A Novel Imaging Mechanism to Determine the At

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The Research group:

The research group at the University of Arkansas is interested in the surface physics of fabricating III-V semiconductor structures such as GaAs and InP. We are particularly interested in the fundamental properties, such as template structure, diffusion, nucleation and growth. The techniques used are STM, MBE, RHEED, X-ray diffraction, and Hall effect (www.uark.edu/misc/mbestm). The theoretical work was done at the Theory Department of the Fritz-Haber-Institute, Max-Planck-Gesellschaft in Berlin, Germany. This group uses density-functional theory calculations mainly for the investigation of the atomic and electronic structure of surfaces, as well as the dynamics of surface processes that constitute the atomistic basis of catalysis and crystal growth. The simulation of STM images forms part of this work as an important tool to study the reconstruction of surfaces (www.fhi-berlin.mpg.de/th/).

The scanning tunneling microscope (STM) has given profound insight into the nature of surfaces on the atomic scale. However, interpreting STM images can be difficult due to several contrast mechanisms such as sample-tip convolution effects or bias-dependent variations in the local density of states (LDOS). These mechanisms can confound the interpretation of image features, especially the determination of the atomic structure. Nowhere is the atomic structure of a surface more technologically important than in the family of zinc blende III-V or compound semiconductors such as GaAs or InP. The (001) oriented surface of these materials is the starting surface for producing a large variety of optoelectronic devices [1]. These devices are produced by epitaxy where layers of atoms are deposited upon an atomically clean surface. Therefore, a far better understanding of the atomic arrangement and stoichiometry of these surfaces is needed for modelling growth, especially when attempting to produce short-period heterostructures where the interfaces constitute a significant fraction of the whole structure. Surprisingly, the atomic structure of the most commonly used III-V surface, the GaAs(001)-(2 × 4) had not been known until recently [2]. Determining its atomic structure required the combination of STM data, first principles theory, and the discovery of a novel imaging mechanism.

Our experimental setup consists of a commercial molecular beam epitaxy (MBE) chamber from Riber. The MBE chamber contains reflection high-energy electron diffraction (RHEED) for monitoring the surface during growth and is equipped with a novel temperature measurement system that measures the band gap of the substrate and is accurate to within ± 2 °C [3]. This chamber is connected *in situ* to an OMICRON room temperature STM [4]. Special sample blocks were made from Mo designed to fit onto the standard 3 inch MBE sample manipulator and hold an OMICRON STM sample plate.

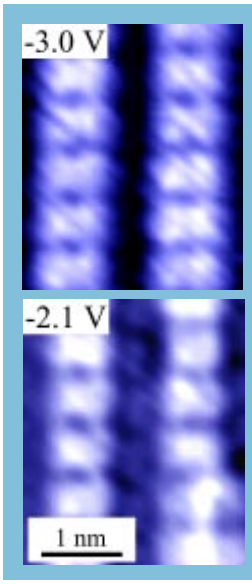

FIG. 1. STM images of the GaAs(001)-(2 × 4) reconstructed surface taken at the (filled state) sample bias as indicated. Notice that at the higher bias (above), the trench structure is not visible, while at the lower bias (below), the trench structure is visible.

Two atomic-scale resolution STM images of a GaAs(001)-(2 × 4) reconstructed surface are shown in Fig. 1 These images were taken from the same region using two different negative sample biases as indicated. A negative sample bias results in electrons tunneling from the filled states of the sample to the tip. The two bright vertical rows running in the [1$\bar{1}$0] direction are the As-dimer rows, which consist of the topmost portion of the surface. The spacing of these rows in the [110] direction represents the "4-by" periodicity of 1.8 nm. Within each row, the distinct peanut-shaped sections have a spacing of 0.9 nm in the [1$\bar{1}$0] direction and represent the "2-by" periodicity. These peanut-shaped sections consist of four As atoms or two side by side As dimers bonded along the [1$\bar{1}$0] direction. The striking difference between the two images is the appearance of the structure between the dimer rows. This structure consists of two As atoms or one As dimer also bonded along the [1$\bar{1}$0] direction and is a full monolayer, or 0.28 nm below the topmost layer of As dimers.

