The role of AsH\textsubscript{3} partial pressure on anti-phase boundary in GaAs-on-Ge grown by MOCVD? Application to a 200mm GaAs virtual substrate

The MIT Faculty has made this article openly available. Please share how this access benefits you. Your story matters.
The role of $\text{AsH}_3$ partial pressure on anti-phase boundary in GaAs-on-Ge grown by MOCVD – application to a 200 mm GaAs virtual substrate

KOHEN David$^{1,*}$, BAO Shuyu$^{1,2}$, LEE Kwang Hong$^1$, LEE Kenneth Eng Kian$^1$, TAN Chuan Seng$^{1,2}$, YOON Soon Fatt$^{1,2}$, FITZGERALD Eugene A.$^{1,3}$

1 Low Energy Electronic Systems IRG (LEES), Singapore-MIT Alliance for Research and Technology, 1 Create Way, Singapore 138602
2 School of Electrical and Electronic Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore
3 Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

* david@smart.mit.edu +6598592078

Abstract

We demonstrate the influence of the arsine partial pressure ($p(\text{AsH}_3)$) on the quality of a GaAs layer grown on Ge substrate by metal organic chemical vapor deposition. The GaAs quality improves with $p(\text{AsH}_3)$ used during the 100 nm thick GaAs buffer layer. By growing a GaAs buffer layer at 630°C with $p(\text{AsH}_3)$ of 5 mbar, we obtain a smooth GaAs layer with a root mean square roughness of 4.7 Å. This GaAs layer does not contain anti-phase boundaries. With these optimized growth parameters, we fabricate a virtual GaAs substrate on a 200 mm silicon wafer as a first step towards the integration of III-V devices on silicon.

Keywords

1 Introduction

Although the lattice mismatch (<0.1%) and thermal expansion coefficient mismatch (<1.6% at room temperature) between GaAs and Ge are small, the polar nature of GaAs makes it difficult to obtain high quality GaAs on Ge. GaAs can be deposited in two different orientations on the non-polar Ge lattice, with one orientation being rotated relative to the other by 90° along the growing axis[1]. When two different GaAs orientations are deposited on the same surface, As-As and Ga-Ga bonds form at the domains boundary and propagate in the growing GaAs layer, creating an anti-phase boundary (APB)[1].

Anti-phase boundaries (APB) result in surface roughening in the form of long crack-like structures[2], depressions in the surface[3] or even stacking faults formation[4,5]. APB also act as recombination centers, thereby reducing the photoluminescence (PL) efficiency of the GaAs layer[6]. While surface roughening is detrimental to majority carrier devices because surface scattering decreases channel mobility, a high recombination rate decreases the performances of minority carrier devices such as solar cells or light-emitting diodes. Therefore, the optimization of the GaAs on Ge growth is a first step towards performance improvements of III-V devices on Ge (or Si).

Different techniques have been proposed and experimentally demonstrated to either suppress or reduce APB in GaAs on Ge. An early proposal was to use a non-polar GaAs growing axis (e.g. on {111} or {211} Ge surface)[7,8]. However, <100> orientated Ge wafers are preferred due to their lower cost, greater availability, and more importantly they open a pathway towards integration of III-V devices on Si (100) wafers that are used in CMOS processing. Although the selective area growth of GaAs inside Silicon V-grooves[9,10] or trenches[11] has been demonstrated to prevent the APB formation, the growth of APB-free blanket GaAs on Ge (or Si) by MOCVD still remains challenging.
Because of the polar nature of the <100> GaAs growth axis, starting on a double-step Ge surface is required\[12\]. One way to obtain a double step Ge surface is to use a slightly misorientated Ge wafer (typically between 2 and 10°). Single-domain GaAs growth on such offcut Ge wafers has been demonstrated previously\[13\]. However, the use of misorientated substrates is an essential but insufficient condition to obtain APB-free GaAs layers. A two-step growth, with a thin GaAs buffer layer with optimized growth parameters, followed by growth of GaAs under more conventional growth conditions, is necessary.

