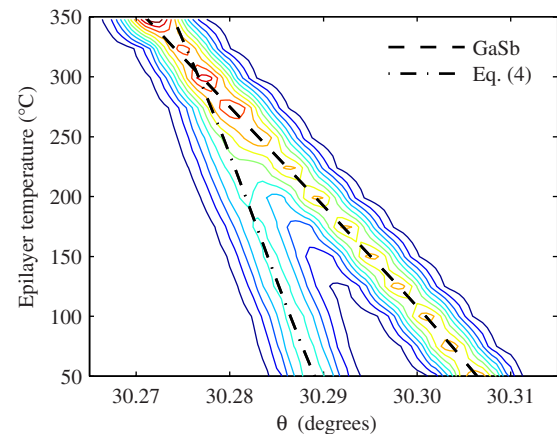


FIG. 2. (Color online) Topographical representation of the temperature shift of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_{0.0671}\text{Sb}_{0.9329}$ and GaSb 004 XRD peaks for a piece of Sb 99-1, with measurements performed at about 25 °C intervals from 50 to 348 °C. The dashed curves show theoretical peak positions calculated from lattice constants found in Ref. 18 (GaSb) and from Eq. (4) ($\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$).

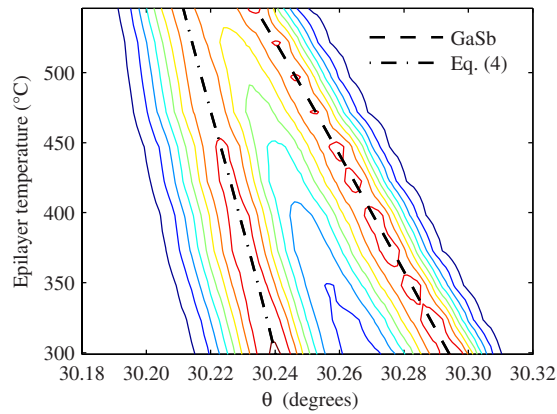


FIG. 3. (Color online) Topographical representation of the temperature shift of 004 peaks for a piece of Sb 122 coated with 100 nm Pt. Measurements were performed at about 25 °C intervals from 299 to 546 °C. The dashed curves show theoretical peak positions calculated from lattice constants found in Ref. 18 (GaSb) and from Eq. (4) ($\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$), with $y = 0.0566$.

from the 004 scans presented in Fig. 3. Due to a high degree of overlap of the epilayer and substrate peaks at most of these temperatures, the usual 70% of peak value method could not be used for extracting the peak position. Instead, a weighted mean over a range of higher intensities was used, with the peak intensity being weighted the most. The As mole fraction ($y=0.0566$) was derived from the best fit to Eq. (4) at 299 °C, which was then used to determine $C_{11,12}$ and δ .

In Table II, the bulk lattice constants derived from measurements are also compared to the bulk lattice constants calculated from Eq. (4) at different temperatures up to 546 °C. It can be seen that the deviation between a derived from measurements and a calculated from Eq. (4) is within $\pm 1 \times 10^{-4}$ Å from 300 to 546 °C. An analysis of the uncertainties involved in the determination of the peak positions

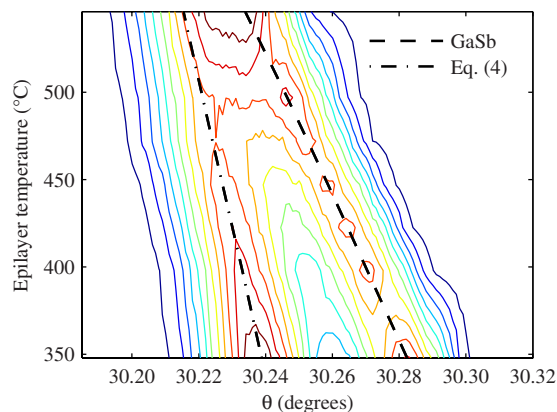


FIG. 4. (Color online) Topographical representation of the temperature shift of 004 peaks for a piece of Sb 122 coated with 200 nm Pt. Measurements were performed at 348 °C, at about 25 °C intervals from 398 to 497 °C, and at 546 °C. The dashed curves show theoretical peak positions calculated from lattice constants found in Ref. 18 (GaSb) and from Eq. (4) ($\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$), with $y=0.0574$. Equation (4) was found to fit the measurements to within $\pm 1 \times 10^{-4}$ Å up to 450 °C (i.e., as far as both peaks are well resolved).

