

New Structural Model of the Si(112) 6×1 -Ga Interface

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Abstract. The current structural model of the Si(112) 6×1 -Ga surface can be described as a self-assembled array of atomic wires. The structure of this surface is investigated using scanning tunneling microscopy, Rutherford backscattering spectroscopy, and density functional theory. It is concluded that the current model is incorrect, and a new model is proposed. In this model, the surface is semiconducting, in contrast to the currently predicted metallic wire array.

INTRODUCTION

Research has shown that upon Ga deposition on pristine Si(112) and subsequent annealing, the surface returns from a faceted surface to its basal (112) orientation [1, 2, 3]. Large anisotropic islands exist on the surface which consist of double-width (111)-like terraces and single (111)-like steps. According to the existing structural model of this reconstructed surface, the Ga atoms adsorb at the step edges within each bulk terminated unit cell and thus form atomic chains running in the $[1\bar{1}0]$ direction [4, 1, 2, 3]. Due to a complex interplay of stresses in the surface reconstruction, vacancies in the Ga atomic chains line up into quasi-periodical vacancy lines resulting in the 6×1 unit cell of the surface reconstruction [2, 3].

Due to the predicted existence of rows of Si atoms with partially filled dangling bonds, the Si(112) 6×1 -Ga surface reconstruction has been described as a surface array of parallel quantum wires [5]. In the present work we investigate this surface by Scanning Tunneling Microscopy (STM), Rutherford Backscattering Spectroscopy (RBS), and Density Functional Theory (DFT). We *disprove* the existing structural model. A new structural model is proposed, with a semiconducting surface instead of the predicted (quasi one-dimensional) metallicity [5].

EXPERIMENTAL

Experiments were carried out in an ultra-high vacuum system (base pressure $< 5 \times 10^{-11}$ mbar) with a Ga deposition source, direct current sample heating facilities and an Omicron variable temperature STM. A Si(112) wafer (orientation $\pm 2^\circ$ of the nominal (112) orientation) was cut into (10×2) -mm² samples and rinsed in acetone and isopropanol. After introduction into UHV the samples were degassed at 500° C overnight and subsequently the sample temperature was slowly raised to 750° C and kept there for 4 hrs. Next, the sample was flashed at 1200° C to remove the native oxide. During resistive heating, the current was directed parallel to the nano-facets of the clean (112) surface (*i.e.* in the $[1\bar{1}0]$ direction) in order to avoid current-induced step bunching. Ga was deposited using a commercial effusion cell with the Si substrate held at room temperature. After Ga deposition the sample was annealed at about $500 \pm 50^\circ$ C. The pressure remained below 2×10^{-10} mbar during sample preparation. STM experiments were performed at room temperature using etched tungsten tips. STM images of the filled and empty electronic states were obtained with a constant current between 0.06 and 0.1 nA and bias voltages between 1 and 2 V.

At the AMOLF institute RBS experiments to determine the amount of Ga atoms per unit cell on the surface were carried out at normal incidence and at a backscattering angle of 165° using a 2.0 MeV He⁺ ion beam of a Van de Graaf accelerator. The beam current was typically about 20 nA.

We have also analyzed theoretically the atomic and electronic structure of several structural models corresponding to Ga-coverages ranging from 5 to 12 Ga atoms per 6×1 unit cell. For this purpose we have used an efficient local-orbital (DFT) technique [6].

Using our first-principles hamiltonian of the surface system, we calculated theoretical STM images of these structures using the DFT local-orbital hamiltonian of the surface together with a non-equilibrium Keldish Green function approach [7] and compared these with the experimental results.

RESULTS AND DISCUSSION

Figure 1 shows a high resolution empty state STM image on a flat terrace of the Si(112) 6×1 -Ga surface. In contrast to the images of Baski *et al.* [2] this image shows *two* parallel rows of atoms per unit cell, intersected by the vacancy lines. The periodicity of the surface structure in the direction perpendicular to the rows of atoms (9.4 Å) is equal to the periodicity of the bulk truncated Si(112) surface. The atomic rows in the unit cell consist of 4 or 5 atoms, which results in 5×1 or 6×1 unit cells, in agreement with the findings of Baski *et al.* [1, 2]. Note that these images evolve towards the experimental STM images of Baski *et al.* when the lower atomic rows disappear from view due to a change of resolution.

