Direct observation of atomic scale surface relaxation in ortho twin structures in GaAs by XSTM

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Abstract
We have studied the (110) GaAs surface of a structure containing ortho twins by cross-sectional
scanning tunnelling microscopy and we have compared the experimental results with *ab initio*
density functional theory calculations and STM simulations. Both experimentally and
theoretically we find that the surface of different twin crystallites are significantly displaced
with respect to each other, parallel to the twin boundary. This result is explained by a surface
relaxation of the atoms in the (110) GaAs surface and the difference between the atomic
configuration of the ortho twins.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

We have investigated the lateral relaxation in nanoscaled ortho twins in a structure containing embedded GaAs nanowires by a combination of cross-sectional scanning tunnelling microscopy (XSTM) and *ab initio* density functional theory (DFT) calculations. Twins are by far the most common type of structural defect in III–V semiconductor nanowire systems. At present twins are considered as one of the major, if not the largest, obstacle for creating perfectly structured and functional nanowires [1–3]. Although twinning of the crystal structure has been widely discussed for example for the growth of crystals from a melt [4], and also discussed as a concept within the broad field of crystal defects [5], it is not as well understood for nanowire systems. Twins found in nanowire systems are formed during the crystal growth and are therefore called growth twins. Twins can also be introduced in a crystal during plastic deformation caused by applying an external stress. In the later case the twins are called deformation twins. In the

case of crystal growth from a melt, the formation of twins and the parameters that influence the occurrence of twins have been discussed by Hurle [4] for example. For the formation of twins during nanowire growth, recent publications show advances in controlling the density of twins and report on parameters that influence their occurrence [6–10]. However, complete prediction and control of the crystal structure and density of twins cannot be achieved at present.

The nanowires in this study were nucleated and grown using gold particles as seeds. The nucleation and growth of the nanowires take place at the interface between the seed particle and the semiconductor surface, and the diameter of seed particles more or less determines the diameter of the nanowires. The preferred growth direction of III–V semiconductor nanowires is $\langle 111 \rangle B$. Twins, with $\{111\}$ twin boundaries perpendicular to the growth direction, are common in these nanowire structures and are usually formed through the whole cross-section of the nanowires. Apart from the differences in the actual growth mechanism, the formation of twins in bulk or bulk-like materials is significantly different. In the case of twins formed during growth from a melt or plastic deformation, the twins are usually formed within the crystal matrix and do not go through the whole crystal. These twins are usually bounded by dislocations and it is only when

these twins reaches the surface of the crystal that they are not associated with dislocations. Dislocations are known to introduce lattice distortions in their vicinity, especially at boundaries between twins, which has been imaged by transmission electron microscopy [11]. When the twinning takes place in the growth direction of the nanowires, forming twin boundaries perpendicular to the growth direction, the crystal structure would, as a first assumption, correspond to an ideal twin structure with ideal (also called coherent) {111} twin boundaries. Consequently, dislocations are not necessarily formed as the twins are formed during the growth of nanowires. This system is therefore interesting to study as it is an example of what could be perfect regarding the symmetry across the twin plane (the interface) between adjacent twins and without the influence of distortions due to dislocations.

The nanowires in figure 1(a) illustrates an ortho twin (also called rotational twin) crystallite by a 60° rotation of a full segment of the nanowire around the [111]*B* growth axis. This corresponds to a reversal in the zinc blende stacking sequence ABCABC to a mirrored stacking sequence of CBACBA in the rotated segment. Each letter A, B and C represents a bilayer of Ga and As atoms bonded together with bonds in the [111]*B* direction. It is worth pointing out that it is only the stacking sequence that is mirrored, not the bonding configuration. The interface between two different stacking sequences is called a twin boundary or a twin plane. The atomic arrangement of the (110) plane is shown in figure 1(b). In this figure, the stacking sequence is CABCAB*C*BACBAC (read from the bottom), where the '*C*' plane is distinguished as the twin plane. The small segment of B*C*B stacking corresponds to the description of a wurtzite-like stacking sequence. Twin defects in nanowires can therefore introduce a local band gap variation as a consequence of the difference between the band gap of wurtzite and zinc blende structures. It is important to note that the twin plane belongs to both twin crystallites and it is theoretically possible to have a perfectly symmetric alignment of the ortho twins (with all nearest neighbour bonds aligned as in a zinc blende crystal), corresponding to an ideal twin boundary. This kind of symmetric twin boundary between ortho twins is shown in the model of figure 1(c). The para twin on the other hand, is a mirroring of the stacking sequence, as well as, of the bonding across the twin boundary. This requires the bonding to be either Ga–Ga or As–As across the twin boundary. The presence of para twins has, as far as the authors know, never been reported or observed for this system and is less likely due to the much higher cost in energy to form the cation–cation/anion–anion bonds necessary for such a twin configuration. The formation of a para twin also requires the growth direction to change from $\langle 111 \rangle B$ to the less favoured $\langle 111 \rangle A$ direction.