Two temperature ranges have been reported for the GaAs buffer layer that allows for the growth of APB-free GaAs layers. One is in the [350-550°C] range\[4,14–17\] and the second one is in the [600-725°C range]\[7,17–20\]. Between these two temperature ranges, growth of a mixed distribution of GaAs domains occurs, leading to the formation of numerous APB\[17\]. Although the lower temperature regime reduces the diffusion of Ge into the GaAs layer\[14\], the higher temperature regime reduces the carbon contamination in the GaAs layer\[21\]. Furthermore, it is frequent to observe diamond-shape APB-related defects at the GaAs/Ge interface with the low-temperature growth regime\[3,15,22\]. In addition, using the higher temperature regime, devices grown on Ge substrates such as lasers and solar cells have shown comparable and even better performances than on GaAs substrate\[18,21\]. This has motivated us to use the higher temperature regime for the GaAs buffer layer.

Arsenic atoms play an important role at the Ge surface by creating As dimers with two possible orientations\[1\] that can lead to two GaAs domains. In addition, the Ge surface exposed to arsine will be covered by a self-limiting As monolayer. Since arsenic has a high vapor pressure, care must be taken to ensure the complete coverage of the Ge surface in order to prevent the formation of APB during the GaAs growth.
There are contradictory reports in the literature about the optimized V/III ratio for the GaAs buffer layer growth [13,19,20,23]. Values ranging from 12 up to 120 have been reported. All the cited studies used MOCVD with AsH₃ as the group V precursor, so it is surprising that such a large range of “optimized V/III ratios” was reported.

This paper investigates the discrepancies in the reported values for the optimized V/III ratio for APB-free growth of GaAs on Ge. We show that it is the AsH₃ partial pressure \( p(\text{AsH}_3) \) during the GaAs buffer layer, and not the V/III ratio, that influences the appearance of anti-phase boundaries (APB). We demonstrate the growth of GaAs on a Ge substrate with a RMS roughness below 5 Å on a 10 × 10 µm² scan, with excellent crystalline and optical quality by using an optimized \( p(\text{AsH}_3) \) of 5 mbar. These optimized growth parameters are used to fabricate a virtual 200 mm GaAs substrate on silicon.

2 Experimental details

Epi-ready <100> orientated Ge and GaAs wafers with a 6° offcut towards the nearest (111) plane were used as starting substrates. The growth of GaAs layers was performed in an AIXTRON Crius MOCVD reactor using TMGa and AsH₃ as precursors and 32 standard liters per minute (slm) of H₂ as carrier gas. An optical pyrometer array measured the temperature at the surface of the wafer. GaAs was grown on Ge substrates using a two-step growth process, which consists of a thinner GaAs buffer layer grown with one set of process conditions, followed by a thicker GaAs epi-layer using a different set of growth conditions (Figure 1).
Figure 1: Schematics of the two-step GaAs growth on Ge. A 100 nm GaAs buffer layer is grown with varying growth parameters. Then a 500 nm thick GaAs epi-layer is grown under conventional GaAs growth parameters.

Each growth began with the wafer baked at 650°C under H₂ for 5 minutes in order to initiate a double-step surface. This was followed by the 100 nm thick GaAs buffer layer, which was initiated with a 5-second pre-flow of AsH₃ followed by the introduction of TMGa at a fixed flow rate of 19 µmol/min or 38 µmol/min. The surface temperature, reactor pressure and V/III ratio were varied for the GaAs buffer layer growth of different samples, as listed in Table 1. Following the GaAs buffer layer, a 500 nm thick GaAs epi-layer was deposited. For all samples, growth of the GaAs epi-layer was carried out at 630°C under a reactor pressure of 100 mbar, with a TMGa flow of 96 µmol/min and a V/III ratio of 46.

