The equilibrium geometry and electronic structure of Bi nanolines on clean and hydrogenated Si(001) surfaces

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Abstract

The equilibrium geometry, electronic structure and the energetic stability of Bi nanolines on clean and hydrogenated Si(001) surfaces have been examined by means of \textit{ab initio} total energy calculations and scanning tunneling microscopy. For the Bi nanolines on a clean Si surface the two most plausible structural models, the Miki or \textit{M} model [Phys. Rev. B \textbf{59}, 14868 (1999)] and the Haiku or \textit{H} model [Phys. Rev. Lett. \textbf{88}, 226104 (2002)], have been examined in detail. The results of the total energy calculations support the stability of the \textit{H} model over the \textit{M} model, in agreement with previous theoretical results. For Bi nanolines on the hydrogenated Si(001) surface, we find that an atomic configuration derived from the \textit{H} model is also more stable than an atomic configuration derived from the \textit{M} model. However, the energetically less stable (\textit{M}) model exhibits better agreement with experimental measurements for equilibrium geometry. The electronic structure of the \textit{H} and \textit{M} models are very similar. Both models exhibit a semiconducting character, with the highest occupied Bi-derived bands lying at \(\sim 0.5\) eV below the valence band maximum. Simulated and experimental STM images confirm that at a low negative bias the Bi–lines exhibit an “antiwire” property for both structural models.

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I. INTRODUCTION

The physical sciences have been moving towards the control of material’s composition and structure at the atomic/molecular level for several decades. In recent years the focus has moved from layer-resolved growth to the control of material structure in all three spatial directions and at length scales down to one nanometer. The control of structure at this length scale will lead to greater control of material properties. However, for a viable technology, new methodologies must be found for assembling large numbers of nano-structured systems on a practical timescale[1]. One way of achieving this goal is to utilize systems that can be assembled or organized in parallel. For systems assembled on surfaces, different terms in the surface free energy can be used to guide the parallel assembly process[2, 3]. On semiconductor surfaces, morphological instabilities that arise from either anisotropic strain fields[4] or growth kinetics[3], can also be used to break symmetry and create dots[5], huts[6, 7] or wires[8–10].

In this paper we shall describe a study of a relatively new nanoline phase (hereafter line) that forms when Bi is deposited onto Si(001) surfaces. This phase has received considerable attention because of its striking structural quality[11–19]. The lines are only 1.5 nm wide and can be grown with aspect ratios of over 350:1. They also have no measurable width dispersion and they can be grown to lengths of up to 500 nm, defect free, without kinks or breaks[11, 12, 14–16, 18, 19]. The conditions under which the lines form are quite unusual because Bi has to be deposited onto Si(001) above the Bi desorption temperature of 500 °C. Understanding the physical factors that govern the nucleation and growth of these lines could possibly lead to methods for fabricating other one dimensional stuctures on Si(001). Furthermore, the Bi–lines assemble into arrays on Si(001), that have aperiodic line spacing, and these arrays could be used to guide or to constrain the self-organization of other atomic or molecular species. The other species could possibly be constrained to lie either between the two parallel rows of Bi dimers, or between the Bi–lines on the Si(001)2×1 terraces.

In Fig. 1 a low magnification STM image of a Si(001) surface covered in Bi–lines is presented. The image covers an area of 1µm × 1µm. The bottom half of the image is dominated by one single terrace and in this terrace the Bi–lines run from top-left to bottom-right. In the upper half of the image there are a number of terraces displaced by single-height steps (a_0/4 = 1.36 Å where a_0 is the cubic lattice constant of Si). The spacing between the
lines is aperiodic and the orientation of the lines rotates by \(\pi/2\) in terraces displaced by a single-height step. The step-edge structure on the Bi–line surfaces is modified by the lines and the way the lines influence the step structure on the Si(001) surface has been described elsewhere [20, 21]. Because of the reasons cited above, the Bi–lines have been studied with: total energy calculations[17, 19, 22–25], the scanning tunneling microscope (STM)[11, 12, 14–16, 18, 19], x-ray photoelectron diffraction and low energy electron diffraction (LEED)[26]. It is known that they comprise two parallel rows of symmetric Bi dimers. Although a number of different models have been proposed for the Bi line structure, none of the structural models is fully consistent with all of the experimental findings.