TABLE II. Sb 122 (100 nm Pt): Comparison of a from Eq. (4) and a calculated from Eq. (1) using literature values of GaSb (Ref. 18) for a_x and values derived from 004 reflection measurements (Fig. 3) for a_z . $\Delta\theta$ is the observed angular separation between the two peaks shown in Fig. 3 and θ is the angular position of the $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_{0.0566}\text{Sb}_{0.9434}$ peak.

Temperature (°C)	$\Delta\theta$ (deg)	θ (deg)	a from Eq. (1) (Å)	Equation (4) (Å)
299	0.054	30.239	6.1134	6.1134
324	0.051	30.236	6.1142	6.1142
348	0.048	30.234	6.1149	6.1149
373	0.044	30.231	6.1157	6.1157
398	0.041	30.228	6.1165	6.1166
423	0.038	30.225	6.1173	6.1174
447	0.035	30.222	6.1181	6.1182
472	0.032	30.220	6.1189	6.1190
497	0.028	30.217	6.1197	6.1198
522	0.025	30.214	6.1206	6.1207
546	0.022	30.211	6.1214	6.1215

and a_{GaSb} suggests that the uncertainty in a derived from the 004 reflection measurements is $\pm 2.4 \times 10^{-4}$ Å, close to the standard error of Eq. (4). We take the above results as a strong indication that Eq. (4) is valid up to around 550 °C. Note that since we have not measured the in-plane lattice constant, these measurements cannot be considered to be absolute proof of validity for Eq. (4) up to 550 °C.

A topographical representation of the temperature shift of 004 peaks up to 546 °C for the piece coated with 200 nm Pt is shown in Fig. 4. Also in this case, Eq. (4) was found to fit the measurements up to 450 °C (i.e., as far as both peaks are well resolved).

The TEC of AlSb has only been reported up to 340 K (Ref. 7) (where it flattens out) and is thus currently the best estimate for the TEC of AlSb at higher temperatures. Using this TEC, we can calculate the lattice constant at higher temperatures from Eq. (3). A comparison of the interpolation of the binary constituents, Eq. (4) ($y=0.0589$) and the derived bulk lattice constants for Sb 130-4 is shown in Fig. 5. It can be seen that the binary interpolation deviates significantly

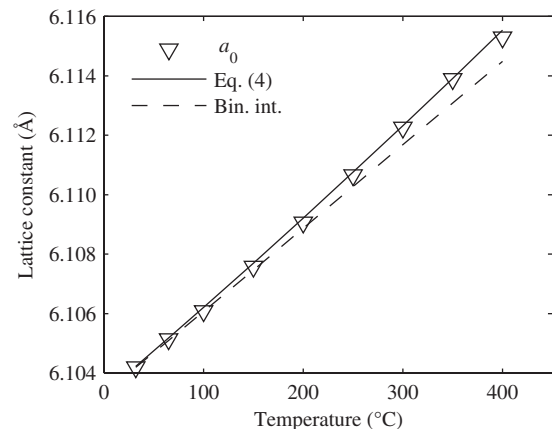


FIG. 5. Derived bulk lattice constants of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_{0.0589}\text{Sb}_{0.9411}$ from experimental data for sample Sb 130-4 compared to Eq. (4) and interpolation of the binary constituents from 32 to 400 °C.

from the measured lattice constants at elevated temperatures, and thus further investigation of AlSb above 340 K is needed.