The (110) GaAs surface of this structure is a good choice to study for two main reasons. Firstly, it gives the possibility to compare the results with what is already known about the ordinary (110) GaAs surface, which is the natural cleavage plane of zinc blende materials and a surface that has been well studied. Secondly, it is generally found that the surface of semiconductor nanowires have {110}- and {112}-oriented macro facets [12–15]. For nanowires, the surface
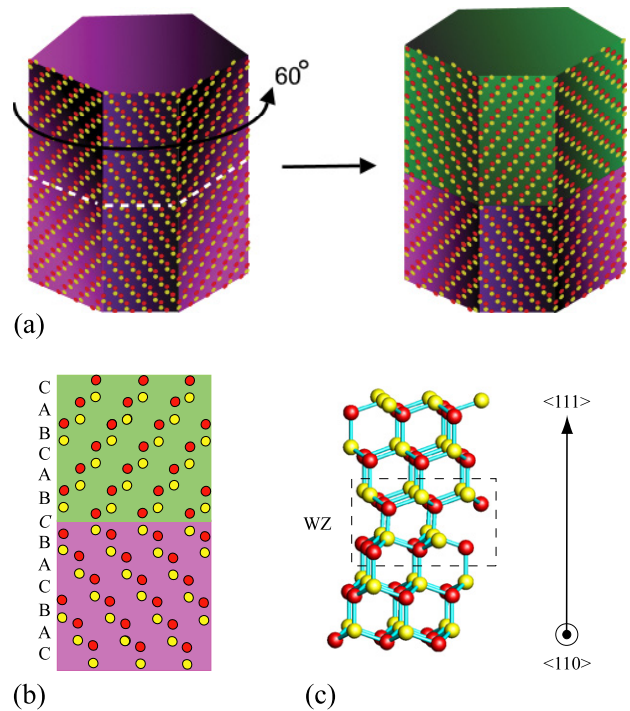

Figure 1. (a) An ortho twin crystallite can be created in a nanowire by rotating a segment by 60° around the [111]*B* growth axis. (b) Insertion of this kind of twinned structure results in a switch from an ABCABC stacking to a CBACBA stacking. Note that there are only surface atoms present in the illustrations in (a) and (b). (c) At the boundary between the two twins, there is a twin plane in which the closest atoms are arranged according to a wurtzite (WZ) bonding configuration. The atomic configuration in this three-dimensional model of the twin structure is slightly rotated from a $\langle 110 \rangle$ perspective for illustrative reasons. (Dark and light grey circles (red and yellow online) illustrate Ga and As atoms, respectively.)

to volume ratio is large and the influence of the surface on, for example, the optical properties can be large [16]. Sensor applications with nanosized structures actually rely on this sensitive influence of the nanowire surface for their functionality [17–19]. In this perspective, the (110) surface of a twinned structure is interesting from both a fundamental research point of view, as well as, from a nanowire application point of view.

For the ordinary (110) GaAs surface (hereafter referred to as the (110) GaAs surface, as opposed to the twinned surface), it is well established that the As surface atoms relax outward and the Ga surface atoms relax inward [20]. The bond length has been found to be more or less preserved, and the relaxation can be described by a rotation of the bond angle and by a buckling angle. In this paper we focus on the lateral (in the (110) surface plane) relaxation of the atoms, which accompanies the rotation of the bond angle (when the bond length is conserved), in a GaAs structure containing ortho twins.