AFM in tapping mode was used to measure the root mean square (RMS) surface roughness. The interface between GaAs and Ge was observed using cross-sectional TEM at 200kV in a FEI Tecnai tool and a FEI scanning electron microscope (SEM). A 488 nm blue laser coupled to a silicon photo-detector probed the light emission properties of the GaAs layer and the GaAs QW structure at room temperature. The GaAs layer thickness was measured using spectroscopic ellipsometry at 65°, 70° and 75° incidence angle over a [0.7-5] eV energy range. To analyze the crystalline quality of the layers, we used a PANalytical
high-resolution X-ray diffractometer equipped with a hybrid 4-bounce Ge(400) monochromator that only let the Cu K\(\alpha_1\) radiation pass through. The detector was used in the channel mode configuration for the fast reciprocal space mapping (RSM) or equipped with a symmetric 3xGe (220) triple-axis analyzer to measure the high resolution RSM.

<table>
<thead>
<tr>
<th>Sample name</th>
<th>Temperature (°C)</th>
<th>V/III ratio</th>
<th>As(\text{H}_3) partial pressure (mbar)</th>
<th>TMGa flow (µmol/min)</th>
<th>Reactor Pressure (mbar)</th>
<th>Growth Time (minutes)</th>
<th>Visual inspection of surface</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>630</td>
<td>234</td>
<td>0.3</td>
<td>19</td>
<td>100</td>
<td>21</td>
<td>Cloudy</td>
</tr>
<tr>
<td>B</td>
<td>680</td>
<td>234</td>
<td>0.3</td>
<td>19</td>
<td>100</td>
<td>21</td>
<td>Cloudy</td>
</tr>
<tr>
<td>C</td>
<td>630</td>
<td>936</td>
<td>1.25</td>
<td>19</td>
<td>100</td>
<td>21</td>
<td>Slightly cloudy</td>
</tr>
<tr>
<td>D</td>
<td>630</td>
<td>936</td>
<td>2.5</td>
<td>38</td>
<td>100</td>
<td>10.5</td>
<td>Specular</td>
</tr>
<tr>
<td>E</td>
<td>630</td>
<td>936</td>
<td>5</td>
<td>38</td>
<td>200</td>
<td>10.5</td>
<td>Specular</td>
</tr>
<tr>
<td>F</td>
<td>630</td>
<td>468</td>
<td>5</td>
<td>38</td>
<td>400</td>
<td>10.5</td>
<td>Specular</td>
</tr>
</tbody>
</table>

Table 1: Process parameters used during the 100 nm thick GaAs buffer layer. All samples are then capped by a 500 nm thick GaAs epi-layer grown at 630°C with a V/III ratio of 46.

3 Results

3.1 Optimization of GaAs on Ge

Sample A, grown with a V/III ratio of 234 at 630°C exhibits a cloudy surface, which is a characteristic of a very rough surface. Indeed, the atomic force microscope (AFM) scan of the surface (Figure 2b) shows numerous pits in the GaAs layer, with a feature size ranging from 100 to 500 nm in both width and length. This leads to a root mean square (RMS) roughness value of 46 nm in a 10 × 10 µm\(^2\) scan. A closer inspection by cross-sectional SEM shows that these pits extend deep into the GaAs layer (Figure 2a). Consequently, the GaAs layer is not continuous but it is composed of islands around 1 µm in length. The measured roughness in this case is likely to be an underestimate of the true RMS roughness,
considering the fact that the AFM tip is not able to probe the bottom of the high aspect ratio pits.

Figure 2: Sample A, the GaAs buffer layer was grown at 630°C with an AsH$_3$ partial pressure of 0.3 mbar, a V/III gas phase ratio of 234. (a) Cross-sectional scanning electron micrograph of sample A. (b) 10 $\times$ 10 $\mu$m$^2$ AFM scan of the GaAs surface. The surface is very rough (with a RMS roughness of 46 nm) and holes (or pits) are observed in the GaAs layer.