To determine the atomic structure of this surface and to understand why the trench structure appears at the lower biases, first

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omic Structure of the GaAs(001)-(2x4) Surface

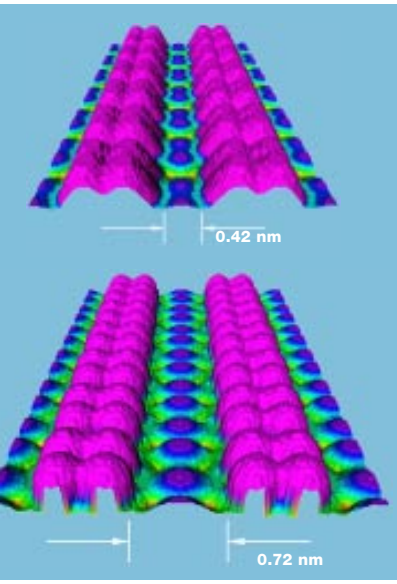

FIG. 2. 3D rendered first-principles theory STM images, or surfaces of constant LDOS, are generated by integrating the LDOS over different energy windows to simulate the high bias and low bias condition. The lower bias image (below) shows the trench width almost doubling.

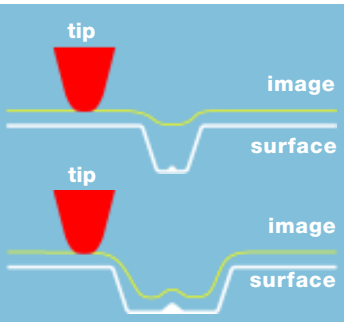

FIG. 3. Schematic diagram showing the electronic-sample sharpening effect. At high biases (above) the trench is narrow while at low biases (below) the trench widens. The wider trench region allows the STM tip to image the trench structure.

principles [5] derived STM images of the β2 structure [6] were calculated and are shown in Fig. 2 [2]. To mimic the filled state bias in the STM images the valence band states of the first-principles calculations were integrated over appropriate energy windows. Similar to the -2.1 V bias STM image, the calculated images show the top-layer As-dimer rows and the structure of the trench. However, the lower bias calculated image shows the width of the trench region almost doubling from 0.42 nm to 0.72 nm. The trench widens as a result of the retracting surface of constant LDOS about the top-layer As-dimer dangling bond orbital.

The increase in the width of the trench explains why the trench structure becomes visible in the STM images at lower biases. It is not the case that the LDOS of the features within the trench is changing with bias. Here, the trench features are exposed at lower biases due to the widening of the trench. This is a novel imaging mechanism that is similar to a tip-sample convolution effect except that the *sample* is changing, not the tip. This is dubbed electronic-sample sharpening and a schematic is shown in Fig 3. These diagrams show the tip imaging the surface under two different biasing conditions. At the lower bias, the width of the trench is increased, allowing the tip to image the structure of the trench which is a full monolayer (0.28 nm) below the surface. It is interesting to observe that the spatial distribution of the tunneling current is wide enough to jump from one side of the trench to the other when the width is 0.42 nm and not wide enough when the trench width is 0.72 nm.

Advances in surface preparation, microscope/tip fabrication and first principles theory have greatly enhanced our ability to quantify surface atomic structure. In addition, this combination helped uncover a new imaging mechanism which provides insight into the fundamentals of STM. Furthermore, it allowed the uncovering of the atomic structure of the technologically important GaAs(001) surface and provided insight into the spatial distribution of the tunneling current. This work was supported in part by the Office of Naval Research Grant No. N00014-97-1-1058 and the National Science Foundation Grant No. DMR-9733994.

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