Atomic structure of the GaAs$(\overline{1}\overline{1}3)B(8\times1)$ surface reconstruction

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Atomically resolved scanning tunneling microscopy and low-energy electron diffraction were used to determine the surface structure of the GaAs$(\overline{1}\overline{1}3)B$ surface prepared by molecular beam epitaxy. An (8×1) reconstruction was found, which forms by exchanging Ga and As atoms analogously to the GaAs(113)$A(8\times1)$ reconstruction proposed by Wassermeier *et al.* [Phys. Rev. B **51**, 14 721 (1995)]. The characteristic components of the *A* and *B* (8×1) surface reconstructions are dimers forming zigzag chains along $[\overline{3}\overline{3}2]$ in two atomic levels. While on the *A* surface the dimers are built of As atoms, on the *B* surface Ga atoms form the dimers. The morphology of the GaAs$(\overline{1}\,\overline{1}\,3)B(8\times1)$ surface is rather smooth and does not show the typical roughness known for the GaAs(113)$A(8\times1)$ surface.

Most semiconductor surfaces undergo reconstructions to lower their surface energy. In the case of compound semiconductors the reconstructions on a given surface orientation might differ in their periodicity and/or in their stoichiometry. It follows that some reconstructions are dominated either by the anions or the cations. Experimentally, the different surface reconstructions on a given surface can be induced by varying the preparation conditions. The most prominent surface on GaAs is the (001) plane for which a large number of reconstructions has been found.[1] In particular, the $(001)(2\times4)\beta2$ (Ref. 2) and the $(001)(4\times2)\beta2$ (Ref. 3) reconstructions are formed by the same kind of atomic arrangement but with exchanged elements. The dominating structural components are rows of As dimers and dimer vacancies for the $(2\times4)\beta2$ and rows and vacancies of Ga dimers for the $(4\times2)\beta2$ reconstruction. Another possible reason for a different arrangement is a more intrinsic property of the zincblende crystal, namely, the polarity of some of its surfaces. For instance, the {111} bulk-truncated surfaces are terminated either by cations (*A* surfaces), or anions (*B* surfaces). One may expect that the surface reconstructions on both planes form by the same structural components but build of the different ions. Instead, the (2×2) reconstructions, which are found on both faces, are completely different: On the *A* surface, the reconstruction is caused by the vacancy of one Ga atom in each unit cell,[4] whereas the reconstruction for the *B* surface arises from the formation of As trimers.[5] This finding also shows the complexity of surface reconstruction on compound semiconductors.

The GaAs$(\overline{1}\,\overline{1}\,3)B$ surface has successfully been employed as a substrate for the growth of quantum structures like quantum dots,[6–12] but the bare surface has not been studied extensively. Although several authors reported on the occurrence of a (1×1) structure[13–15] and also of a (2×1) reconstruction[16] on the GaAs$(\overline{1}\,\overline{1}\,3)B$ surface, no structural model has been proposed so far which fulfills the electron counting rule (ECR).[17] In addition, it has been reported that the surface prepared by molecular beam epitaxy (MBE) is not stable, but decomposes into facets of low-index surfaces.[18,19] We believe therefore that a detailed study on the surface structure is highly desirable.

In this contribution we report for the first time an (8×1) reconstruction for the GaAs$(\overline{1}\,\overline{1}\,3)B$ surface and present a structural model for this surface. Our model is in agreement with the ECR and should therefore be energetically favorable. We show that the GaAs {113} planes possess a reconstruction which forms analogously for the Ga and As terminated faces as in the case of the $(001)(2\times4)\beta2$ and $(4\times2)\beta2$ reconstructions, but its origin lies in the surface orientation rather than in the surface preparation. To our knowledge analogously formed structures, which are caused by the polarity of the surfaces have not been observed on GaAs up to now.

Our samples were prepared by MBE and studied *in situ* with low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM; Park Scientific Instruments, VP2). A detailed description of the ultrahigh vacuum (UHV) system is given elsewhere.[20] Samples with a typical size of 10×10 mm^2 were cut from GaAs(113) 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 oxide desorption samples were additionally cleaned by several ion bombardment and annealing 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. After growth, the sample temperature was kept at 500 °C while the As source was cooled down to room temperature. Then the samples were cooled with a temperature change of 1 K s^{-1} to 300 °C and, after the base pressure of the growth chamber was less than 3×10^{-9} mbar 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.