Sample B was grown at a 50°C higher growth temperature compared to sample A. The growth resulted in a hazy (or cloudy) surface as well. Microscope inspection revealed the presence of surface pits, which is the characteristic of anti-phase boundaries (APB). The surface pits of sample A (Figure 2b) and B look similar to the results of Wu et al[23]. However, unlike their results, we were unable to obtain APB-free GaAs on Ge growth solely
by varying the growth temperature. This was despite the fact that sample A and sample B
were grown with a V/III ratio of 234, which is higher than the recommended minimum values
found in the literature[13,19]

Instead, we have found that the large range of optimized V/III ratio in the literature
can be explained by the different reactor pressures used in these studies. Indeed, according to
equation 1, the arsine partial pressure $p(\text{AsH}_3)$ is proportional to the reactor pressure.

$$p(\text{AsH}_3) = p(\text{reactor}) \times \frac{\text{flow(AsH}_3)}{\text{total gas flow}} \quad (1)$$

where $p(\text{reactor})$ is the reactor pressure, and total gas flow includes the carrier gas, TMGa
and AsH$_3$ flow.

Therefore, under similar carrier gas and AsH$_3$ flow, $p(\text{AsH}_3)$ can vary by one order of
magnitude between an atmospheric pressure (AP) MOCVD and a reduced pressure MOCVD.
For instance, Tyagi et al. mention a carrier gas flow of 4 slm[19] (a typical value for an AP-
CVD reactor). Assuming a similar AsH$_3$ flow to ours (800 sccm), Tyagi’s $p(\text{AsH}_3)$ would be
more than 15 times higher than ours, even though the V/III ratio might be approximately the
same. This demonstrates that the V/III ratio alone does not completely specify the reactor
environment under which the growth is carried out.

From our experiments, we found that it was not the V/III ratio but the arsine partial
pressure $p(\text{AsH}_3)$ that had the most influence on the surface morphology in our set of
experiments. As an example, Figure 3 shows Nomarski microscope images of three different
GaAs growth conditions, corresponding to sample C, D and E. The only difference was
$p(\text{AsH}_3)$ during the 100 nm thick buffer layer. The V/III ratio and growth temperature were
the same for all three samples. For sample E, the reactor pressure was raised from 100 mbar
to 200 mbar in order to increase $p(\text{AsH}_3)$ without changing the AsH$_3$ mass flow (and
accordingly V/III ratio), according to equation 1.
Figure 3: (a) Schematic of the grown samples. The 100 nm thick GaAs buffer is grown under a V/III ratio of 936 and with varying arsine partial pressure. (b-d) Nomarski microscope image of the samples C, D and E respectively with the GaAs buffer layer grown under an arsine partial pressure of (b) 1.25 mbar, (c) 2.5 mbar and (d) 5 mbar. Numerous surface pits are observed for sample C and D (some are highlighted by an arrow) whereas no pits are detected for the sample E. The scale bar is 10 µm for all Nomarski images.

With $p(\text{AsH}_3)$ of 1.25 and 2.5 mbar, although specular to the eye, the GaAs surface is not smooth and contains pits with a density in the order of $10^5$/cm$^2$ (Figure 3b and 3c). Whereas the sample grown at $p(\text{AsH}_3)$ of 5 mbar is free of surface defects and appears smooth when viewed under a Nomarski microscope (Figure 3d). The surface was further analyzed by plan-view SEM (not shown here) and no pits or crack-like structure were detected.

The surface of the GaAs (sample E) consists of elongated terraces orientated along the $<110>$ direction (Figure 4) with an average width of 27 nm and a height of 4.4 nm. A similar surface morphology has been observed previously[4,15]. Given that the double atomic steps
of the Ge surface are 2.7 nm apart, this suggests that step bunching occurs during the growth of GaAs[15,24]. A larger AFM scan was taken and an RMS roughness value of 4.7 Å was measured on a 10 × 10 μm² scan. This roughness is more than two times lower than the previously reported roughness of GaAs on Ge using an intermediate quantum dot layer to block the propagation of APB-related defects[2]. Thus, together with the crystalline quality improvement, the surface roughness also decreases when \(p(\text{AsH}_3)\) increases.

![AFM image](image)

**Figure 4**: 1 × 1 μm² AFM image of the GaAs on Ge substrate (sample E). Elongated terraces are observed along \(<110>\) with an average width of 27 nm.