2. Experimental details

GaAs $\langle 111 \rangle B$ nanowires were fabricated from aerosol gold particles with a diameter of 40 nm, using metal-organic

vapour phase epitaxy (MOVPE) growth on a GaAs(001) substrate. After the growth of the nanowires at 450 °C, the temperature in the growth chamber was increased to 630 °C and a sequence of AlGaAs and GaAs layers were grown to embed the grown nanowires completely. Twins, originally formed in the nanowires, propagate out into these embedding layers [21]. A detailed description of the growth can be found in [22]. The samples were cleaved inside a UHV chamber kept at a base pressure of $<1 \times 10^{-10}$ mbar. We thereafter studied the cleaved surface by STM, using a commercial Omicron STM 1 microscope situated inside the same UHV chamber. The imaging was performed in constant current mode at a negative sample bias around -2 V (filled state imaging) and at a feedback current of around 0.1 nA. The STM tips that were used in this study were electrochemically etched polycrystalline tungsten tips. By imaging the cleaved surface, we were able to locate and image the interior of the nanowires as well as to study the twin structures with atomic resolution. The method of accessing and studying the interior of nanowire structures has been described in more detail elsewhere [21–23]. The identification of what we refer to as the apparent positions of the surface As atoms in our STM measurements in this paper, was done by analysing the positions of the brighter areas in the as-acquired filled state STM images, after the images were checked and corrected for thermal drift and calibration errors. The bright areas/spots in these STM images were marked manually by circles, centred on these brighter areas/spots. After using this method of identifying the apparent positions of the surface As atoms, measurements of the distances between these positions were performed.

2.1. Theoretical calculations and STM simulations

Theoretical calculations of an ortho twinned GaAs structure, as imaged by XSTM, were performed by *ab initio* DFT calculations with the Vienna *Ab initio* Simulation Package (VASP) [24, 25] using Perdew–Ernerzhof–Burke (PBE) [26] functionals within the projector augmented wave (PAW) [27] method. STM images were simulated as described previously [28, 29]. An ortho twinned structure was modelled in the [1$\bar{1}$1] direction with a segment of 3 GaAs layers in one twin orientation placed in between two segments (each consisting of 3 GaAs layers) of the other (ortho) twin orientation, forming a twin structure with two twin boundaries (figure 4(a) shows the model). A slab thickness perpendicular to the (110) surface of 5 layers was used, resulting in a total of 128 atoms in the unit cell. The vacuum gap was set to 10 Å and the total unit cell size was 25.9 Å × 4.6 Å. The 4 top most (110) GaAs layers were allowed to relax freely to establish the structure with the lowest energy. The starting point for the relaxation was a high symmetry structure with a bonding configuration across the twin interface as indicated in figures 1(b) and (c). For comparison, a structure of un-twinned GaAs was also modelled and relaxed within the same theoretical framework, including the relaxation of the (110) GaAs surface. The relaxed surface was used to simulate STM images.
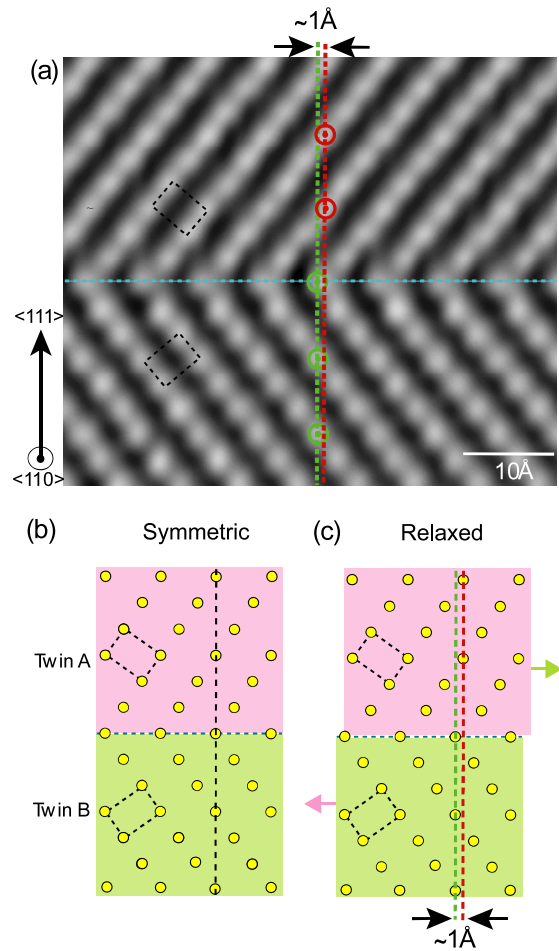

Figure 2. (a) Filled state STM image of a single twin boundary. Unit cells of the top and bottom twin are drawn in the image (black dashed rectangles). The left dashed line (green online) perpendicular to the twin plane follows the As atoms in the bottom twin and the right dashed line (red online) follows the As atoms in the top twin. The As atoms in the boundary follow the bottom twin. (b) Symmetric (unrelaxed) model of the As atoms in the twin structure. (c) Distorted (relaxed) model of the As atoms in the twin structure as suggested from our STM images.

