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View online: http://dx.doi.org/10.1063/1.4945598
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Atomic structure and stoichiometry of In(Ga)As/GaAs quantum dots grown on an exact-oriented GaP/Si(001) substrate

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(Received 16 October 2015; accepted 25 March 2016; published online 4 April 2016)

The atomic structure and stoichiometry of InAs/InGaAs quantum-dot-in-a-well structures grown on exactly oriented GaP/Si(001) are revealed by cross-sectional scanning tunneling microscopy. An averaged lateral size of 20 nm, heights up to 8 nm, and an In concentration of up to 100% are determined, being quite similar compared with the well-known quantum dots grown on GaAs substrates. Photoluminescence spectra taken from nanostructures of side-by-side grown samples on GaP/Si(001) and GaAs(001) show slightly blue shifted ground-state emission wavelength for growth on GaP/Si(001) with an even higher peak intensity compared with those on GaAs(001). This demonstrates the high potential of GaP/Si(001) templates for integration of III-V optoelectronic components into silicon-based technology. © 2016 AIP Publishing LLC.

Here, we present XSTM studies on the atomic structure

The incorporation of III-V laser structures on Si(001) substrates is highly desirable for Si photonics and on-chip interconnects.1–4 However, despite considerable interest, direct growth of III-V semiconductors on Si is plagued by high dislocation densities of 105–108 cm−2, which act as non-radiative recombination centers that greatly limit device performance.5 Often, III-V laser structures are grown on slightly off-cut Si(001) substrates6–7 in order to eliminate anti-phase domains, but for an integration into complementary metal-oxide-semiconductor (CMOS) technology, the growth on exactly oriented Si(001) substrates8–12 is highly preferable.

In order to optimize the device quality, a fundamental understanding of the atomic structure and the electronic properties is of major importance. However, compared with growth on III-V substrates, relatively little is known about the atomic structure and stoichiometry of III-V nanostructures for laser devices grown on silicon substrates.13,14

Cross-sectional scanning tunneling microscopy (XSTM) is a powerful method to investigate the structural details of III-V nanostructures, e.g., size, shape, and stoichiometry, grown on different III-V substrates.15–17 A clean cross-sectional III/V{110} surface for XSTM investigations can easily be prepared by cleaving the III-V(001) substrate in an ultrahigh-vacuum (UHV) chamber. In case of III-V layers grown on a Si(001) substrate, the preparation of III-V/Si{110} surfaces is not as trivial and frequently results in {111} oriented terraces on the silicon substrate, also deteriorating the quality of the III-V/{110} cleavage surface. Thus, only a few XSTM studies on in-situ cleaved Si{110} surfaces are yet reported.18

Here, we present XSTM studies on the atomic structure and stoichiometry of InAs/InGaAs quantum-dot-in-a-well

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metallic behavior, while for GaAs and GaP, clear plateaus of \( V \) with zero slope can be seen. Furthermore, the larger extension of the plateau in case of GaP compared with GaAs is in agreement with its larger bulk band gap. An additional structural investigation of the GaP/Si and GaAs/GaP interfaces as well as a more detailed analysis on the spectral shape, e.g., as the additional shoulders, will be given elsewhere.

Figure 1(a) shows a sketch of the entire sample structure, while an XSTM overview image of the GaAs/GaP/Si interface is presented in Fig. 1(b). From the latter, one can easily distinguish between the III-V layers and the silicon substrate due to the different densities and orientations of surface steps. On the silicon surface, many steps—oriented along the \( <110> \) directions—can be seen, while the GaP and GaAs surfaces are almost free of steps. The GaAs/GaP interface shows a high crystal quality despite of the lattice mismatch. The three different materials can also be distinguished by analyzing the different electronic properties by taking current-voltage (\( I-V \)) curves in the scanning tunneling spectroscopy (STS) mode [Fig. 1(d)]. As expected, the \( I-V \) curve for Si shows an almost metallic behavior, while for GaAs and GaP, clear plateaus with zero slope can be seen. Furthermore, the larger extension of the plateau in case of GaP compared with GaAs is in agreement with its larger bulk band gap. An additional structural investigation of the GaP/Si and GaAs/GaP interfaces as well as a more detailed STS study will be presented elsewhere.

