Atomic structure of the GaAs$(\overline{113})B$ surface

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The GaAs$(\overline{113})B$ surfaces were prepared by molecular-beam epitaxy and were *in situ* studied by low-energy electron diffraction and scanning tunnelling microscopy. We present results for two different surface structures, the recently observed (8×1) reconstruction and an As-rich structure. For the (8×1) reconstruction we confirm a model that consists of Ga dimer zigzag chains along [332] in two atomic levels. We report on the reflection high-energy electron diffraction (RHEED) during growth. RHEED oscillations are observed mainly with the electron beam along [$\bar{1}$10] from which it is concluded that growth occurs through two-dimensional nucleation and propagates along [332]. The As-rich structure represents a remarkable case intermediate between a stable singular and an unstable facetted surface: Locally, As adatoms and dimers create a $1\times$ and a $2\times$ periodicity but long-range order does not exist; nevertheless, the surface comprises large terraces that are separated by well-developed steps.

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I. INTRODUCTION

The understanding of growth mechanisms of compound semiconductors is of considerable interest for both fundamental physics and device technology. In particular, the spontaneous occurrence of three-dimensional islands, that form by the Stranski-Krastanov growth mode in lattice-mismatched heterostructures, has attracted much interest for the direct synthesis of devices exhibiting low-dimensional electron confinement.[1] So far, on the InAs/GaAs system most of the research has concentrated on the growth of quantum dots on (001) oriented substrates. However, there are also some studies on the formation of quantum disks[2] and quantum dots grown on $(113)B$ oriented substrates.[3–8] Most remarkably, spontaneous ordering effects of the islands depending on the In content were reported by Xu *et al.*[8] However, the understanding of the mechanisms, involved in the growth process, requires a detailed knowledge of the atomic arrangement on the bare surface itself.

So far, the bare GaAs$(113)B$ surface has not been studied extensively.[9–14,16–18] Early reports on ion bombardment and annealing (IBA) prepared samples revealed a (1×1) structure in the low-energy electron diffraction (LEED) pattern and it was concluded that the surface does not reconstruct.[10] These results were confirmed by Scholz *et al.*,[12] but for samples prepared by molecular-beam epitaxy (MBE) facetting of the surface was observed. Also, Setzer *et al.*[13] observed facetting on MBE-prepared GaAs$(113)B$ samples and proposed that the surface decomposes into facets of low-index orientation, which form regular pyramids. These findings were supported by scanning electron microscopy and, in addition, by first-principles calculations.[9] In contrast, we have recently found an (8×1) reconstruction on MBE prepared GaAs$(113)B$ samples using reflection high-energy electron diffraction (RHEED) and scanning tunnelling microscopy (STM).[14] It is interesting to note, that this reconstruction forms analogously to the GaAs$(113)A(8\times1)$ surface.[15] More recently, the $8\times$ periodicity on MBE-prepared samples was confirmed by RHEED and STM in spite of lacking atomic resolution of the latter.[18]

Besides the studies on MBE prepared surfaces, samples grown by metalorganic vapor phase epitaxy (MOVPE) did not show facetting.[16,17] Instead, the surface morphology was found to be similar to that of the GaAs(001) surface, showing wide terraces separated by monolayer steps. Based on STM and RHEED results Kawase *et al.*[16] proposed a (2×1) structural model.

The above studies demonstrate that a detailed study of the surface structure that is able to explain all the experimental findings is still lacking. Consequently, we report herein a systematic study of the structural properties of the GaAs$(113)B$ surface prepared by MBE under different conditions and examined *in situ* by electron-diffraction techniques and STM. Two structures were found on this surface, which differ in their stoichiometry and in their periodicity. In addition, we discuss the influence of the atomic arrangement on the surface morphology.

Our paper is organized as follows: We start with a short introduction into the surface geometry of GaAs(113) surfaces in Sec. II, followed by some notes on our experiment in Sec. III. In Sec. IV we briefly introduce the (8×1) reconstruction and discuss the RHEED oscillations observed. In detail we describe the results for the As-rich phase in IV B and discuss the transition between the two phases in IV C before we end with our conclusion.

II. SURFACE GEOMETRY

The structure of the bulk-truncated GaAs$(\overline{113})B$ surface is shown schematically in a ball and stick model in Fig. 1. The primitive unit cell is rhombohedric as marked by the dashed rhombus in the top view of the surface. In Fig. 1(a) the unit cell contains the same number of Ga and As atoms, but the coordination of both is different. The Ga atoms are twofold coordinated, whereas the As atoms are in a $(111)B$-like configuration being threefold coordinated. Alternatively, a second termination of the surface is possible, whose unit cell is marked by the dashed rhombus (B') in Fig. 1(b). In this case, the unit cell is comprised only of As atoms; one, which is twofold coordinated, in the topmost layer, the second,

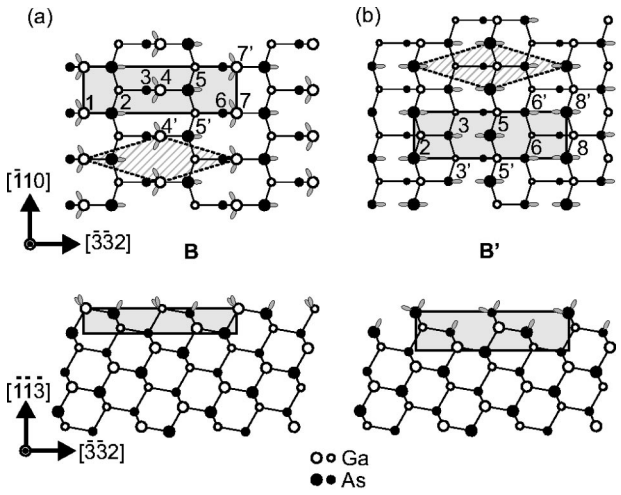

FIG. 1. (a) GaAs$(\overline{113})B$ bulk-truncated structure *B*, (b) alternative cut B'.