Sample E was further analyzed by observing the cross-section under TEM (Figure 5). The interface between the Ge substrate and the GaAs layer is abrupt, without any signs of APB features at the interface or in the GaAs layer.
**Figure 5:** Cross-sectional transmission electron micrograph of the GaAs on Ge using optimized AsH$_3$ partial pressure for the initiation layer (sample E), in double beam condition with a $<220>$ diffraction vector. No anti-phase boundary or dislocations are detected.

The tilt and strain state of the GaAs layer were calculated using two reciprocal space mapping measured by XRD (Figure 6), according to the method developed by Chauveau[25]. The tilt of the GaAs layer in reference to the Ge substrate is 0.0071° in the [-110] direction, which is in the opposite direction of the substrate offcut. This tilt value is comparable to the one reported by Knuuttila for a GaAs grown at 620°C[15]. A tensile strain value of 0.078% is found for the GaAs layer, meaning that the 600 nm GaAs layer is almost fully strained to the Ge substrate, but the relaxation process has started to occur by the formation of misfit dislocations[1].
Figure 6: Reciprocal space map of the GaAs on Ge sample E taken at the (a) (004) and (b) (-2-24) diffraction plane. The interference fringes can be observed in the (004) RSM.

Our experiments clearly show that the V/III ratio alone does not determine whether APBs form. Indeed, the samples D and E were grown under the same V/III ratio but only sample E shows a smooth APB-free GaAs layer. Rather, we demonstrated that \( p(\text{AsH}_3) \) is the main factor influencing the formation of APB. Samples E and sample F were grown under the same \( p(\text{AsH}_3) \) but with different V/III ratios. Both show smooth surfaces without pits. The analysis of sample E confirmed that no APB are observed in the GaAs layer.

There are several hypotheses for the dependence of the GaAs layer morphology and crystalline quality on the arsine partial pressure \( p(\text{AsH}_3) \). First, a low V/III ratio (and consequently a low \( p(\text{AsH}_3) \)) can induce three-dimensional growth when initiating heterovalent epitaxy on non-polar surfaces, as demonstrated for GaP on Si growth by Suzuki et al.[26]. Second, the As adsorption at the [-110] step is dependent on \( p(\text{AsH}_3) \) and temperature[27]. Below a critical \( p(\text{AsH}_3) \), there might be incomplete surface coverage of the Ge by As, leading to surface sites where Ga atoms might adsorb once TMGa is introduced into the reactor for GaAs growth, thus leading to the formation of APB. Brammertz et al already mentioned that a high As partial pressure is needed in order to prevent the As desorption from the Ge surface[28]. Under our growth conditions, the critical \( p(\text{AsH}_3) \) lies between 2.5 and 5 mbar. We expect this critical \( p(\text{AsH}_3) \) to be lower at reduced growth.
temperature because the As desorption at the step edges reduces with temperature[27]. A complete mapping of the process conditions (temperature and \( p(\text{AsH}_3) \)) that are necessary to obtain smooth and APB-free GaAs can be performed if epitaxy at different temperatures is desired, but is not the focus of this paper.

3.2 GaAs quantum well

To further investigate the suitability of the GaAs on Ge layer as a template for further III-V growth, a GaAs QW, cladded by two AlGaAs layers, was grown on another GaAs on Ge sample obtained using the optimized GaAs growth conditions (corresponding to sample E). The AlGaAs was deposited using a TMAI/TMGa molar flow ratio of 0.3, resulting in an AlGaAs composition of 24% Al, as measured by XRD and photoluminescence (PL). The GaAs QW had a nominal thickness of 10 nm.