Figure 1(c) shows overlapping XSTM overview images starting from the undoped GaAs and AlAs layers towards the first two DWELL layers. The AlAs layer can be identified as a dark stripe due to the larger band gap of AlAs compared with GaAs, while the DWELL layers appear as bright stripes. The highest contrast within these stripes is related to the quantum dots (QDs) located within the In\(_{0.15}\)Ga\(_{0.85}\)As layers. The bright appearance of the DWELL layers as compared with the surrounding GaAs matrix results from a combination of the electronic contrast and of the compressive strain due to the lattice mismatch of about 7% between InAs and GaAs. The latter results in an elastic outward relaxation after sample cleavage, that can be probed with the STM tip and is highest at the DWELL centers. It should be noted that the third DWELL layer was located directly at a pronounced surface step and could thus not be imaged.

The PL analysis presented in Fig. 2 compares the optical properties of the side-by-side grown samples on GaP/Si(001) and GaAs(001) substrates. For each sample, PL spectra were taken at different positions in order to study the sample homogeneity. The DWELL ground-state emission for growth on GaP/Si varies between 1270 and 1275 nm, while for growth on GaAs, it varies between 1305 and 1310 nm. Thus, the spectra for growth on GaP/Si(001) are slightly blue shifted with respect to the growth on GaAs substrate. Such a blue shift was already observed and attributed to the residual compressive strain in the GaAs buffer layer on Si substrate, resulting in slightly smaller QDs. Higher PL peak intensities for growth on GaP/Si substrates compared with growth on GaAs substrates were observed, not only for this specific sample but also for several samples with varying growth parameters, all showing good PL efficiency. A more detailed analysis on the spectral shape, e.g., as the additional shoulders, will be given elsewhere.

Figure 3 shows XSTM images of DWELL 1 and DWELL 2 with several slightly differently appearing QDs. The roughly truncated-pyramidal shape of the QDs is marked by dashed lines in Figs. 3(b) and 3(c) for guiding the eye. It should be noted here that in filled-states images the image contrast induced by strain relaxation dominates, resulting at first view in a rounder appearance of the QDs. However, a detailed inspection of the contrast reveals a shape very close to a truncated pyramid.

![Graph showing the comparison of PL spectra for DWELL structures grown on GaP/Si(001) and bulk GaAs(001)](image)

**FIG. 1.** (a) Schematic of the sample structure grown on GaP/Si(001) substrates. Growth on GaAs(001) substrates starts at the dashed line. (b) XSTM overview image of the GaAs/GaP/Si interface region, taken at a sample voltage of \( V_s = +2.5 \) V and a tunneling current of \( I_t = 40 \) pA, and (c) assembly of XSTM overview images of the InAs/InGaAs DWELL-structure, taken at \( V_s \) between \(-3.0 \) V and \(-3.5 \) V and \( I_t = 20 \) pA. (d) \( I-V \) curves of Si (squares), GaAs (triangles), and GaP (circles) acquired at a stepped (110)-cleavage surface (not shown here) with the tip position stabilized at \( V_{\text{stab}} = -1.4 \) V and \( I_{\text{stab}} = 70 \) pA.

![Graph showing the comparison of PL spectra for DWELL structures grown on GaP/Si(001) and bulk GaAs(001)](image)
Within the evaluated scan area extending across \( \sim 0.9 \mu m \), a total number of about 30 QDs are analyzed. QDs with heights up to 28 ML (\( \sim 8 \) nm) and base lengths between 15 and 25 nm are observed. This wide range of apparent base lengths is connected to the randomly distributed cleavage positions so that the actual average base length is closer to 25 nm, leading to a density of about \( 6(\pm 2) \) \( \times 10^{10} \) cm\(^{-2} \). These structural findings are quite similar to the averaged values for DWELL structures grown on a GaAs(001) substrate with emission wavelengths slightly below 1.3 \( \mu m \).\(^{19}\)

In Fig. 3(c), the bright feature (labeled with A) with monoatomic step height in the center of the QD is most likely a cleavage-induced defect, as it was already observed in XSTM investigations of the highly strained diluted-nitride system.\(^{23}\) Such cleavage-induced defects could appear as bright objects or also as dark depressions, e.g., as the feature labeled B in Fig. 3(c). It should be noted that features labeled C are no defects but can be attributed to a slight contamination after cleavage.