3. Results

Figure 2(a) shows an experimental STM image of an ortho twinned (110) GaAs surface. Open circles have been placed on a few of the apparent positions of the As atoms in this STM image. Figure 2(b) illustrates how these atoms should line up along a vertical line along the ⟨111⟩ direction according to a symmetric (bulk-like) arrangement. From our STM measurements we observe that within a twin domain, the apparent positions of the surface As atoms line up as expected from the symmetry of the (110) GaAs surface. However, as seen from figure 2(a), the marked apparent positions of the surface As atoms that belong to twin domains of different orientations do not line up perfectly along the ⟨111⟩ direction. This can be seen by the small separation between the two vertical lines in the figure. In figure 2(c), we illustrate a relaxed model of how the As atoms in the (110) surface of one of the twin domains are displaced with respect to an adjacent
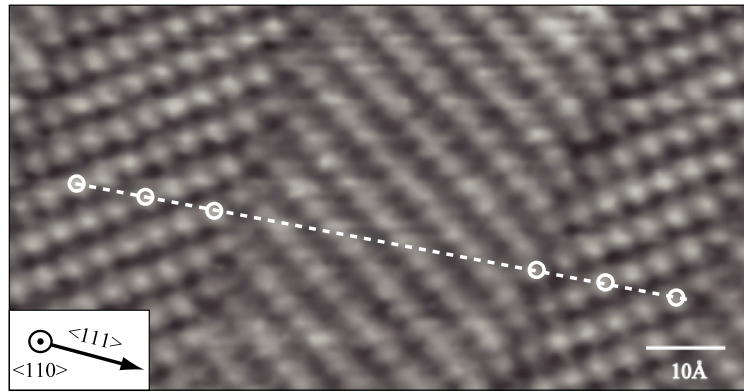
Figure 3. An STM image showing three twin segments within the same area of imaging. The apparent positions of the surface As atoms in domains of the same twin orientation line up, as indicated by the circles and dashed line, while twins of different orientations are slightly shifted (as shown in figure 2).

domain of a different orientation, as suggested from our STM measurements. No apparent relaxation perpendicular to the ortho twin boundary can be observed. That is, the distance between the atomic planes in the $\langle 111 \rangle$ direction is observed to be constant and as expected from a GaAs zinc blende structure. From our STM measurements, we observe a displacement of $1.0\text{ Å} \pm 0.3\text{ Å}$ in the $\langle 112 \rangle$ direction between the apparent positions of the surface As atoms in domains of different twin orientation (i.e. the distance between the vertical lines drawn as in figure 2(a)). The STM image in figure 3 shows that the apparent positions of the surface As atoms that belong to the same twin orientation are aligned in the $\langle 111 \rangle$ direction. In other words, we observe that the apparent positions of the surface As atoms in different domains of the same twin orientation are not displaced with respect to each other.

We find an excellent agreement when comparing the experimental and simulated STM images of similar sized ortho twins, see figure 4. Furthermore, from the simulations we find that the intensity maxima in the simulated STM image coincide with the geometric positions of the As atoms in the relaxed structure. This is crucial for the analysis of our experimental data as it can be very difficult to separate between electronic and geometric effects in STM experiments [30, 31]. In the work by Bass *et al* [31] it was also observed that the intensity maxima in simulated STM images corresponded exactly to the position of the As atoms in the top layer at negative sample bias (filled state imaging). However, for a positive sample bias (empty state imaging) the intensity maxima were shifted away from the positions of the Ga atoms. The fact that we have not done any intentional doping of our material is known to introduce additional difficulties when using positive sample bias during STM imaging of GaAs surfaces [32]. By focusing on performing filled state STM imaging we thereby simplify our high resolution STM imaging. In addition, our experimental STM images can be strongly correlated with the actual positions of the atoms in the surface according to our simulations and in agreement with Bass *et al* [31]. From our theoretical calculations we can further examine the relaxation of the atoms by directly comparing the positions of the atoms in the relaxed structure to their positions in the unrelaxed structure.
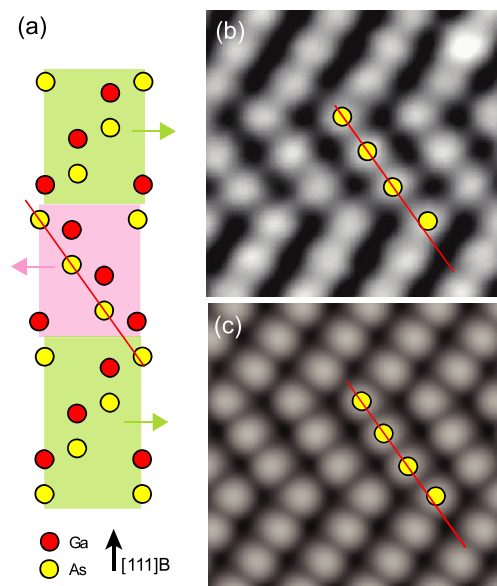