According to the current structural model [4, 2, 5], the highest row should be the row of Ga atoms adsorbed at the stepedge in the bulk terminated unit cell, and the lowest row of atoms can only be designated to the row of Si atoms with the partially filled dangling bonds. To our knowledge, this is the first observation of this second line of

atoms. According to Refs. [4, 2], these lines of Si atoms should be continuous in the [110] direction (*i.e.* parallel to the high row of Ga atoms), and the vacancy line should have a mirror symmetry plane running exactly through the middle of the vacancy line, see Fig. 3 in Ref. [5] and Fig. 2 in Ref. [2]. However, the lines of Si atoms are not continuous inside the quasi-periodic vacancy lines; *i.e.* there exists a vacancy also in this row of atoms (see Fig. 1). Due to the zig-zag arrangement of the atoms in the two chains of atoms, this leads to an asymmetry in the vacancy line (*cf.* the right inset of Fig. 1). This is in clear contrast with the symmetric structural model, which therefore needs to be reconsidered.

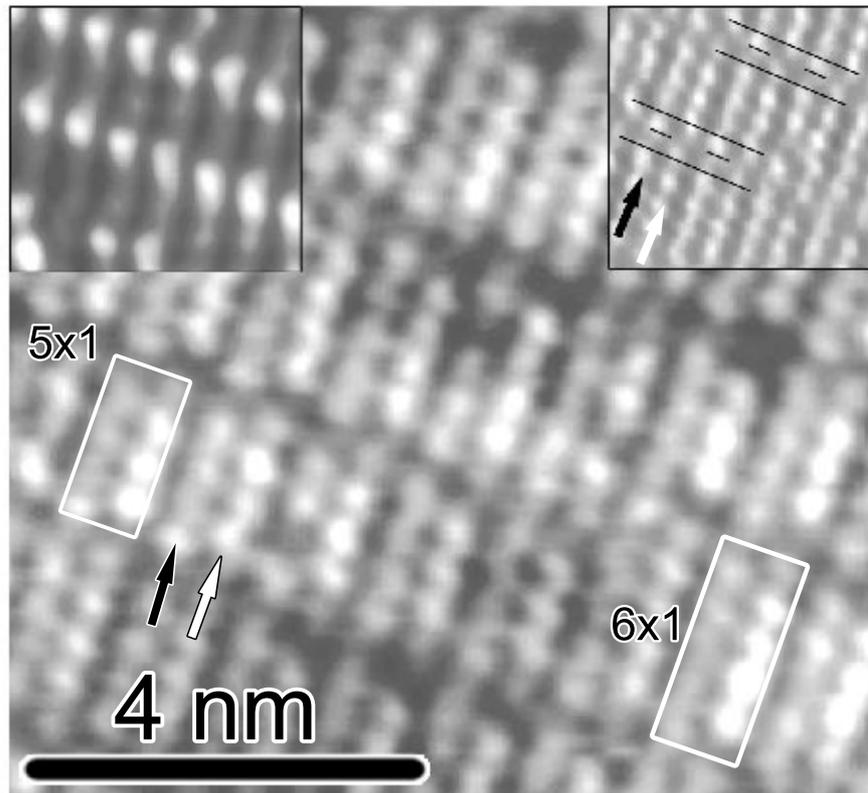


FIGURE 1. Atomic resolution empty state image of the Si(112) 6×1 -Ga surface ($V_{\text{sample}} = +2$ V, $I = 70$ pA). 5×1 and 6×1 unit cells are indicated. Two parallel chains of atoms are observed per unit cell: one chain appears slightly higher (white arrow) than the other (black arrow). The right inset (filtered) shows the asymmetry in the vacancy lines, which are defined by the black lines running through the last atoms neighbouring the vacancy line. The left inset shows a filled state image ($V_{\text{sample}} = -2$ V, $I = 100$ pA). Higher intensity blobs are visible in the vacancy lines.