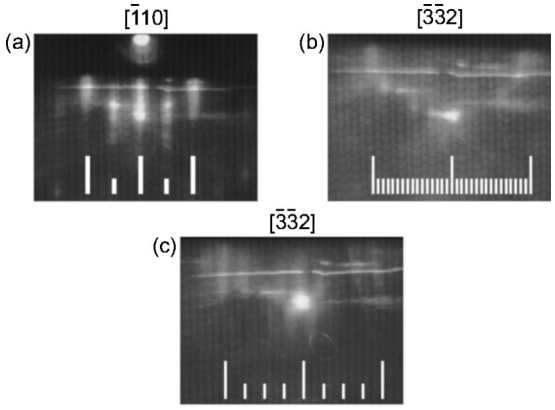

FIG. 2. RHEED pattern during MBE growth of GaAs$(\overline{113})B$ (a) along [110], (b) along [332], (c) along [332], after annealing in As flux.

which is threefold coordinated, in the third atomic layer. It is interesting to note that the calculated surface energy for the B'-truncated structure is lower than the surface energy of the *B*-truncated surface, even for Ga-rich environment.[9] For a simpler description of the experimental findings, it is more convenient to use a face-centered unit cell, shown by the hatched rectangles in Figs. 1(a) and 1(b). Even though the size of the unit cell is doubled, its rectangular shape will make the periodicity of the reconstructions in the reciprocal space more obvious. The dimension of this unit cell is 4.0 Å in the [110] direction and 13.3 Å along [332].

III. EXPERIMENT

The experiments were carried out in a multichamber ultrahigh vacuum (UHV) system, which has been described in detail elsewhere.[19] In brief, it consists of a small MBE chamber with RHEED optics, a STM (Park Scientific Instruments, VP2) chamber, and an UHV analysis chamber with an Ar-ion gun for sputter cleaning, a LEED optics, and a photoelectron spectrometer. These chambers are connected by an UHV transfer line including a small loading chamber.

Samples with a typical size of 10×10 mm^2 were cut from GaAs(113)*B* oriented wafers [*n* type, Si doped, carrier concentration $(1.4–4.8)\times10^{18}$ cm^{-3}, Wafer Technology]. Before the samples were introduced into the UHV, they were degreased with propanole. After removing the native oxide layer at 580 °C, samples were additionally cleaned by several IBA cycles. Homoepitaxial layers 20–50 nm thick were grown by MBE at a temperature of 530 °C. The As_2:Ga beam equivalent pressure ratio was 15. During growth, the RHEED pattern showed a broadened (00) beam along the [332] azimuth indicating a weakly developed $8\times$ periodicity in the [110] direction. Perpendicularly, at a beam incident along [110] only the bulk diffraction spots appeared. Both RHEED pattern and schematically drawn bars giving the position of the diffracted beams are shown in Fig. 2. We note that the longer bars indicate the position of the diffracted beams of the primitive unit cell.

Two different structures were obtained by different quenching procedures after growth. A more Ga-rich phase was acquired by keeping the sample temperature at 500 °C while the As source was cooled down to room temperature. As we will show below, this structure is the aforementioned (8×1) reconstruction. An As rich phase occurred by annealing the sample at a temperature of 450 °C while the As_2 flux was kept constant for several minutes, yielding a mixed $(2\times1)/(1\times1)$ structure. After the respective treatment, the sample temperature was decreased to 300 °C, while the MBE sources were cooled down, and at a pressure below 3×10^{-9} mbars, the samples were transferred to the analysis chamber. The samples were allowed to cool down to room temperature and were kept in this chamber for at least 1 h before further investigation. STM images were acquired in constant current mode with tunneling currents between 0.075 and 0.2 nA and sample voltages between -2 and -3.5 V. The spatial resolution was worse for positive bias voltage (empty-state images) so that these measurements could not contribute further details.

IV. RESULTS AND DISCUSSION

A. The (8×1) structure

The GaAs$(\overline{113})B(8\times1)$ reconstruction was found by keeping the sample temperature slightly lower than the temperature during growth. Hereafter, the $8\times$ RHEED pattern already observed during growth at an electron beam incident in [332] direction arose more clearly. This finding indicates that this structure is developed during MBE growth. The RHEED pattern in the [110] incident showed only a period, equivalent to 6.5 Å in real space, which corresponds to half of the length of the bulk-truncated unit cell in this direction. We note that due to the face-centered unit cell only spots appear in the reciprocal space image for which $h+k$ is even. Thus, this spacing corresponds to a $1\times$ period. The corresponding periodicities were also found in the LEED pattern, which was reported in Ref. 14. From these results, we conclude the reconstruction forms a periodicity of (8×1) with respect to the face-centered unit cell.

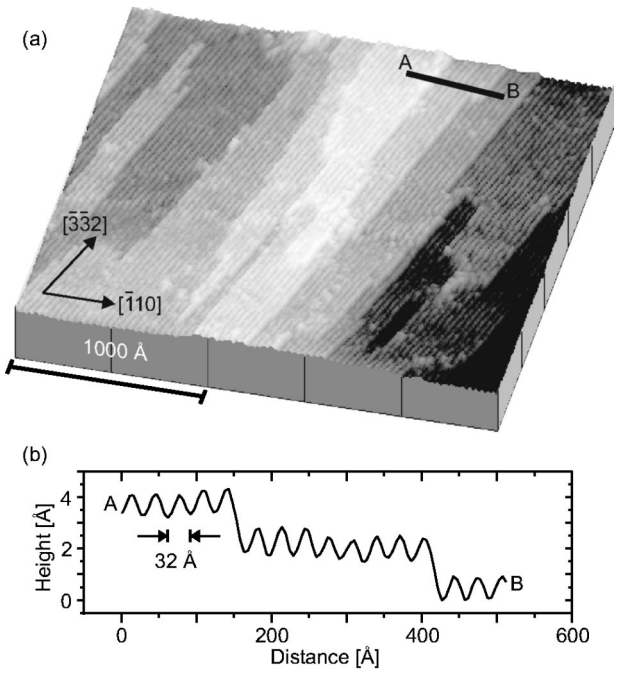

FIG. 3. (a) Large-scale 3D STM image of the GaAs(113)*B*8×1 reconstructed surface, sample bias voltage −2.8 V, sample current 0.15 nA. (b) Height profile along *AB* in (a). The step height is 1.7 Å.