Figure 4. (a) Model indicating the distortions of the structure. (b) Experimentally obtained STM image of a twin structure very similar to the simulated one. (c) Simulated STM image of a twin segmented structure in the $[1\bar{1}1]$ direction. Guide lines for visualizing the misalignment of the atoms across the twin boundary have been added to the illustration in (a), the STM image shown in (b) and the simulated STM shown in (c). Note that these guide lines do not pass through the As atoms at the lower twin boundary, indicating the relaxation as all these atoms should be on this line in the unrelaxed model.

Quantitatively, we find a theoretical mean value of $0.4 \pm 0.2\text{ Å}$ for the displacement of the surface As atoms in the $\langle 112 \rangle$ direction between different ortho twinned segments. We will now compare the results from our theoretical calculations, our STM data and previously published values for the relaxation of the (110) GaAs surface. Our results, together with data from [31] are therefore presented in tables 1 and 2. Δx is the lateral (in the (110) plane) displacement in the $\langle 112 \rangle$ direction (parallel to the twin plane) and Δy the lateral (in the (110) plane) displacement in the $\langle 111 \rangle$ direction (perpendicular to the twin plane), see figure 5. The arrows in figure 5(c) illustrate the
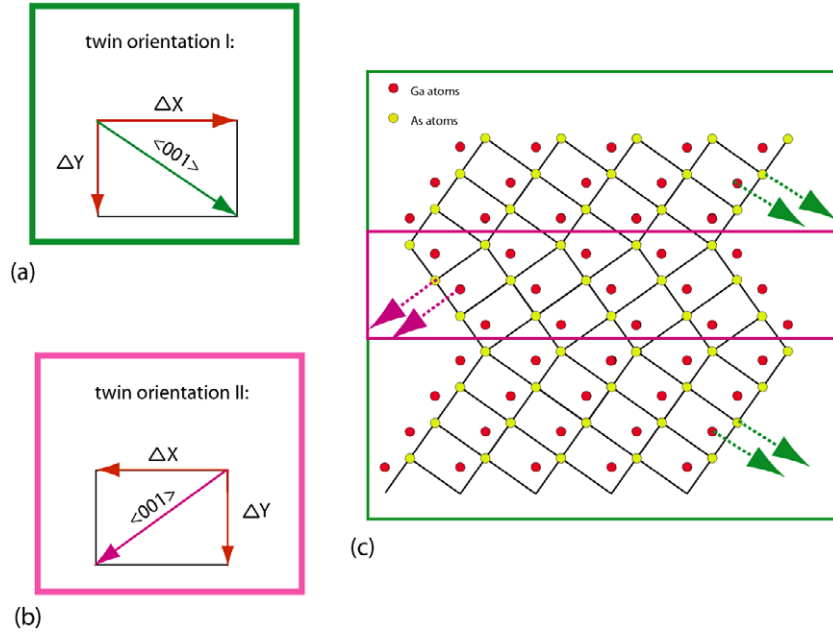
Figure 5. An illustration of the directions of the relaxation in the (110) GaAs surface with respect to the two different twin orientations. It also shows the directions of the distortions, Δx and Δy, that are presented in tables 1 and 2. The direction of Δx is parallel to the twin boundary and $\langle 112 \rangle$, the direction of Δy is parallel to the growth direction and $\langle 111 \rangle$.

Table 1. The lateral surface relaxation.