RBS measurements of the amount of Ga on the surface were performed *ex situ*. From the amount of backscattered ions and the size of the 6×1 unit cell (*i.e.* $9.407 \times 23.042 \text{ \AA}^2$) an amount of 9 ± 1 Ga atoms per 6×1 unit cell is determined. This is significantly higher than 5 Ga atoms per 6×1 unit cell in the current structural model, confirming that indeed this model is incorrect.

Using these experimental results, several candidate structural models for this surface were analyzed using a local-orbital DFT code to obtain the relaxed atomic geometry and

corresponding electronic structure. Fig. 2 shows the two most stable structures found in these calculations. A full row of 6 Ga atoms would result in large stress due to the unequal covalent radii of Ga and Si. To relieve this strain, approximately every 6th Ga atom is missing. These Ga vacancies can be filled with two basic 'building blocks'; either a (smaller) Si atom fills the empty Ga spot, or two Si atoms rebond to form a Si dimer leaving a 'real' Ga vacancy. The two most stable structures are very close in total energy. Both contain two rows of 5 Ga atoms (brown) adding up to 10 Ga atoms per 6×1 unit cell, consistent with the RBS results. One structure contains a dimer in each Ga row (model A) and the other contains a dimer in the Ga row at the step-edge and a Si replacement in the other Ga row (model B). As discussed in Refs. [3, 2], this local structure develops into a long range ordered 6×1 periodicity due to a complex interplay of surface stresses which lines up these vacancies in quasi periodical vacancy lines.

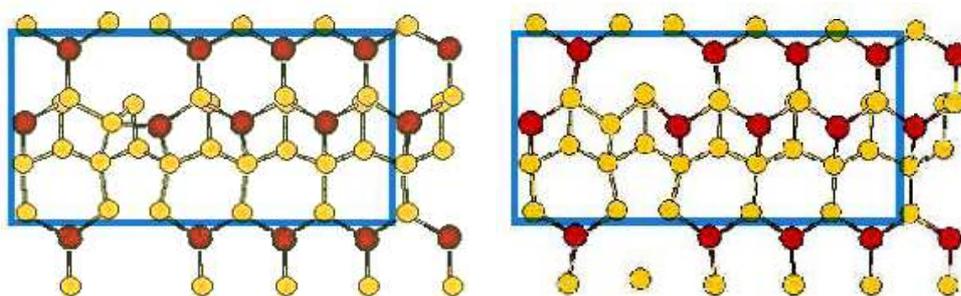


FIGURE 2. Topview of two candidate new structural models. Ga (brown) and Si (yellow) atoms form a 6×1 reconstruction (unit cell indicated in blue). Left: model A, right: model B.

The simulated empty state STM images, calculated from these structural models are shown in Fig. 3. These images both are reasonably consistent with the experimental images, and show the required asymmetry in the vacancy line (cf. Fig. 1). In both models, all Si dangling bonds are saturated as a consequence of the higher Ga coverage, resulting in a semiconducting surface. Therefore, this surface cannot be described as an array of metallic quantum wires.

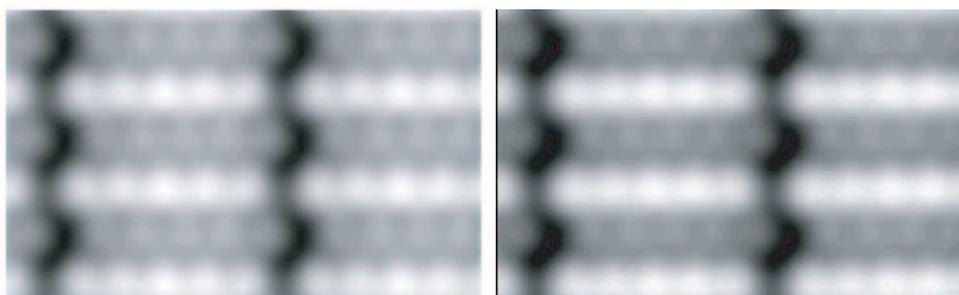


FIGURE 3. Simulated empty state STM images. Left: model A, right: model B.

CONCLUSION

A new structural model for the Si(112) 6×1 -Ga surface has been devised. It turns out that the higher Ga coverage on this surface (as compared to the previous model) saturates all Si dangling bonds, leaving the surface a semiconductor.

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