A three-dimensional STM image of an 2500×2500 Å^2 area is shown in Fig. 3. Large flat terraces are visible at this scale. The step-height amounts to 1.7 Å, which corresponds to the height difference of three atomic levels of the (113) plane. Within the terraces, rows extend over more than 1000 Å running from the bottom to the top of the image. The distance between the rows is 32 Å and corresponds to the 8× periodicity observed in the RHEED pattern. Figure 4 exhibits a high-resolution STM image, which shows the atomic arrangement of the reconstruction more clearly. The rows are composed of series of protrusions forming zigzag chains along [332] in two levels. The lower zigzag chains are phase shifted in the [332] direction with respect to the topmost zigzag chain. With the help of the high-resolution STM images, we have developed a structural model for the GaAs(113)*B*(8×1) surface, which is depicted in Fig. 5. In the topmost layer, Ga dimers are formed, arranged in zigzag chains along [332]. A second zigzag chain in the third atomic layer is also built of Ga dimers with the dimers shifted in the [332] direction by a quarter of the unit cell with respect to the topmost Ga dimers. Between those middle dimer chains a trench is formed containing threefold coordinated Ga and threefold coordinated As atoms in the fifth and sixth atomic layer, respectively. Hence, the reconstruction is comprised of six atomic layers, with an entire corrugation within the unit cell of 3.4 Å.

Most remarkably, the GaAs(113)*B*(8×1) structural model presented above is exactly analogous to the (8×1) reconstruction known for the GaAs(113)*A* surface.[15] It just results by exchanging the anions by the cations and vice versa. Although it seems trivial that analogous structures form on the two faces of a polar surface, such a case has not been observed for GaAs before. One may ask at this point whether we have mixed up the *A* and *B* faces. This is not the case since the two faces are of very different morphology. Whereas the *B* face exhibits extended and flat terraces (see Fig. 3), the *A* face exhibits a distinct waviness on the same scale including 10-ml-deep holes.[20]

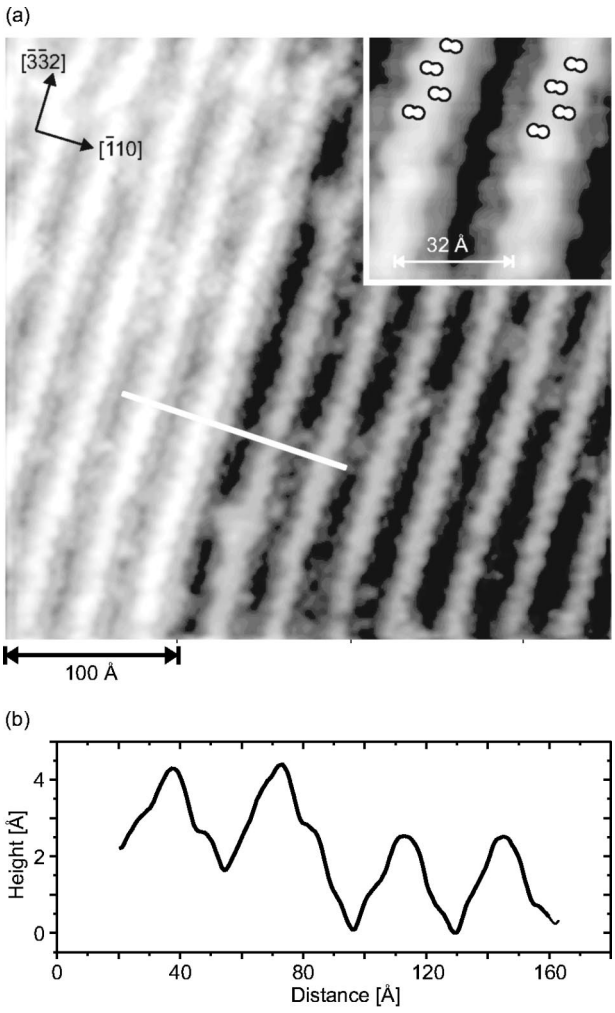

FIG. 4. (a) High-resolution STM image of the GaAs(113)*B* surface showing a step edge. Same parameter as for Fig. 3. (b) Height profile along [110].

Looking at the large scale STM image of the GaAs(113)*B*(8×1) surface shown in Fig. 3, it becomes clear, that the step structure on the surface is highly anisotropic. While steps edges along [332] are extremely long, the step edges in the perpendicular [110] direction are relatively short. In general, steps are considered to play an important role in growth mechanisms, since they often act as incorporation centers. Thus, they influence directly the surface morphology. The fingerlike step structure on the GaAs(113)*B*(8×1) surface suggests that growth occurs mainly by propagation along [332]. In order to clarify this point we have monitored the evolution of the specular RHEED spot intensity in dependence of time and azimuthal direction.