Naitoh et al. [11, 12, 15, 16] constructed the first structural model of the line. Their model (\(N\) model) was based upon constant-current topographical images that were acquired with STM. They measured the separation of the two parallel Bi dimers rows to be \(\approx 3.8\ \text{Å}\) and their model was constructed to reproduce this separation. Miki et al. [14, 27] also acquired constant-current topographical images of the lines with STM and estimated the separation of the Bi dimer rows to be significantly larger and closer to \(\approx 6\ \text{Å}\). A missing dimer line was inserted between the Bi dimer rows to increase the separation of the rows[14, 27]. The equilibrium geometry proposed by Miki et al. (\(M\) model) was subsequently confirmed by x-ray photoelectron diffraction (XPD) experiments [26]. \textit{Ab initio} total energy calculations [17, 24] confirmed that the \(M\) model is energetically more favorable than the \(N\) model. Additionally, in Ref. [17] a new line geometry, the Haiku or \(H\) model, was proposed that was found to be even more stable than the \(M\) model. Comparisons of experimental constant-current topographical images and theoretical STM simulations, that used the atomic configuration of the \(H\) model and the Tersoff-Hamman approximation, were found to be in good agreement.

However, the results of recent XPD [26] and X-ray standing wave (XSW) experiments [28], do not provide support for the \(H\) model which, after all, is the minimum energy atomic geometry. Moreover, the \(H\) model, which is based on B-type steps on the As-terminated Ge(001) surface, requires a significant rearrangement of subsurface atoms. Although it is the minimum energy structure, it is possible that the energy barriers associated with bond breakage and atom rearrangement prohibit its formation at the relatively low growth temperatures that are used (< 600°C). Clearly some more work has to be done to resolve these issues.

If the Bi–line system is to be used as a template for assembling other line structures, it
is important to consider the effect of hydrogen passivation of the Si(001) surface since it is more reactive than the Bi-line. Thus, the electronic structure, energetic stability, and the equilibrium atomic geometry of the Bi-lines on the hydrogenated Si(001) surface are also important issues to be investigated.

In this paper, we present a combined theoretical and experimental investigation of the Bi-lines on both the Si(001) and the hydrogenated H/Si(001) surfaces. In the \textit{ab initio} theoretical calculations we have considered the two most plausible structural models ($M$ and $H$) that were introduced above for the Bi-lines. The energetic stability of the $H$ model for Bi-lines on Si(001) has been confirmed. Similarly, our total energy results indicate that the $H$ model is also the energetically most stable for the Bi-lines on the H/Si(001) substrate. The equilibrium geometry for both $M$ and $H$ models have been detailed and compared with the experimental findings. Finally the electronic structure of the Bi-lines has been investigated by means of STM simulations and electronic structure calculations. The experimental investigations have been carried out for negative biases (occupied states). STM images of the Bi-line surfaces are more difficult to acquire in positive bias (unoccupied states) for reasons that we have discussed in detail elsewhere [29]. The experimental and theoretical results have been analysed carefully to present a coherent picture of the electronic features of the Bi-line system.

II. THEORETICAL AND EXPERIMENTAL METHODS

The theoretical calculations were performed in the framework of the density functional theory, within the local density approximation (LDA) using the Ceperley-Alder correlation [30] as parameterized by Perdew and Zunger [31]. The electron-ion interaction was treated by using norm-conserving, \textit{ab initio}, fully separable pseudopotentials [32, 33]. The wave functions were expanded in a plane wave basis up to the kinetic energy cutoff of 12 Ry. This energy cutoff was found to be totally adequate for our studies: the total energy and the equilibrium atomic geometry were well converged within 0.1 eV/(2×8) cell and ±0.02 Å, respectively. To simulate the Bi-covered Si(001) surface we used a repeated slab method, with a supercell containing ten atomic layers of Si and a vacuum region equivalent to twice the cubic lattice constant. We modelled the system by considering a unit cell with 2×8 periodicity. In order to test convergence of results we also made calculations with a 2×12
surface unit cell. The Si dangling bonds at the other side of the slab were saturated by a layer of hydrogen atoms. The sampling of the surface Brillouin zone was performed using a set of 4 special $k$ points. A dipole correction method [34, 35] was employed to annul the effect of the spurious electrostatic field which arises due to the inequivalence of the two surfaces in the periodic slab geometry. To obtain the equilibrium geometry, atoms in the eight topmost layers were fully relaxed to within a force convergence criterion of 12 meV/Å.