Figure 7 depicts the PL spectra of the QW structure grown both on GaAs and Ge substrates. The PL spectra are similar in shape, with a FWHM of 18 nm, proving the high optical quality of the GaAs layers on both substrates. In the presence of APB, the GaAs PL linewidth has previously been reported to be doubled compared to single domain GaAs[29]. This therefore confirms that our optimized GaAs on Ge growth conditions result in the formation of high quality single-domain GaAs on Ge.
Figure 7: Room temperature PL spectrum of a 10 nm thick GaAs quantum well (QW) cladded by Al$_{0.24}$Ga$_{0.76}$As layers on Ge and GaAs substrate. Both spectra were taken under the same PL conditions with a 488 nm blue laser diode operating at 30mW. The curves are shifted vertically for clarity. The peak wavelength is 838.4 nm on GaAs substrate and 839.2 nm on Ge substrate. The FWHM for both samples is 18 nm and the intensity are comparable, demonstrating a comparable optical quality.

3.3 Application to a 200 mm GaAs on silicon substrate

To extend our study, the optimized growth conditions of GaAs on Ge were used to fabricate a 200 mm GaAs virtual substrate on a starting Si wafer. Using our previous knowledge on the two-step growth of Ge on Si[30], 1 µm of Ge was deposited on a 200 mm Si (100) wafer, followed by 1 µm of GaAs (100 nm of buffer and 900 nm of epi-layer) and a thin capping layer of AlGaAs. The AlGaAs capping helps in passivating the GaAs surface so that room temperature PL can be measured[31].

As shown in the cross-sectional TEM image (Figure 8), the interface between GaAs and Ge is free of crystalline defects, and no sign of anti-phase boundaries (APB) are detected in the GaAs layer. This compares favorably with a report of the latter structure grown by MBE, in which APB were detected at the GaAs/Ge interface[32]. The contrast at the Si/Ge interface is due to the abrupt relaxation of the 4.2% lattice mismatch creating an array of misfit dislocations. Our previous work[30] has shown that the threading dislocation density (TDD) in the Ge layer is in the range of low-$10^7$ cm$^{-2}$, and we expect a similar TDD to be propagated in the GaAs layer.
Figure 8: (a) Cross-sectional transmission electron microscope image of the GaAs on Ge on Si sample, observed under the <022> two-beam diffraction condition. The interface between GaAs and Ge is abrupt and free of crystalline defects. No anti-phase boundaries were detected in the GaAs layer. Misfit dislocations are visible at the Ge/Si interface with one threading dislocation segment extending in the Ge layer. (b) 5 × 5 µm² atomic force microscope image of the surface of the GaAs/Ge/Si sample. The root mean square roughness is 8.3 Å. The cross-hatch pattern is due to the strain field generated by the misfit dislocations at the Ge/Si interface along the <110> direction.

The GaAs surface is smooth with an 8.3 Å RMS roughness measured on a 5 × 5 µm² scan area, as shown in Figure 8b. The surface morphology is very similar to the GaAs layer on Ge substrate, with steps visible in the [1-10] direction. However, the roughness is higher
than the GaAs on Ge substrate. This is due to the underlying roughness of the Ge layer on Si, measured at 7.5Å RMS in our previous study[30].

Two important observations can be made of our results. First, the roughness of the GaAs layer is similar to the roughness of the underlying Ge layer, as opposed to the work from Waldron et al. in which the roughness doubled between the GaAs and the Ge layer[33]. Second, a low RMS roughness value (below 1 nm, see Figure 8), similar to the work of Zhou et al can be achieved, without using an intermediate polishing step and a GaAs regrowth[4], therefore simplifying the growth process.

Figure 9: Room-temperature photoluminescence spectrum of the GaAs layer showing the GaAs peak energy at 1.415 eV with a FWHM of 31 nm

The high optical quality of the resulting GaAs layer is demonstrated by the low FWHM value of the room temperature PL spectra (Figure 9). The GaAs peak wavelength is at 1.415 eV with a linewidth of around 31 nm, a typical value corresponding to the parabolic band-to-band recombination. This FWHM value is similar to the recently published results of GaAs on Silicon using aspect ratio trapping technique[11] and confirms the high optical
quality of the grown layer. The peak wavelength is red shifted by 15 meV compared to a GaAs reference film measured under the same conditions in our PL system. This red shift can be explained by the strain state of the GaAs layer.