The occurrence of spot-intensity oscillations are attributed to a layer by layer growth mode.[21] Within this growth model

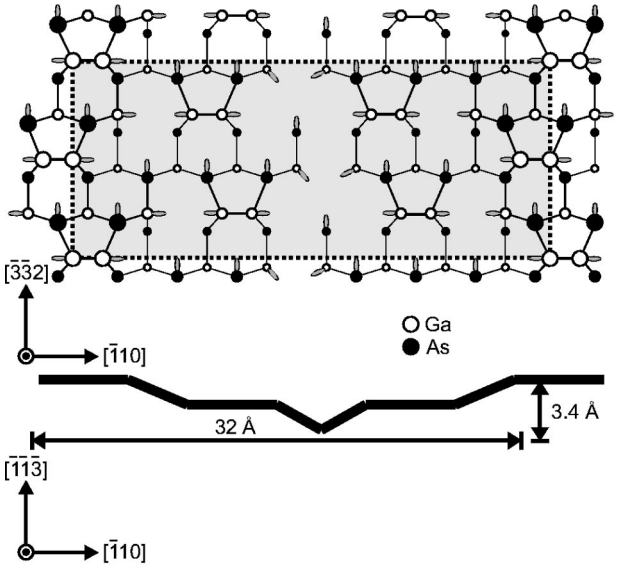

FIG. 5. Model of the GaAs$(\overline{113})B8\times1$ reconstruction.

the period of the oscillations corresponds to the growth of one monolayer, i.e., a complete layer of Ga and As. In contrast, the step-flow growth mode does not show oscillations.[22] Moreover, it was suggested by Neave *et al.*[21] that the growth direction parallel to the surface may also be specified with the help of RHEED intensity oscillations. According to Neave *et al.*,[21] step edges perpendicular to the electron beam weaken the beam intensity through diffuse elastic scattering. This effect is maximal for maximum step length, i.e., at 1/2 ML in two dimensional (2D) nucleation. For GaAs(113)*B*, if the step length is large along [332], strong oscillations are expected for the beam along [110] and vice versa.

Interestingly, the GaAs$(\overline{113})B$ surface exhibits very long steps along [332]. As expected, therefore, we observed RHEED oscillations mainly when the electron beam was directed parallel to [110], and only to a minor degree in the perpendicular direction as shown in Fig. 6(a). Consequently, we conclude that growth occurs through 2D nucleation and that the islands are more extended along [332]. For comparison we have measured the RHEED intensity oscillations, as shown in Fig. 6(b), on a (001) oriented GaAs substrate along [110] under the same growth conditions. It is interesting to note that the period of the oscillation on the (001) surface is less than twice the period of the oscillations on the GaAs(113)*B* surface. This is in agreement with the fact that the monolayer step height on the GaAs(113)*B* plane is 1.7 Å, while on the (001) surface it is 2.8 Å. Our result demonstrates that the growth conditions known for an (001) oriented substrate are also applicable for this high-index surface.

Although RHEED oscillations have been observed by other groups on [113]*B* surfaces[18,23–25] the azimuthal variations are still controversial. Lubyshev *et al.*[25] observed a maximum amplitude with the electron beam along [332]. Although this azimuthal dependence is reversed with respect to ours, they came to the same conclusion that ''the surface grows through propagation and coalescence of pronounced

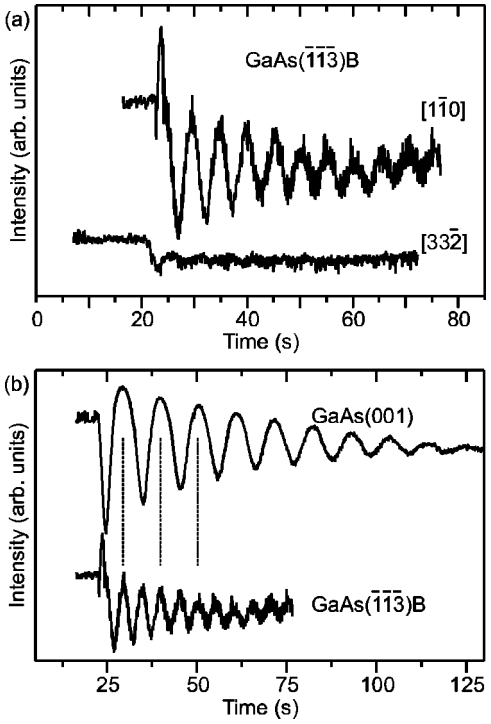

FIG. 6. GaAs$(\overline{113})B$ RHEED oscillation of the (00) beam, (a) different azimuths, (b) comparison with GaAs(001).

2D nucleation along the $[33\overline{2}]$ direction.'' Brandt *et al.*[23] observed also RHEED oscillations without presenting them or noting the azimuth. They derived the monolayer period of 0.17 nm in agreement with our observation. Wang *et al.*[18] observed strongest amplitudes of RHEED oscillations for incident electrons along [332]. This discrepancy to our result is likely due to a different surface morphology; their surface is much rougher than ours as evidenced from their STM images.

The growth along $[33\overline{2}]$ can be explained with the help of the electron counting rule[26] (ECR) in a similar way as recently discussed by Geelhaar *et al.* for GaAs(113)$A(8\times1)$.[27] The ECR is a helpful tool in separating out surface structures of expected low total energy; it is a rule and not a law and there are exceptions as discussed recently.[28] Geelhaar *et al.*[27] suggested to apply the ECR to models of 1D islands. The 1D islands extend infinitely in one direction, whereas in the perpendicular direction they are constructed as small as possible. It results that only islands along [332] fulfill the ECR, while islands in the perpendicular direction do not. This suggests that structures protruding from step edges along [332] are energetically unfavorable and, therefore, do not occur. Hence, step edges along [332] are straight, and thereby no RHEED oscillations are observable in this azimuth. In the perpendicular direction, step edges are rough, giving rise to the oscillation of the RHEED intensity until one layer is fully completed. Thus, growth propagates mainly along [332], i.e., along the rows of zigzaging Ga dimers, giving rise to the fingerlike step edges on the GaAs$(\overline{113})B(8\times1)$ surface.