Our experimental study was performed with a home-built beetle-type STM[36, 37] using a Pt-Ir tip sharpened by field emission. The Si(001) wafers (Virginia Semiconductor, Inc.) were n-type, phosphorus doped, with resistivities in the range 5.2-7.2 Ωcm and misorientation angle $|\theta| < 0.5^\circ$. They were diced into rectangular samples with a width of 6 mm and a length of 17 mm. Following an overnight degas, atomically ordered surfaces were prepared by resistively heating the samples to 1260 °C for 40 s while maintaining the chamber pressure below $2 \times 10^{-9}$ Torr, annealing at 1000 °C for 180 s, and then slowly cooling down the sample at a rate of 1 °C/sec. All sample temperatures were measured using an infrared pyrometer (Land Instruments International). Lines were created by depositing 0.5 - 4.5 ML of Bi on a clean silicon surface at a rate of about 0.07 ML/min in the desorption regime (T $> 500$ °C). The samples were subsequently annealed for an additional 10-40 minutes.

### III. RESULTS AND DISCUSSION

Figure 2(a) is a schematic representation of the $M$ line model. In this model, the Bi–lines are composed of two parallel rows of Bi dimers that lie along the [110] crystallographic direction, and they are separated by a missing dimer line. The lateral distance between the Bi dimers in the $M$ model is 6.62 Å. In the $H$ model, shown in Fig. 2(b), the Bi dimers also assume the role of the fundamental building block of the line structure and the Bi dimers are also separated by a missing dimer line. However, the distance between the Bi dimers is 6.32 Å, which is 0.29 Å smaller than the row separation in the $M$ model. Moreover, the $H$ model exhibits a missing dimer line adjacent to each Bi dimer, and the Si substrate below the line is reconstructed, forming fivefold and sevenfold Si rings.

In order to determine the most stable configuration for the Bi–lines on the clean Si(001) surface, we compared the total energies between these two models by using the following
expression:
\[ \Delta E = E[H] - \{ E[M] + 2\mu_{\text{Si}}^{\text{bulk}} \}. \]

Here \( E[H] \) (\( E[M] \)) represents the calculated total energy of the \( H \) model (\( M \) model), and \( \mu_{\text{Si}}^{\text{bulk}} \) is the chemical potential of Si bulk. In order to keep the same criterion for the total energy convergence, \( \mu_{\text{Si}}^{\text{bulk}} \) was calculated by using the same procedure as used for the surface (Bi–line) calculations. We find that the \( H \) model is energetically more favorable than the \( M \) model by 0.37 eV/dimer, which is in agreement with the recent theoretical result by Owen et al. [17]. We have verified the convergence of our calculated \( \Delta E \) with respect to: (i) energy cutoff for the plane wave expansion, (ii) number of special \( k \) points for the Brillouin zone sampling, and (iii) size of the surface unit cell. Our results are summarized in Table I.

We next considered the formation of Bi–lines on the hydrogenated Si(001) surface. The \( M \) and \( H \) nanoline models are shown in Figs. 3(a) and 3(b), respectively. As expected the Si dimers become symmetric due to the hydrogen adsorption, while the equilibrium geometries of the Bi–nanolines are slightly perturbed by the hydrogen adsorption. Comparing the total energies we find that the \( H \) model is energetically more stable than the \( M \) model. We calculated a total energy difference of 0.57 eV/dimer. Therefore, from the perspective of total energy, the \( H \) model is more stable on both the clean Si(001) surface and the H/Si(001) surface. The relative stability of the \( H \) model over the \( M \) model results from a better surface relaxation for the former model. Two prominent signatures of the difference in surface relaxation are: the vertical height between the top layer and the third layer Si atoms, and the lateral movement of Bi atoms towards the missing dimer in between.