	Δx in the (110) GaAs surface according to DFT calculations	Δx in the (110) GaAs surface according Bass *et al* [31]	Δy in the (110) GaAs surface according to DFT calculations	Δy in the (110) GaAs surface according Bass *et al* [31]	Δx in the twinned (110) GaAs surface according to DFT calculations	Δy in the twinned (110) GaAs surface according to DFT calculations
Ga	0.3 Å[a]	0.327 Å	0.2 Å[a]	0.229 Å	0.4 Å[a]	0.3 Å[a]
As	0.1 Å[a]	0.119 Å	0.1 Å[a]	0.0832 Å	0.2 Å[a]	0.1 Å[a]

[a] Error estimation $\pm$0.1 Å (the error bars in the DFT simulation are due to the limitation of the unit cell in z-direction).

Table 2. Comparison of the lateral surface relaxation.

	Δx twinned (110) GaAs surface minus Δx ordinary (110) GaAs surface	Δy twinned (110) GaAs surface minus Δy ordinary (110) GaAs surface	Shift in $\langle 112 \rangle$ direction between two different twins according to relaxation in ordinary (110) GaAs surface	Shift in $\langle 112 \rangle$ direction between two different twins according to DFT calculation of the twinned structure	Experimentally measured shift in $\langle 112 \rangle$ from STM filled state imaging
Ga	0.1 Å[a]	0.0 Å[a]	0.6 Å[c]	0.7 Å[c]	—
As	0.1 Å[a]	0.1 Å[a]	0.2 Å[c]	0.4 Å[c]	1.0 Å[b]

[a] Error estimation $\pm$0.1 Å.
[b] Error estimation $\pm$0.3 Å.
[c] Error estimation $\pm$0.2 Å.

directions of the lateral relaxation in the (110) GaAs surface according to the data that has been reported earlier in the literature [20]. It is important to note that the directions of the total relaxation in a surface of two different ortho twin orientations are two equivalent $\langle 100 \rangle$ directions. When two regions of different ortho twin orientations are compared, as in this study, the relaxation in respective twin domain are rotated relative to each other. As is seen in figures 5(a) and (b), the total relaxation in the respective $\langle 100 \rangle$ directions can be divided into two components. One of the components, Δy in figure 5, is in the same direction for both twin domains and perpendicular to the twin boundary. The other component, Δx in figure 5,

is parallel to the twin boundary, but in opposite direction for the two different ortho twin orientations. In table 2, the displacements Δx and Δy (according to the notation in figure 5) for the twinned and the (110) GaAs surface are compared and the total shifts in the $\langle 112 \rangle$ direction between different ortho twin domains in the surface are presented.

From table 1 it can be seen that our theoretical results of the (110) GaAs surface agree well with the previous results of Bass *et al* [31] (first to fourth columns). We find that the lateral relaxation of the atoms in the twinned (110) GaAs surface do not differ, within the uncertainty of the calculations, from what we find from the (110) GaAs surface (first and second

columns of table 2). There is a difference in the order of a tenth of an Å between the shift in $\langle 112 \rangle$ direction for the different twins in the (110) GaAs surface and the twinned (110) GaAs surface (third and fourth columns of table 2). This difference is within the uncertainty of our calculations and therefore we do not consider this difference. Experimentally, we measure the shift in the ortho twinned (110) GaAs surface to be in the same direction as we find from our calculations but slightly larger (see fourth and fifth columns of table 2). Further, we find from the calculations that the lateral relaxation is larger for the Ga atoms than for the As atoms (see third and fourth column of table 2), in agreement with previously reported data for the relaxation of the (110) GaAs surface [20]. We find that the atoms within a twin domain relax according to the atomic configuration of their nearest neighbouring atoms, also when being very close to or in the actual twin boundary, and in agreement with what we observe from our STM measurements. The distortion that we observe both experimentally and find from our theoretical calculations lies in the twin plane and the bonding configuration between its Ga and As atoms.