B. The As-rich phase

As-rich surfaces play an important role in the growth of InAs quantum structures on GaAs, since these structures are

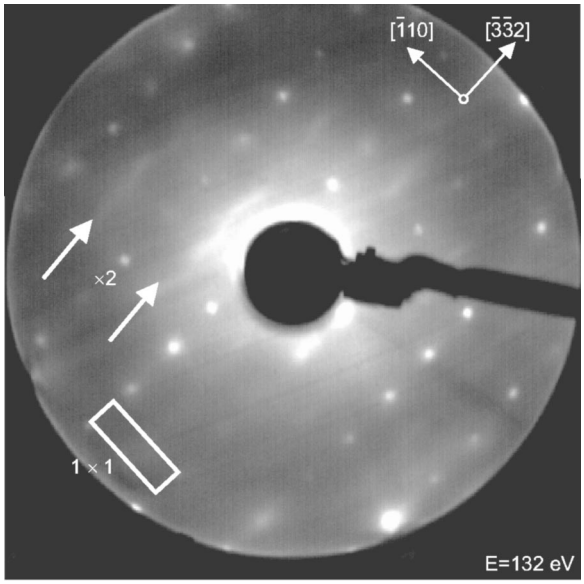

FIG. 7. LEED pattern of the As-rich structure of the GaAs(113)*B* surface.

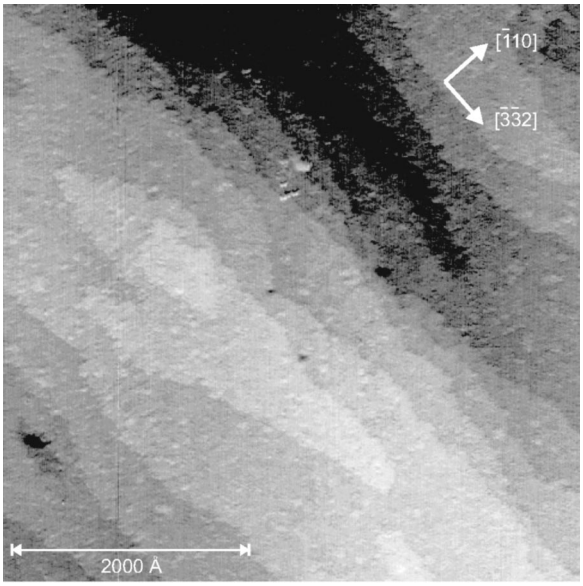

FIG. 8. Large-scale STM image of the As-rich structure of the GaAs(113)*B* surface. Sample bias voltage −2.8 V, sample current 0.125 nA.

usually grown under As-rich conditions and at lower growth temperatures due to the lower desorption temperature of In atoms. In addition, there is a common interest in As-rich surfaces since they play an important role in growth processes in metalorganic chemical vapor deposition.[29] We have, therefore, prepared the GaAs(113)*B* surface by annealing the samples after growth maintaining the As flux. It is well known, that the double As layer phase of GaAs(001), namely, the $c(4\times4)$ surface, can be prepared by MBE under the same conditions.[30,31]

During the anneal process, while decreasing the sample temperature to 450 °C, the RHEED pattern [Fig. 2(c)] in the [332] direction changed at a temperature of approximately 470 °C from a broad (00) spot to a streaky pattern. The spacing of the streaks corresponds to twice the period of the unreconstructed unit cell. This periodicity doubling was also observed by Kawase *et al.*[16] and was attributed to the dimerization of As atoms on the surface. The RHEED pattern in the perpendicular direction remained the same showing the bulk diffracted beams. A further decrease of the sample temperature did not cause a significant change of the RHEED pattern.

After annealing, in the LEED-pattern, shown in Fig. 7, basically only the bulk diffraction spots are clearly visible. However, very weak stripes extending along [332] are visible in between the rows of the bulk diffracted beams, indicating a poorly ordered 2× periodicity on the surface. Moreover, the spots are relatively broad and a considerable amount of background scattering is present. In different experiments, during which the quenching procedure was varied by lowering the cooling rate and varying the As flux, the LEED pattern showed always high background due to diffuse elastic electron scattering. This indicates a low degree of order on the MBE prepared surface in spite of annealing. However, from the RHEED and the LEED pattern we conclude that at least small domains of (2×1) symmetry are present on the surface.

Some information on the morphology of the surface can be derived from the STM image in Fig. 8. At this scale—the image shows a 5000×5000 Å^2 area of the surface—large terraces can be recognized. Linescans across the terraces revealed a step height of 1.7 Å, the same amount as observed on the (8×1) reconstructed surface. On samples grown by MOVPE the surface showed a similar morphology in STM images and atomic force microscopy images.[16,17] It is interesting to note that although the electron-diffraction patterns indicated a poor surface quality, the STM images revealed well-developed single layer terraces. However, looking closely at the image, there is a significant number of holes and single layer islands within the terraces, which may explain the high background in the electron-diffraction pattern. Figure 9 shows a high-resolution STM image of an 250×250 Å^2 area within a terrace. Despite of the apparently somehow disordered surface structure, rows running from the upper left-hand side to the lower right-hand side, extended along [110], are visible. We note that on this surface the rows are oriented perpendicularly to the rows observed on the GaAs(113)*B*(8×1) surface. The spacing of the rows is 6.5 Å, which corresponds approximately to half the length of the unit cell in [332] direction. This distance is also in accordance with the RHEED and LEED results, which showed only a 1× period in this direction. Since the unit cell is face centered, the 1× period of the diffracted beams in the RHEED pattern corresponds to half the length of the unit cell.