The strain state of the GaAs layer has been measured by XRD (Figure 10). We found that the GaAs layer has an in-plane lattice constant of 5.6621 Å and an out-of-plane lattice constant of 5.6435 Å. Compared to the unstrained GaAs lattice constant of 5.6532 Å, the GaAs layer grown on the Si-on-Ge template is 0.16% strained (tensile strain). This tensile strain, originated from the thermal expansion mismatch between the silicon substrate (2.6 ppm/°C) and the GaAs layer (5.7 ppm/°C), will produce an up-shift of the light holes valence band and a down-shift of the conduction band at the Γ point[34] according to the following equations:

\[
\Delta E_c = 2a_c \left( 1 - \frac{C_{12}}{C_{11}} \right) \varepsilon \quad (2)
\]

\[
\Delta E_{lh} = \left[ -2a_v \left( 1 - \frac{C_{12}}{C_{11}} \right) - b \left( 1 + 2 \frac{C_{12}}{C_{11}} \right) \right] \varepsilon \quad (3)
\]

With \(C_{11}\) and \(C_{12}\) are the stiffness constant of GaAs, \(a_c\) and \(a_v\) are the conduction band and valence band hydrostatic deformation potential respectively, \(b\) is the shear deformation potential and \(\varepsilon\) is the biaxial strain. The numerical application is shown in Table 2. The calculated bandgap reduction is 20 meV which agrees with the experimental value of 15 meV. The large range of reported for of \(a_c\) and \(a_v\)[35] can explain the small difference.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a_c)</td>
<td>-7.17</td>
<td>eV</td>
</tr>
<tr>
<td>(a_v)</td>
<td>-1.16</td>
<td>eV</td>
</tr>
<tr>
<td>(b)</td>
<td>-2</td>
<td>eV</td>
</tr>
<tr>
<td>(C_{11})</td>
<td>1221</td>
<td>GPa</td>
</tr>
<tr>
<td>(C_{12})</td>
<td>566</td>
<td>GPa</td>
</tr>
<tr>
<td>(\varepsilon)</td>
<td>0.16</td>
<td>%</td>
</tr>
</tbody>
</table>
\[
\begin{align*}
\Delta E_c & \quad -12 \quad \text{meV} \\
\Delta E_{lh} & \quad 8 \quad \text{meV} \\
\Delta E & \quad 20 \quad \text{meV}
\end{align*}
\]

Table 2: Parameters used in the calculations of the bandgap lowering due to the strain in the GaAs layer and the resulting conduction band downshift, light hole valence band upshift and the net resulting bandgap reduction. The 20 meV value matches the 15 meV red shift measured experimentally.

Figure 10: Reciprocal space map of the GaAs on Ge-on-Si sample taken along the (004) and (-2-24) diffraction plane. The large RSM (a) and (c) were taken using an array detector while the zoomed-in RSM (b) and (d) were measured using an analyzer crystal placed in front of the detector. The GaAs layer is under 0.16% tensile strain. This tensile strain is accumulated during the cooldown from growth temperature, due to the thermal lattice mismatch between the silicon substrate.
The GaAs thickness uniformity has been measured by spectroscopic ellipsometry (Figure 11). The average GaAs thickness is 1041 nm with a standard deviation of 20 nm, proving the high uniformity of the growth process.

Figure 11: GaAs layer thickness mapping on the 200 mm wafer measured with spectroscopic ellipsometry. The average GaAs layer thickness is 1041 nm and the standard deviation is 20 nm.

4 Conclusion

In conclusion, we have demonstrated that the arsine partial pressure $p(AsH_3)$, and not the V/III ratio, is the key factor influencing the heteroepitaxy of GaAs on Ge in the high temperature regime. We have shown that below a critical $p(AsH_3)$, the GaAs layer contained surface pits extending down in the GaAs layer. The crystalline quality of the GaAs layer increases together with $p(AsH_3)$. By using a $p(AsH_3)$ of 5 mbar, we have obtained very smooth GaAs layers without anti-phase boundaries and that are of a high crystalline and optical quality.