First we describe the bulk-truncated structure of GaAs$(\overline{1}\overline{1}3)B$, which is shown schematically in Fig. 1 in top view and side view. The primitive unit cell is rhomboedric but for simplicity we follow Wassermeier *et al.*[21] and use a face-centered rectangular unit cell to achieve a shorter nota-

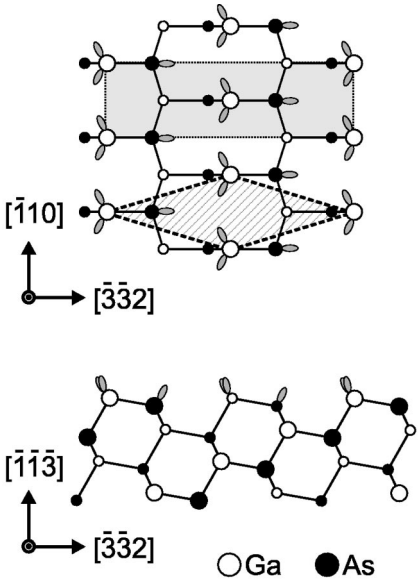

FIG. 1. Ball and stick model for the bulk-truncated GaAs$(\overline{1\,1\,3})B$ surface.The gray rectangle shows the face centered unit cell, the primitive unit cell is marked by the dashed rhombus. (a) Top view. (b) Side view.

tion for the reconstructed surface.[22] 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 $(\overline{1\,1\,1})B$-like configuration being threefold coordinated.

The periodicity of the (8×1)-reconstructed $(\overline{1\,1\,3})B$ surface is clearly visible in the LEED pattern which is shown in Fig. 2. The reflection spots are sharp indicating a well ordered surface. Both the reconstruction (8×1) and the face-centered bulk-truncated (1×1) unit cells are indicated. The size of the reconstruction unit cell in real space is 32.0×13.3 Å^2. The LEED pattern exactly matches the (8×1) pattern observed on the GaAs(113)A surface.[23] A STM image of a 2500×2500 Å^2 area is shown in Fig. 3. Large flat terraces can be seen at this scale. The step height between the terraces is 1.7 Å . Within the terraces, rows extend over more than 1000 Å, running from the upper left-hand side to the lower right of the image. The distance between the rows is 32.0 Å and corresponds to the $8\times$ periodicity observed in the LEED pattern.

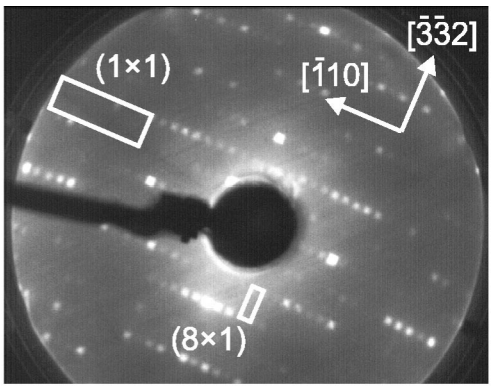

FIG. 2. LEED pattern of the GaAs$(\overline{1\,1\,3})B(8\times1)$ surface. $E=83$ eV.

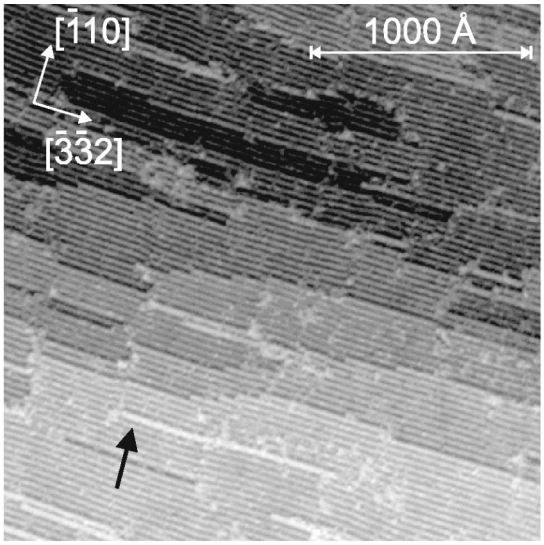

FIG. 3. Filled states ($U=-2.8$ V, $I=0.13$ nA) STM image of the GaAs$(\overline{1\,1\,3})B(8\times1)$ surface.