In order to understand the twofold periodicity of the electron-diffraction patterns one has to look in more detail at the STM images. We have, therefore, zoomed into three different images taken from different areas of a terrace, which are shown in Figs. 10(a)–10(c). In Fig. 10(a) two rows of elongated protrusions are visible running along [110]. The spacing of the rows is approximately 13 Å and the elongated features are separated along [110] by 8 Å. The distances as

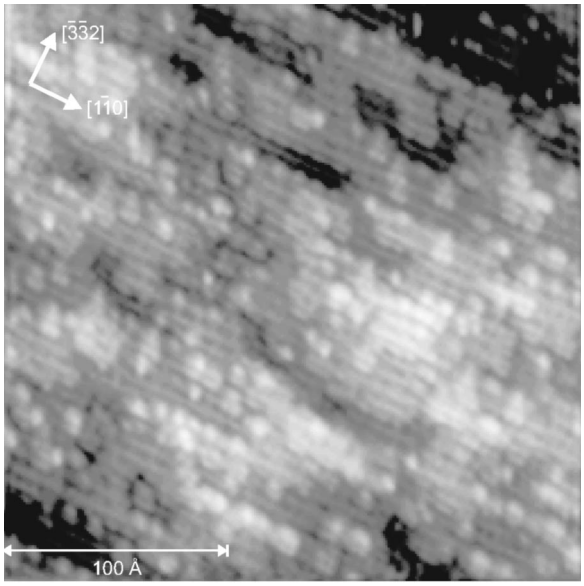

FIG. 9. High-resolution STM image of the As-rich structure of the GaAs(113)*B* surface. Sample bias voltage −3.25 V, sample current 0.12 nA.

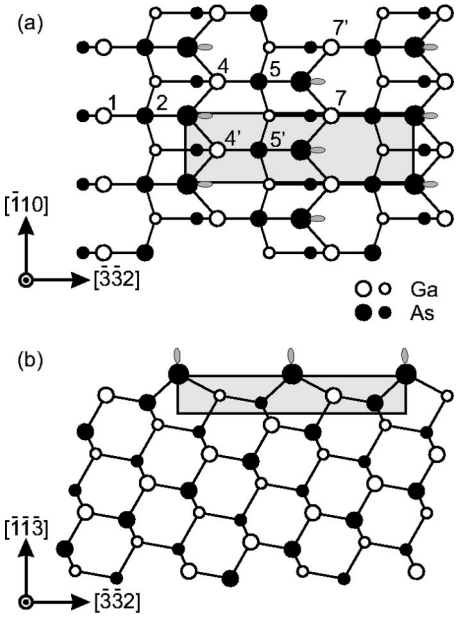

FIG. 11. (1×1)-reconstruction model for the As-rich GaAs(113)*B* surface as proposed by Stiles and Kahn (Ref. 10).

well as the orientation suggest to assign these features to As dimers. Thus, the arrangement of these dimers to a row along [110] gives rise to the observed 2× periodicity in the diffraction patterns. A second atomic arrangement within the terrace is depicted in Fig. 10(b). This image reveals rows of protrusions separated by 6.5 Å extended along [110]. The spacing of the protrusions within a single row is only 4 Å and suggests to assign these protrusions to single As adatoms. Also, there are some extra adsorbed As dimers visible as bright elongated features, but these dimers are part of a layer above the single As atoms, as revealed by line scans across the image. The third image shows an island, which is build of a row of As dimers extended along [110] and an adjacent row of single As atoms, demonstrated by the line scans I and II in Fig. 10(d). While on the line scan labeled I two humps separated by approximately 3.5 Å build a unit of the row, the line scan II is built up of single humps separated by 4 Å. These results revealed that the surface is almost completely comprised of rows extended along [110], which are built up of either single As atoms or As dimers.

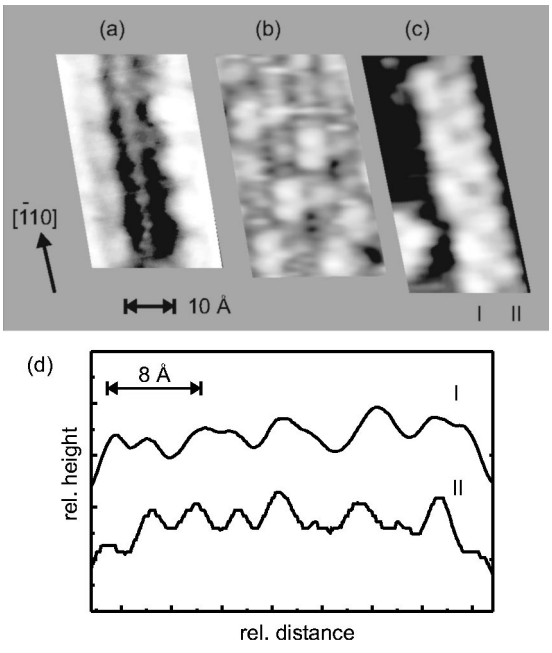

FIG. 10. High-resolution STM images of the As-rich structure of the GaAs(113)*B* surface. (a), (b), (c) different local areas in the image of Fig. 9. (d) line scan along [110] of (I) As-dimer row and (II) As-adatom row.

Based on the experimental findings different structural models can be taken into consideration to explain the results. First, the rows of single As atoms and the almost 1× period observed in the LEED pattern, agrees well with the structural model proposed by Stiles and Kahn.[10] This (1×1) structural model, shown schematically in Fig. 11, results by adding As atoms bonded in the threefold hollow site to the bulk-truncated *B* surface (c.f. Fig. 1). However, this model does not satisfy the ECR. Counting all the electrons within the unit cell, only 3 3/4 electrons are available to be distributed into two orbitals. The lack of 1/4 electron charge might be the reason for the disorder of the surface. The defects on the terraces, i.e., the holes and the islands, yield Ga atoms to appear at the surface, which by emptying their dangling bonds give additional charge into their surrounding and thereby charge neutrality might be achieved.