Having established the energetic stability of the \( H \) model, we compared the equilibrium geometries of the \( M \) and \( H \) models with available experimental results. For both structural models, the Bi dimer bond length [3.10 Å (\( M \) model) and 3.07 Å (\( H \) model)] is in good agreement with the XRD result by Shimomura et al.[26]: 3.0 ±0.3 Å. Due to the formation of a missing dimer line between the Bi–lines, the first sublayer Si atoms are rebonded, forming Si dimers perpendicular to the Bi–lines. In the \( H \) model, the bond length of the first sublayer Si dimer, 2.48 Å, is slightly smaller than that obtained for the \( M \) model, 2.52 Å. As a consequence, the Bi dimers are shifted toward the central missing dimer line by 0.47 Å and 0.63 Å for the \( M \) and \( H \) models, respectively. Both results are in accordance with the XRD measurements by Shimomura et al, with better agreement for the \( H \) model. They find a lateral shift (toward the center of the line) of 0.7±0.3 Å. The same experimental group

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verified that the Bi dimers are higher than the Si dimer plane by $0.3 \pm 0.2$ Å. Further XSW measurements [28] indicate a vertical distance of $0.26$ Å for the Bi dimers, in agreement with the previous XRD results. For the $M$ model, we calculated a vertical distance of $0.65$ Å between the Bi dimers and the topmost Si dimer plane, which is in reasonable agreement with the experimental XRD results. In contrast, the same agreement has not been verified for the $H$ model: we find a vertical distance of $1.40$ Å between the Bi dimers and the topmost Si dimer plane. For the Bi–lines on the hydrogenated Si(001) surface, the vertical distance between the Bi dimers and the Si dimer plane is $0.55$ Å for the $M$ model, and $1.33$ Å for the $H$ model. Therefore, concerning the equilibrium atomic geometry, we can infer that the $M$ model, although energetically less stable than the $H$ model, exhibits better agreement with the recent XRD and XSW measurements [26, 28]. Experimental XRD and XSW studies of Bi–lines on the H/Si(001) surface would provide complementary information that may help to resolve some of these issues.

In Figs 4(a) and 4(b) we present the calculated density of states (DOS) in and around the silicon bulk fundamental band gap for the $M$ and the $H$ models, respectively. The DOS was calculated by considering the four special $k$ points used for the Brillouin zone sampling. In both diagrams, the zero energy was chosen to be coincident with the highest occupied $v1$ peak. In the energy range -1 eV to +2 eV, there is a great deal of similarity in the DOS for the two models, except that the $v4$ peak is shifted to a slightly lower energy for the $H$ model.

The electronic charge distribution of the $v1$ peak for the $M$ model is shown in Fig. 5(a) (along the Bi dimer) and 5(d) (along the nearest neighbor Si dimer). It is clear that the main contribution to the $v1$ peak comes from the up atom of the Si dimer [Fig. 5(d)]. The contribution from the Bi dimers is a factor of ten smaller. Similar electronic distribution has been verified for $v2$ (not shown). At $\approx 0.4$ eV below $v1$ the $v3$ peak is formed with almost equal contributions from the $\pi^*$ orbitals of the Bi dimers [Fig. 5(b)] and the $\pi$ orbitals from the Si dimers [5(e)]. On the other hand, for the $v4$ peak (lying at $\approx 0.58$ eV below $v1$) the major contribution comes from the Bi dimers [compare Figs. 5(c) and 5(f)].