4. Discussion

The result of our calculations of the relaxation in the (110) GaAs surface is in strong agreement with what has been reported previously, in terms of both direction and magnitude. This is important to point out, as we compared our result of both the direction and the magnitude of the relaxation in the ortho twinned (110) GaAs surface with our results of the relaxation in the (110) GaAs surface. In figure 5, we illustrated how the difference in the crystal orientation for ortho twins can result in a rotation of the direction of the surface relaxation, taking into account what is known about the surface relaxation in the ordinary (110) GaAs surface and due to the atomic arrangement for an ortho twinned structure. We showed that when the total relaxation of the (110) GaAs surface is divided into two components, the relaxation in Δy (along $\langle 111 \rangle$) is the same for both twin orientations, whereas the relaxation in Δx (along $\langle 112 \rangle$) is in opposite directions for twins of different orientation. We believe that this explains the direction of the shift in the $\langle 112 \rangle$ direction between the atoms in the ortho twinned (110) GaAs surface that we have observed experimentally, and have found from our calculations and simulation. When comparing the shifts in the $\langle 112 \rangle$ direction between different ortho twins calculated from the (110) GaAs surface and the twinned (110) GaAs surface we found no significant difference. The relaxation that we find from our calculations in the ortho twinned (110) GaAs surface is therefore in strong agreement with what is known about the relaxation in the (110) GaAs surface, considering both the direction and the magnitude. Furthermore, the relaxation that we find in the surface layer from our DFT calculations is decreased substantially when looking at the layers below the surface layer for both the twinned and the ordinary GaAs structure. This is in complete agreement with the interpretation that a surface related relaxation is present in the investigated structure and that our results are not related to distortions of the atomic arrangement in the bulk of the material. It is worth

pointing out that an increase in the thickness of the slab in the calculation does not affect the relaxation of the atoms in or near the surface, which further supports the interpretation of a surface related relaxation.

It is interesting to note that the atoms are found to relax according to the atomic configuration of their nearest neighbouring atoms and that the atoms in the twin plane seem to follow distinctly one of the ortho twin domains. For example, if the atoms are arranged in different ortho twin domains, as shown in figure 5(c), the As atoms in the twin plane follow distinctly the relaxation of the atoms in the lower adjacent twin domain. This can be explained by looking at their closest neighbouring atoms, which are indeed arranged according to their corresponding ortho twin orientation. The Ga atoms in this figure are also arranged according to their neighbouring atoms, which belongs to the upper adjacent twin domain. These Ga atoms therefore follow the relaxation of this twin orientation, in contrast to the As atoms in the same twin plane that follow the lower adjacent twin domain. The bonding configuration between the Ga and the As surface atoms in the twin plane must therefore be different compared to the bonding configuration between the Ga and As surface atoms in a bilayer that is present within a twin domain.

So far we have only discussed the surface relaxation of ortho twinned structures. Let us now shortly discuss what we expect to find from a para twinned structure. To illustrate the case of para twinning in the crystal structure, the lower twin in figure 5(c) would be mirrored across the twin boundary to form a para twin domain, thereby forming As–As bonds across the twin boundary. In this para twin configuration, the Δx relaxation would be instead in the same direction for both twins, whereas the Δy relaxation would be in opposite directions and away from the boundary. There should therefore, according to this model of surface relaxation, not be any shift in the $\langle 112 \rangle$ direction between two para twins. In the $\langle 111 \rangle$ direction there are two factors that could influence the distance between the As atoms across the boundary. Firstly, the As–As bond length would most probably be different from that of the As–Ga. Secondly, the surface atoms would relax away from the boundary, where the spacing between the As atoms at the boundary are highly unlikely to be identical to the in-twin distance. It is worth pointing out that we observe no difference in the spacing of the As atoms across the twin plane, further supporting the identification of the twins in the present study as ortho twins.

5. Conclusions

We have studied the (110) GaAs surface of a structure containing ortho twins introduced by nanowire growth using XSTM and we have compared the experimental data with theoretical *ab initio* density functional theory calculations and STM simulations. We conclude that the apparent positions of the As in the STM images correspond to the geometric positions of the atoms, making the interpretation of the images straight forward. Both experimentally and theoretically, we find that the atoms in the surface of different twin crystallites are significantly displaced with respect to each other, parallel

to the twin boundary. The displacement is explained by a surface relaxation of the atoms in the (110) GaAs surface and the difference between the atomic configuration of ortho twins. Further, the results presented in this work suggest that the twin boundary in these nanowire structures may be more or less ideal. In addition, the results also suggest that the dislocations normally associated with twinning of the crystal structure in bulk materials are not present in nanowires. The surface of nanowires is difficult to explore on the atomic scale. The results presented in this paper are therefore important as these give an insight to the possible surface arrangements of {110}-oriented facets of GaAs nanowires, and maybe also other III–V zinc blende nanowires as most of these nanowires indeed contain twins.

Acknowledgments

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