Figure 4 exhibits a high resolution STM image revealing the atomic arrangement of the reconstruction more clearly. The characteristic components which form the rows are series of protrusions forming zigzag chains along $[\overline{3\,32}]$ in two levels. The height difference between the chains is 1.7 Å, which corresponds to the height difference of three (113) atomic layers. The lower zigzag chains are phase shifted in the $[\overline{3\,32}]$ direction with respect to the topmost zigzag chain. These lower zigzag chains are separated by a trench, whose depth is approximately 1 Å, with respect to the middle zigzag chains. The entire corrugation height within the reconstruction is about 2.7 Å.

In order to explain the experimental findings, we propose a structural model for the GaAs$(\overline{1\,1\,3})B(8\times1)$ reconstructed surface, which is depicted in Fig. 5. The topmost components of the reconstruction are Ga dimers, which form a zigzag chain extended along $[\overline{3\,32}]$. In the third atomic layer there are also series of Ga dimers aligned to zigzag chains, but the dimers are shifted by a quarter of the unit cell with respect to the topmost dimers. Between those middle

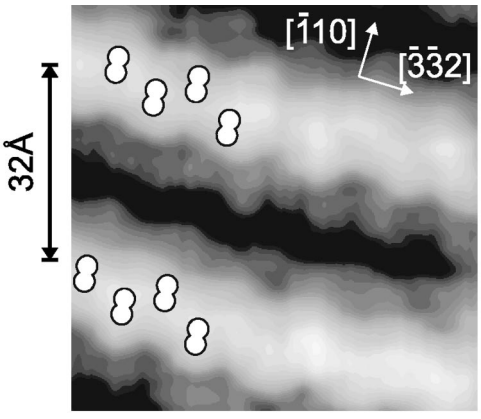

FIG. 4. High resolution filled states ($U=-2.5$ V, $I=0.14$ nA) STM image showing the atomic structure of the GaAs$(\overline{1\,1\,3})B(8\times1)$ surface.

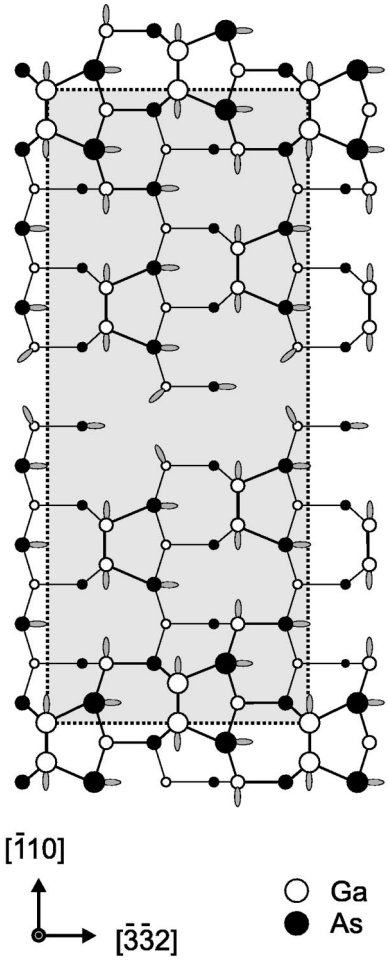

FIG. 5. Reconstruction model of the GaAs$(\overline{1\,1\,3})B(8\times1)$ surface. Atoms of lower levels are depicted by smaller circles.

dimer chains a trench is formed containing threefold coordinated Ga and threefold coordinated As atoms in the fifth and sixth atomic layer, respectively. Altogether, six atomic layers are involved in the reconstruction. The corrugation height within the unit cell is 3.4 Å. The discrepancy between the corrugation height in the model and that obtained by the STM measurements (2.7 Å) is probably caused by the finite size of the tip, which does not reach the lowest atoms in the narrow trench. Counting the number of valence electrons according to the ECR (3/4 from Ga atoms and 5/4 from As atoms), a total amount of 44 electrons (32 Ga atoms and 16 As atoms) have to be distributed in 22 orbitals (6 Ga dimers and 16 As dangling orbitals), yielding fully occupied As dangling orbitals and emptied Ga orbitals. Thus, the ECR is fulfilled leaving the surface semiconducting.