Second, in order to explain the twofold period in the electron-diffraction patterns, a structural model containing As dimers has to be considered. We note that a model based on Ga dimers would be in disaccordance with the excess As preparation conditions. An As dimer model was already proposed by Kawase *et al.*[16] and is depicted in Fig. 12. This model results from the bulk-truncated surface *B′* (c.f. Fig. 1), by adding As dimers bonded to the surface As atoms. The

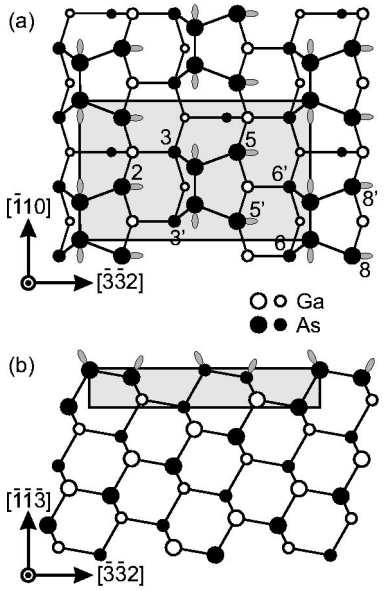

FIG. 12. (1×1)-reconstruction model for the As-rich GaAs(113)*B* surface as proposed by Kawase *et al.* (Ref. 16).

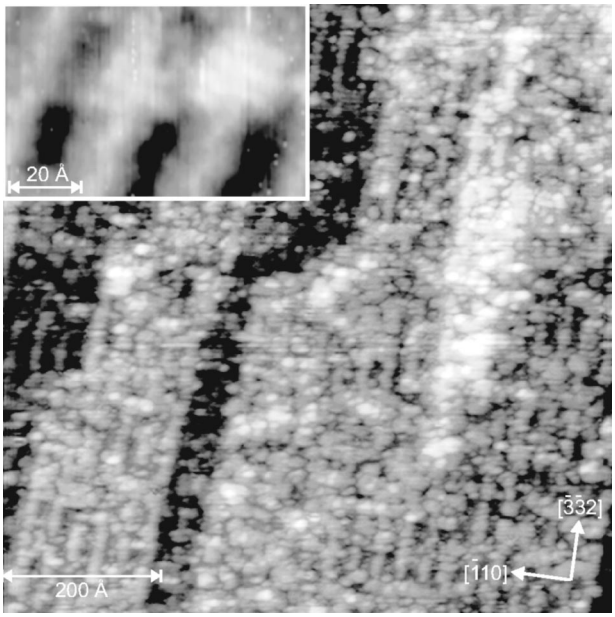

FIG. 13. STM image of the GaAs($\bar{1}\bar{1}3$)*B* surface at the transition between the (8×1) and the As-rich structure.

As dimers are thus aligned to rows along [$\bar{1}$10]. The unit cell is comprised of two As dimers bonded to As atoms and four threefold coordinated As atoms. Within the picture of the ECR, one electron is lacking per (2×1) unit cell and thus, the ECR cannot be satisfied. Hence, also this model requires the existence of disorder to achieve charge neutrality.

In summary, the following picture of the As-rich phase arises: Locally, two different structural motifs occur. In direction [332] As adatoms and dimers create a short-range 1× or 2× periodicity, respectively. Both structures violate the ECR. In addition, the surface is perturbed by holes that expose Ga atoms. A long-range order does not exist on the surface. Therefore, we conclude that, opposed to the (8×1) phase, the As-rich phase is not a stable reconstruction.

Surfaces of single crystals in general are conventionally divided into singular and unstable ones. While singular surfaces are characterized by extended planar areas and a long-range order, unstable surfaces facet into neighboring low-energy surfaces.[33] However, the As-rich phase of the GaAs(113)*B* surface does not fit into either category. Although it lacks a long-range order and violates the ECR suggesting that it is of a high surface energy, the surface comprises large terraces that are separated by well-developed single steps. Facets of a different orientation do not occur at all. Similar observations have been reported for other surfaces, too: On GaAs(113)*A*, an As rich preparation yields also an absence of a long-range ordered reconstruction.[32] Locally, As dimers [as in the GaAs(113)*A*-(8×1) reconstruction] were observed with separations corresponding to 2×, 3×, and 5× periodicities, but none of these structures fulfills the ECR. The surface is fairly rough (terraces are very small), but there are not any facets. The Si(103) surface is stable against faceting, but it is rough and disordered.[34] STM images revealed that even on a nanometer scale the surface is not ordered. Local structural elements were not identified. In order to properly describe these cases, it seems necessary to introduce a third, new category of surfaces: Those that are characterized by the absence of any long-range crystallographic order but do not facet, either. A detailed understanding why such a surface can be energetically favorable would require, of course, a theoretical study. However, it is unclear to us if a disordered structure could be described by present theoretical techniques at all. For compound semiconductors we would like to point out that the aforementioned observations are in accord with our recent conclusion that reducing the number of dangling bonds is more important than reaching a semiconducting ground state, as ensured by fulfilling the ECR.[35] Also, on GaAs the As dimer reduces the surface energy apparently very effectively. This structural motif occurs on all known stable GaAs surfaces whose bulk-truncated structure is at least partly (001)-like [GaAs(001),[36] GaAs(113)*A*,[15,9] GaAs(113)*B* [this paper], GaAs(114)*A*,[37] and GaAs(2 5 11) (Ref. 35)].

C. The (8×1) to As-rich phase transition

As indicated by the RHEED pattern, the actual growth structure seems to be the (8×1) reconstruction, whereas the As-rich phase structure develops after annealing in As flux and lowering the sample temperature. Therefore, we concluded that the latter structure developed just by adsorbing As atoms on the surface under rearrangement of the Ga dimers.