A. Error sources

Uncertainties include errors in x , y , and T . For sample Sb 141-2, x was measured by using a 200 nm $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ calibration layer. A simulation of the 004 XRD peaks for sample Sb 141-2 using the LEPTOS software package from Bruker AXS resulted in $x=0.911$. Assuming an uncertainty of $\Delta x = \pm 0.02$ around $x=0.90$, at 30 °C, y would be determined within $\pm 1.5 \times 10^{-3}$ from the actual As mole fraction in the sample (according to binary interpolation). This shift in y would, however, not be detrimental to Eq. (4). The error would mainly impact Eq. (4) through the thermal coefficients b_2 and b_3 since the thermal expansion for, e.g., $x=0.88$ would slightly differ from $x=0.90$. An estimation of the uncertainty in $a(T)$ for a deviation in x , Δx , of 0.02 can be evaluated by comparing the deviation in $a(T)$, $\Delta a(T)$, at the lowest (30 °C) and highest (400 °C) temperature measured using

$$\begin{aligned} \Delta a(T) &= \frac{da(T)}{dx} \times \Delta x \\ &\simeq \frac{a_{\text{Al}_{0.90}\text{Ga}_{0.10}\text{Sb}}(T) - a_{\text{GaSb}}(T)}{0.9} \times 0.02, \end{aligned} \quad (7)$$

where Eq. (4) is used for $a_{\text{Al}_{0.90}\text{Ga}_{0.10}\text{Sb}}$ ($y=0$) and data in Ref. 18 are used for a_{GaSb} . The difference between Δa at 30 and 400 °C was found to be $\mp 1.0 \times 10^{-4}$ Å for $x=0.90 \pm 0.02$, which is the best estimate for the contribution of this error.

The uneven thermal expansion of the hot plate, causing thermally induced tilt, also contributes to the temperature-related errors. Investigation suggests that the contribution to the incident angular offset is approximately 0.01° in θ when going from 50 to 350 °C. This contribution is, however, included in the incident angle offset calculations mentioned in Sec. III. It is assumed that the angular offset is constant for the measurement series (6–13 measured epilayer and substrate peaks) at each temperature, which lasts about 1.5–2 h. The angular offsets for the peak positions seem random for the different measured peaks, suggesting that there is no steady drift in the angular offset at constant temperature.

The temperature dependence of C_{11} and C_{12} can also contribute to thermally induced errors. However, as mentioned in Sec. II, this temperature dependence is weak and is ignored. For strained GaAs, this error would be approximately 1×10^{-4} Å in the lattice constant a under similar conditions. If the other binary constituents have temperature dependences in C_{11} and C_{12} of the same order, the total error would be approximately the same.

Many of these errors are hard to quantify. For the majority of the measurements (90%), the calculated values for a were within $\pm 2 \times 10^{-4}$ Å of the values predicted by Eq. (4) (and 96% within 2.7×10^{-4} Å). The discussed error sources may both increase and decrease the value for a , and they are all within $\pm 2 \times 10^{-4}$ Å. Since we have performed over 50 mea-

surements on four samples with potentially slightly differing Al mole fractions (x), $\pm 2 \times 10^{-4}$ Å is probably the best estimate for the deviation in the fit for the bulk lattice constant of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$. In addition, measurements on sample Sb 99-1 show that Eq. (4) can be used for y up to at least 0.067 and measurements on Sb 122 show that Eq. (4) can be used up to around 550 °C.

V. CONCLUSIONS

Measurements of the lattice constant of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ from 30 to 398 °C for $y = 0.003$ – 0.059 were performed. A polynomial function for the bulk lattice constant was derived from a fit to the resulting data. Measurements on Pt-coated samples at higher temperatures indicate that the polynomial function is valid up to around 550 °C. We have shown the lattice matching condition for growth of $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}_y\text{Sb}_{1-y}$ lattice matched to GaSb. At 450 °C–550 °C, an As mole fraction of 0.063–0.061 should be used. An interpolation of the binary constituents (Al,Ga)(As,Sb) was shown to give a poor fit to the bulk lattice constant at elevated temperatures, probably due to the lack of data in literature for the thermal expansion coefficients, especially for AlSb.

ACKNOWLEDGMENTS

Thanks are due to Mike Pochet for assistance in improving the language of this article. This project was partly funded by the Research Council of Norway under Contract No. 177610/V30.

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