We have also demonstrated the feasibility of 200 mm GaAs virtual substrate fabrication on Si, by employing an intermediate Ge layer. The surface roughness (below 1
nm) was low and comparable to the underlying Ge layer, without requiring any polishing
step. We have demonstrated the high optical quality of the GaAs layer with the narrow
lineshape obtained by photoluminescence. This GaAs-on-Si virtual substrate can be used as a
starting wafer for the growth of III-V electronic and optical devices.

Bibliography

[1] S.M. Ting, E. a. Fitzgerald, Metal-organic chemical vapor deposition of single domain GaAs
on Ge/Ge[sub x]Si[sub 1−x]/Si and Ge substrates, J. Appl. Phys. 87 (2000) 2618.

InAs/GaAs quantum dots on germanium-on-insulator-on-silicon (GeOI) substrate with high

al., Structural investigation of MOVPE-grown GaAs on Ge by x-ray techniques, Semicond.

density and smooth surface on Si substrate, J. Semicond. 35 (2014) 073002. doi:10.1088/1674-
4926/35/7/073002.

microstructure origin and evolution for GaAs grown on Ge/Si 1− x Ge x /Si substrate, J. Phys.

temperature photoluminescence study of thin epitaxial GaAs films on Ge substrates, J. Appl.


[9] Q. Li, K.W. Ng, K.M. Lau, Growing antiphase-domain-free GaAs thin films out of highly

chemical vapor deposition growth of high quality GaAs on Si(001), Appl. Phys. Lett. 105

quantum well selectively grown by metal organic chemical vapor deposition on Si(100) 300


epitaxy growth process to reduce Ge outdiffusion from the Ge substrate, Appl. Phys. Lett. 92

doi:10.1143/JJAP.44.7777.

of GaAs on Ge substrates by inserting a thin low temperature buffer layer, Cryst. Res.

[17] S.M. Ting, E. a. Fitzgerald, Metal-organic chemical vapor deposition of single domain GaAs
on Ge/Ge[sub x]Si[sub 1−x]/Si and Ge substrates, J. Appl. Phys. 87 (2000) 2618.


and Ga prelayers on the metal-organic chemical vapor deposition of GaAs/Ge, J. Electron.

organic chemical vapor deposition and its application to high efficiency photovoltaic devices,

MOVPE grown GaAs solar cells using different substrates and group-V precursors, J. Cryst.

[22] P. Wanarattikan, S. Sanorpim, S. Denchitcharoen, K. Uesugi, S. Kuboya, Influences of two-
step growth and off-angle Ge substrate on crystalline quality of GaAs buffer layer grown by

surface morphology in Ga(In)As epilayers on Ge grown by MOVPE for multi-junction solar

grown on GaAs (001) vicinal surface by metalorganic vapor phase epitaxy, Japanese J. Appl.
418
Physi
419
420
measurements in metamorphic high electron mobility transistor structures by combination of
421
x-ray reciprocal space mapping and transmission electron microscopy, J. Appl. Phys. 93
422
423
424
[27] G.B. Stringfellow, Organometallic Vapor-Phase Epitaxy, Elsevier, 1999. doi:10.1016/B978-
425
012673842-1/50006-5.
426
427
[29] Y. Ohmachi, Y. Shinoda, S. Oku, GaAs/Ge Crystal Growth on Si and SiO2/Si Substrates,
428
germanium epitaxial film on silicon (001) with germane precursor in metal organic chemical
429
[31] G. Brammertz, Y. Mols, S. Degroote, V. Motsnyi, M. Leys, G. Borghs, et al., Low-
temperature photoluminescence study of thin epitaxial GaAs films on Ge substrates, J. Appl.
430
431
Heterogeneous Integration and Fabrication of III-V MOS Devices in a 200mm Processing
432
[34] Y. Sun, S.E. Thompson, T. Nishida, Strain effect in semiconductors: Theory and device
433
Acknowledgement

This work was supported by the National Research Foundation (NRF) of Singapore through the Singapore-MIT Alliance for Research and Technology’s (SMART) Low Energy Electronic Systems (LEES) IRG.