In previous XSTM studies of MBE grown DWELL structures and of MOVPE grown In\(_{0.80}\)Ga\(_{0.20}\)As QDs covered by an In\(_{0.10}\)Ga\(_{0.90}\)As layer, also the formation of the so-called nanovoids during growth was reported, especially in case of larger QD sizes.\(^{19}\) Such nanovoids, characterized by a material hole, are also found within both DWELL layers, by XSTM (not shown here), as well as by transmission electron microscopy.\(^{24}\) Interestingly, 17 \( \pm 6\) % and 14 \( \pm 3\) % nanovoids, and about 65 \( \pm 15\) % and 20 \( \pm 5\) % cleavage-induced defects are imaged at DWELL 1 and DWELL 2, respectively. Since both layers are grown using identical growth parameters, a similar occurrence would be expected based on DWELL growth alone. Thus, it is most likely that defects are also related to dislocations running from the GaP/ Si substrate or the GaAs/GaP interface towards the sample surface and being partially stopped by the strained DWELL layers. It should be noted that the incorporation of strained layers (or even DWELL layers) below the active region as the so-called dislocation filter layers is already used in order to improve the device quality of laser structures grown on silicon substrates.\(^{3,6}\)

In Fig. 4(a), a close-view XSTM image of an atomically resolved QD from DWELL 2 is presented. The roughly truncated-pyramidal QD shape is highlighted by dashed lines, as also illustrated in the sketch in the inset image. The shape of its In-rich center, characterized by straight boundaries as marked by dotted lines, is similar to a reversed truncated cone.

Figure 4(b) shows the variation of the local lattice parameter as a function of the position along growth direction.\(^{21}\) By comparing the resulting graphs with simulations of the strain relaxation of two-dimensional quantum wells, the local In concentration \( x \) is obtained.\(^{25}\) The local stoichiometry is determined for the QD shown in Fig. 4(a), separately for the center and its sides, as shown in the XSTM inset image [Fig. 4(b)], and compared with the In\(_{0.13}\)Ga\(_{0.87}\)As layer between the QDs, labeled as wetting layer (WL). The In\(_{0.13}\)Ga\(_{0.87}\)As layer between the QDs has a maximum In concentration of about 15% at its base, slightly decreasing along growth direction. A much higher In concentration is found in the QD. For the QD sides, a maximum In concentration of about 70% is observed, while the highest In concentration of up to 100% is located in the upper QD center. A similar In distribution was already observed for In\(_{0.5}\)Ga\(_{0.5}\)As/GaAs QDs.\(^{26}\) It should be noted that the reason for the data points exceeding the value for

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**FIG. 3.** XSTM filled-states images of (a), (b) DWELL 2, and (c) DWELL 1, showing QDs with roughly a truncated-pyramidal shape, as indicated by the dashed lines for guiding the eye. In (c), QDs with cleavage-induced defects (labeled A and B) are observed. A few rounder bright spots (exemplarily marked, labeled C) are attributed to a slight surface contamination after cleavage. The XSTM images are taken at (a), (b) \( V_S = -2.7 \) V, and (c) \( V_S = -3.0 \) V, and at \( I_T = 20 \) pA.

**FIG. 4.** (a) XSTM filled-states image of a QD at DWELL 2, taken at \( V_S = -2.8 \) V and \( I_T = 20 \) pA. The DWELL shape is marked by dashed lines and the In-rich region by dotted lines, further illustrated by the inset sketch. (b) Determination of the local lattice parameter (left axis) as a function of the position along growth direction and the corresponding In concentration (right axis) of the QD center (circles), the QD sides (squares), and the WL (triangles). The graphs from QD center and QD side are determined within the areas marked by the boxes in the XSTM inset image. The uncertainty of the obtained In concentrations amounts to about 10%.
pure InAs is related only to the local bending of the cleavage surface due to the high compressive strain in this system.\textsuperscript{21} The region of the In-rich center and the total QD height derived from the image contrast is marked in Fig. 4(b), being in nice agreement with the variation of the local lattice parameter.

In conclusion, we presented XSTM and PL data of III-V nanostructures grown on exactly oriented GaP/Si(001) substrates. The preparation of a (110) cleavage plane through the GaAs/GaP/Si layer structure allows the study of the atomic structure and stoichiometry of In(Ga)As/GaAs QDs, revealing lateral sizes close to 25 nm, heights up to 8 nm, and an In concentration of up to 100%. In addition, a comparative PL study of side-by-side grown DWELL structures on GaP/Si(001) and GaAs(001) samples exhibits a slight blue shift to a ground-state emission wavelength above 1.27 µm together with an increase in the PL peak intensity for growth on GaP/Si(001). These properties demonstrate the high potential for integration of such III-V nanostructures into silicon-based technology.

The authors thank the Deutsche Forschungsgemeinschaft for financial support of Project No. LE3317/1-1, U. W. Pohl for fruitful discussions, M. Dähne for providing the XSTM setup, and A. Beyer and R. Straubinger for characterization of the sample orientation. Work at UT-Austin was supported by a Multidisciplinary University Research Initiative from the Air Force Office of Scientific Research (AFOSR MURI Award No. FA9550-12-1-0488).

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