The above model is exactly analogous to the (8×1) reconstructed GaAs(113)A surface,[21] it results just by exchanging the anions by the cations. Nevertheless, we note that both GaAs$(\overline{1\,1\,3})B(8\times1)$ and GaAs(113)$A(8\times1)$ reconstructed surfaces present essentially the same STM images. This seems to be surprising on first note, but is in good accordance with other studies: Since the STM images (Fig. 3, Fig. 4) were collected applying negative sample voltage with respect to the tip, the filled dangling bonds of As atoms in the second and in the fourth atomic layer are imaged. In contrast, on the GaAs(113)$A(8\times1)$ surface the As dimers, which are the characteristic components of the reconstructed surface, are imaged under these tunneling conditions. A similar situation is found for the GaAs(001)$(4\times2)\beta2$ surface, where in filled-states images the As atoms in the layer underneath the topmost Ga dimers are visible.[24] In addition, our STM images of the GaAs$(\overline{1\,1\,3})B(8\times1)$ reconstruction are in good accordance to empty state images collected on the GaAs(113)$A(8\times1)$ surface, which shows practically the same STM images as in the case of filled state.[21] In that case the Ga atoms of the second and fourth layer are imaged, since they have one unoccupied dangling bond each.

The morphology of the reconstructed GaAs$(\overline{1\,1\,3})B(8\times1)$ surface is extraordinarily anisotrop, as revealed by the large-scale STM image (Fig. 3). The step edges along $[\overline{3\,3\,2}]$ are extremely straight, while those in the perpendicular direction are quite rough. Similar anisotropic step edges are also found on the GaAs(113)$A(8\times1)$ surface as recently discussed by Geelhaar *et al.*[25] It is therein proposed to explain the anisotropy by applying the ECR to models of one-dimensional (1D) islands. These models are created in such a way that all included atoms are, if possible, in a binding configuration as they would be in the reconstruction. In one direction the islands extend infinitely, and perpendicularly they are constructed as small as possible. The result was that islands extended along $[\overline{3\,3\,2}]$ fulfill the ECR, but islands elongated perpendicularly do not. Thus, structures protruding from steps along $[\overline{3\,3\,2}]$ would be energetically unfavorable, which explains why these step edges are so straight. The same formalism can be applied to the (8×1)-reconstructed GaAs$(\overline{1\,1\,3})B$ surface. On islands extended along $[\overline{3\,3\,2}]$ no additional atoms occur that are in a coordination different from those in the reconstructed unit cell. Thus, one-dimensional islands along $[\overline{3\,3\,2}]$ fulfill the ECR. For islands perpendicularly extended, i.e., along $[\overline{1}10]$, more atoms possessing additional dangling bonds have to be created yielding a violation of the ECR. Thus, the anisotropic step edge structure of the GaAs$(\overline{1\,1\,3})B(8\times1)$ surface can also be understood with the help of the ECR. Most remarkably, the STM image (see Fig. 3) shows indeed a 1D island, marked by the arrow, which propagates only in $[\overline{3\,3\,2}]$. These findings suggest that growth occurs by 2D-nucleation and propagation mainly along $[\overline{3\,3\,2}]$.

The only notable difference between the A and the B surfaces is the corrugation of the surface on a mesoscopic scale. On the GaAs(113)$A(8\times1)$ surface an up and down stacking of dimer zigzag chains occurs yielding an undulated shape of the surface on a mesoscopic scale.[21,25,26] The width of the GaAs(113)$A(8\times1)$ terraces along $[\overline{1}10]$ is rarely extended over more than five unit-cell lengths. In contrast, the terrace widths on the $(\overline{1\,1\,3})B(8\times1)$ surface are usually found to be extended over more than ten unit-cell lengths in the $[\overline{1}10]$ direction. The surface morphology is thereby smoother than that of the A surface. Although the step edge anisotropy is present on both A and B surfaces, indicating similar growth behavior, the mesoscopic scale morphology is indeed different. A comparative study of the influence of growth conditions on the morphology on both surfaces should be performed to substantiate this difference. However, this finding

shows to what extent the surface morphology can be influenced directly by the atomic arrangement on the surface reconstruction.

In conclusion, we have studied the MBE-prepared GaAs(1 1 3)B surface *in situ* by LEED and STM and found an (8×1) reconstruction. We propose a structural model in analogy to the (8×1) reconstruction of the GaAs(113)A surface. The characteristic zigzag chains on the GaAs(1 1 3)$B(8\times1)$ reconstruction are built of Ga dimers, instead of As dimers which are observed on the GaAs(113)A reconstructed surface. To our knowledge the (8×1) is the first reconstruction on GaAs exhibiting this analogy caused by the polarity of the surface. Finally, opposed to the the findings on the GaAs(113)$A(8\times1)$ surface the surface morphology of the GaAs(1 1 3)$B(8\times1)$ surface is smooth and should therefore be quite suitable in device technology.

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