Similar electronic charge distribution has been verified for the $H$ model in Fig. 6. The $v1$ and $v2$ peaks exhibit a very weak contribution from the Bi dimers, being mainly concentrated along the Si dimers. In contrast, the $v3$ peak, located at 0.5 eV below $v1$, has almost equal electronic contributions from the $\pi^*$ states of the $p$ orbitals of the Bi dimers [Fig. 6(b)],
and the π states of the Si dimers [Fig. 6(e)]. The peak $v_4$ lies at 0.78 eV below $v_1$, with the main electronic contribution from the π bonding states localized along the Bi dimers [Fig. 6(c)] and also a contribution from the σ-like orbitals of the Si dimers that is a factor of ten smaller [Fig. 6(f)]. These results, for both structural models, are in accordance with the experimentally verified quantum antiwire property of the Bi–lines on the Si(001) surface *viz*: (i) For low bias voltage, the STM image of the Bi–lines is darker than the Si dimer plane for tunneling current from electronic states near the fundamental band gap [38], and (ii) with increased bias voltage, the Bi–lines become brighter than the Si dimers. Based upon our calculated electronic structure, we find that for low bias voltages the tunneling electrons come from the $v_1$ and $v_2$ peaks which are mainly localized on the Si dimers, and for increased voltages the electronic contribution from $v_3$ and $v_4$ peaks becomes dominant. The electronic states responsible for these features are mainly localized along the Bi dimers, at approximately 1 eV below the valence band maximum at $v_1$.

For the Bi/Si(001) system the tail of the peak $v_1$ (centred 0 eV) is only marginally separated from the tail of the peak centred between 0.4-0.5 eV. Upon hydrogen passivation of the surface Si dangling bonds the peaks $v_1$ and $v_2$ (due largely to Si dimer atoms) are almost washed out. Similarly, the small peaks in the range 0.5–1 eV for the Bi/Si(001) (cf. Fig. 4) are also washed out when the Bi/H/Si(001) system is considered. Thus there opens a finite gap, which is roughly equal to the bulk Si band gap. For the $M$ model, Fig. 7(a), we find a DOS peak ($v_3$) at -0.4 eV within the valence band. The electronic distribution of this peak is depicted in in Fig. 8(a), where the main contribution comes from the π* states of the Bi dimers. Similarly, Fig. 7(b) exhibits the DOS diagram for the $H$ model. We find a DOS peak ($v_4$) lying at -0.5 eV within the valence band. The π hybridization of $v_4$ along the Bi dimer is shown in Fig. 8(c), with small contribution from the passivated Si dimers in Fig. 8(d). We will find these results for the electronic structure of the Bi–lines on Si(001) and H/Si(001) substrates useful in analyzing the STM constant-current topographical images presented below.

By using the Tersoff–Hamann approximation [39], we simulated the STM images of the occupied states for the Bi–lines on the Si(001) and H/Si(001) substrates. We have considered three energy intervals below $v_1$: 0.20, 0.75 and 1.7 eV. For the energy interval of 0.2 eV the greatest contributions come from the electronic states of $v_1$ and $v_2$ peaks, indicated in Fig. 4. Within this small energy interval the simulated STM images for the $M$ and $H$ models, shown...
in Figs. 9(a) and 10(a), respectively, clearly show that the Si dimers are brighter than the Bi–lines for both Si(001) and H/Si(001) substrates. However, this feature is more evident for the H model. Increasing the energy interval to 0.75 eV, the Bi–lines exhibit approximately the same brightness as the Si dimers (see Figs. 9(b) and 10(b)). Finally, for the energy interval of 1.7 eV below \( v \), the Bi–lines become brighter than the Si dimers (see Figs. 9(c) and 10(c)). The increase of the brightness along the Bi–lines, as a function of the energy interval below \( v \), is in agreement with the experimentally obtained STM images for the Bi–lines on the Si(001) substrate, shown in Fig. 11. In this diagram, the Bi–lines are darker than the Si dimer plane for an applied bias voltage of -1.5 V [Fig. 11(a)]. Increasing the bias voltage up to -1.75 V [Fig. 11(b)], the Bi–lines exhibit the same brightness compared with the Si dimers, and for bias voltage of -2.0 and -2.25 V, Figs. 11(c) and 11(d), respectively, the Bi–lines become brighter than the Si dimers. An in-depth discussion of the electronic origin of contrast reversal in bias-dependent STM images of the Bi–lines on the Si(001) substrate has been presented elsewhere [38].