In order to study the transition between the structures, we have kept the sample, which showed a (8×1) structure in the RHEED pattern, under As flux and simultaneously decreased the sample temperature. Immediately after the disappearance of the 8× pattern, we have transferred the sample to the STM chamber.

Figure 13 shows a STM image of the transition structure. The surface still shows the rows of Ga-dimer zigzag chains running from the bottom to the top of the image. However, a

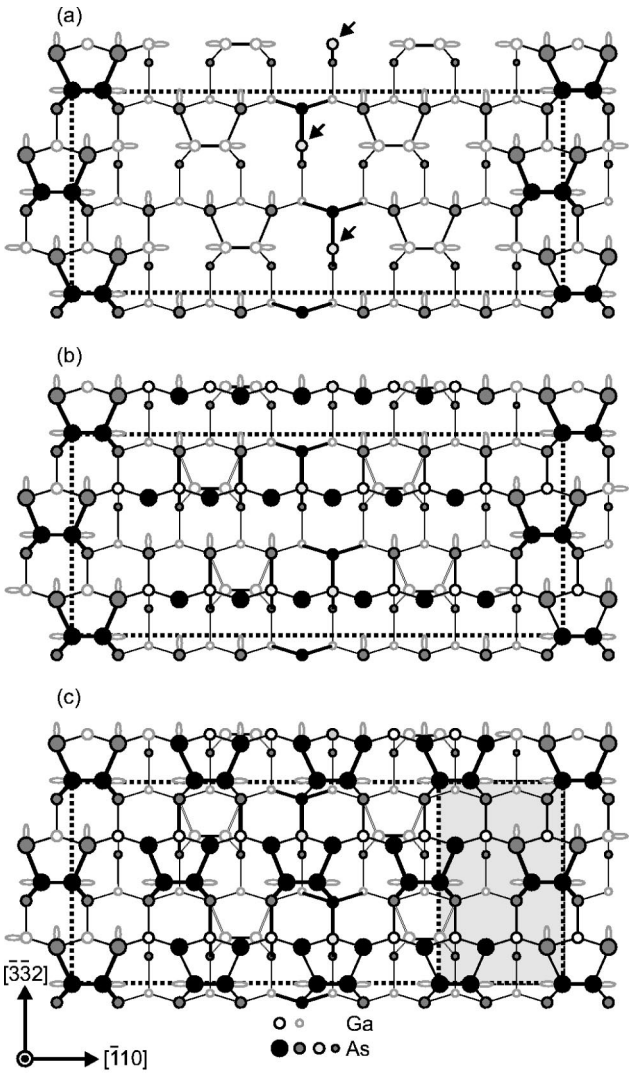

FIG. 14. Schematic sketch of the transition between the (8×1) and the (2×1) model of Kawase *et al.* (Ref. 16) on the GaAs(113)*B* surface. Arrows indicate the added Ga atoms from the Ga dimer, exchanged by As dimers in the highest zigzag row (see text).

considerable amount of disordered structures are present. The inset in the upper left of the image shows a high-magnification image of the disordered structures. There are some short rows of humps oriented perpendicularly to the Ga-dimer zigzag chains. From the tunneling conditions as well as from the structure discussed above, we conclude that these structures are the As dimers and the rows of As adatoms. The image reveals that the transition between the (8×1) to the As-rich phase occurs by filling the trenches of the (8×1) structure with As adatoms and subsequent As dimer formation. Of particular interest is that it is indeed possible to fill the entire trench of the (8×1) structure, which extend to six atomic layers in depth, without additional Ga atoms. The transition is presented in the sequence of Fig. 14(a)–14(c). First, by exchanging the upper Ga dimers with As dimers, the resulting Ga atoms may be included in the trench as indicated by the arrows in Fig. 14(a). This ensures the stoichiometry of the bulk. Second, As atoms attach to the surface and build a layer within the trench. And finally, a second layer of As atoms attach at the surface yielding As dimer formation. Following this transition, the As dimers automatically bound to As atoms as proposed by the model of Kawase *et al.*[16]

V. CONCLUSIONS

Two different phases were observed on the MBE prepared GaAs(113)*B* surface: a (8×1) reconstruction and an As-rich structure. For the (8×1) reconstruction we have proposed recently an adapted Wassermeier model[15] in which As is exchanged by Ga and vice versa.[14]. The characteristic components of this model are Ga dimers forming zigzag chains along [332] in two atomic levels. Step edges are extremely smooth along [332] and rough in the perpendicular [110] direction. This is explained by applying the ECR that strongly favors growth along [332] but disfavors nucleation into [110] direction. This growth asymmetry is nicely reflected in the RHEED oscillations that were observed most strongly when the electron beam was directed along [110] but much weaker in the perpendicular direction. Therefore, we conclude that the growth occurs through two-dimensional nucleation with the islands largely extended along [332], i.e., propagating mainly along [332].

Surfaces of single crystals in general are conventionally divided into stable singular and unstable ones. While singular surfaces are characterized by extended planar areas and a long-range order, unstable surfaces facet into neighboring low-energy surfaces. However, the As-rich phase of the GaAs(113)*B* surface does not fit into either category but represents a remarkable intermediate case: Locally, two different structural motifs occur; As adatoms and dimers create a 1× and 2× periodicity along [332] but a long-range order does not exist; nevertheless, the surface comprises large terraces that are separated by well-developed single steps. Therefore, we conclude that, opposed to the (8×1) phase, the As-rich phase is not a stable reconstruction. In order to properly describe these cases, it seems necessary to introduce a third, new category of surfaces: Those that are characterized by the absence of any long-range crystallographic order but do not facet, either. A detailed understanding why such a surface can be energetically favorable would require, of course, a theoretical study. However, it is unclear to us if a disordered structure could be described by present theoretical techniques at all.

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