Comparing the calculated and the experimentally obtained STM constant-current topographs, we can conclude the following:

(i) The inversion of the brightness (across the Bi–lines) occurs within an energy interval of \( \approx 1 \) eV in the experimentally obtained STM images, as well as in the theoretical simulations. Since the STM measures the local density of states, throughout the calculation of the averaged surface corrugation, we inferred the “electronic width” of the Bi–lines. The surface corrugation was obtained by computing the vertical height (i.e. vertical position of the “tip”) along the lines indicated in Fig. 9(c) or 10(c).

(ii) We find an “electronic width” of \( \approx 15 \) Å for both structural models, as shown in the shaded regions in Figs. 9(d) and 10(d). The experimental STM line profiles suggest that the line occupies 4 surface unit cells; \( 4a_\circ = 15.4 \) Å where \( a_\circ = a_c/\sqrt{2} = 3.84 \) Å and \( a_c \) is the lattice constant of Si (5.43 Å). However, it must be remembered that the tip composition is unknown in these experiments and this could introduce a systematic error to the width determination. For example, it is quite likely that there are Si atoms at the tip apex (\( sp^3 \) hybrid orbitals) and the Tersoff-Hamman approximation assumes that the tip wavefunctions involved in tunneling process have \( S \) symmetry.

(iii) We have also compared the lateral distance (\( d \)) between the two peaks that arise from the two parallel rows of Bi dimers. For the \( M \) model we find \( d \) equal to 6.6 Å, which is
in agreement with the calculated equilibrium distance between the Bi–lines: 6.62 Å in Fig. 2(a). Similarly, for the \( H \) model we find \( d = 6.4 \) Å, which also agrees with the calculated equilibrium distance between the Bi–lines (6.32 Å in Fig. 2(b)). The lateral separation extracted from the STM line profile (Fig. 12) is \( (6.2 \pm 0.5) \) Å. Consequently, the calculated widths both lie within the range defined by the experimental value and the experimental uncertainty.

The simulated STM images for both models of the Bi–lines on the hydrogenated Si(001) surface are presented in Figs. 13(a) and 13(c), respectively. As expected, due to the hydrogen passivation of the Si dimers, the Bi–lines are brighter than the the Si dimers plane. The calculated surface corrugations are shown in Figs. 13(b) and 13(d), where we find an “electronic width” of \( \approx 15 \) Å for \( M \) and \( H \) models, respectively. For the lateral distance \( d \), we find 6.63 Å and 6.24 Å for the \( M \) and \( H \) models, respectively.

IV. CONCLUSIONS

Using \textit{ab initio} calculations, we have examined the two most plausible atomic arrangements for Bi–lines structures on clean Si(001) and H/Si(001) surfaces. The total energy results indicate that the Haiku geometry (\( H \) model) is more stable than the Miki geometry (\( M \) model) for both clean and hydrogenated Si(001) substrates. However, the equilibrium atomic geometry of the \( M \) model is in better agreement with recent x-ray measurements. Further structural investigations of the Bi–lines on the H/Si(001) surface may lead to a conclusive determination of the line structure.

The electronic structure of the two systems is quite similar. For the Bi–line system on Si(001), the highest occupied states lie mainly along the topmost Si-dimers on the \( 2 \times 1 \) terraces, while the electronic states originating from the Bi–dimers are located between 0.5 and 0.8 eV below the valence band maximum. For the Bi–lines on H/Si(001), the highest occupied states that are attributed to the Si dangling bonds are suppressed due to the hydrogen passivation. In this case, the Bi-derived states, along the Bi–lines, are positioned between 0.4 and 0.5 eV below the valence band maximum.

The simulated STM images of the Bi–lines on Si(001) for both structural models reproduce the main features of the experimental constant-current STM images. For example, the “antiwire” property of the Bi–lines at low negative bias has been confirmed and the
calculated width of the Bi dimer rows is in excellent agreement with the STM value for both structure models.

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TABLE I: Total energy difference, $\Delta E$ (in eV/dimer), as a function of the (i) energy cutoff for the plane wave expansion, (ii) number of special $k$ points for the Brillouin zone sampling, and (iii) size of the surface unit cell: $2 \times n$.

<table>
<thead>
<tr>
<th>$2 \times n$</th>
<th>8 Ry/2-$k$</th>
<th>8 Ry/4-$k$</th>
<th>12 Ry/2-$k$</th>
<th>12 Ry/4-$k$</th>
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<tr>
<td>$2 \times 8$</td>
<td>$-0.38$</td>
<td>$-0.39$</td>
<td>$-0.36$</td>
<td>$-0.37$</td>
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<tr>
<td>$2 \times 12$</td>
<td>$-0.36$</td>
<td>–</td>
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FIG. 1: Large-area image of Si(001) ($\approx 1 \mu m \times 1 \mu m$) acquired at $V_{\text{sample}} = -2.25$ V (occupied states) showing long Bi-lines self-organizing in aperiodic line arrays. This image contains terraces that are displaced by single-height steps (1.36 Å). The line orientation on neighboring terraces rotates by $\pi/2$, mirroring the rotation of the Si surface dimers.
FIG. 2: Atomic structure of the Bi–lines on the Si(001) surface. (a) Miki (M) model and (b) Haiku (H) model. The positions are in Å. The light gray (black) circles represents the Si (Bi) atoms. In the Top view only the topmost Si and Bi atoms are represented by solid lines.
FIG. 3: Atomic structure of the Bi–lines on the hydrogenated Si(001) surface. (a) M model and (b) H model. The positions are in Å. The light gray (black) circles represents the Si (Bi) atoms. In the Top view only the topmost Si, H and Bi atoms are represented by solid lines.
FIG. 4: Calculated density of states for the Bi–lines on the Si(001) surface: (a) $M$ model, and (b) $H$ model. The labeling scheme ($v1 - v4$) is explained in the text.

FIG. 5: Electronic distribution of the $v1$, $v3$ and $v4$ states (indicated in Fig. 4) for the $M$ model, along the Bi dimers (a)–(c) and Si dimers (d)–(f): $v1$ (a) and (d), $v3$ (b) and (e)$v4$ (c) and (f). Units, $e/\text{bohr}^3$. 
FIG. 6: Electronic distribution of the $v1$, $v3$ and $v4$ states (indicated in Fig. 4) for the $H$ model, along the Bi dimers (a)–(c) and Si dimers (d)–(f): $v1$ (a) and (d), $v3$ (b) and (e), $v4$ (c) and (f). Units, $e/\text{bohr}^3$.

FIG. 7: Calculated density of states for the Bi–lines on the H/Si(001) surface: (a) $M$ model, and (b) $H$ model. The labeling scheme is explained in the text.
FIG. 8: Electronic distribution of $v_3$ for the $M$ model along the Bi dimers (a) and along the hydrogen passivated Si dimers (b). Similarly, the electronic distribution of $v_4$, for the $H$ model, along the Bi dimers (c) and hydrogenated Si dimers (d). Units: $e/\text{bohr}^3$. 
FIG. 9: Simulated constant current STM images of the occupied states, for the $M$ model considering three energy intervals within the valence band: 0.2 eV (a), 0.75 eV (b) and 1.7 eV (c). In (d) we present the vertical position of the “tip” along the (solid and dashed) lines in the simulated constant-current topographical image. The vertical and horizontal positions are given in Å.
FIG. 10: Simulated constant current STM images of the occupied states, for the $H$ model considering three energy intervals within the valence band: 0.2 eV (a), 0.75 eV (b) and 1.7 eV (c). In (d) we present the vertical position of the “tip” along the (solid and dashed) lines in the simulated constant-current topographical image. (c). The vertical and horizontal positions are given in Å.
FIG. 11: Sequentially acquired images in the same region showing the bias dependence of the apparent height of Bi–lines. The image area is 300 Å × 300 Å; sample biases are (a) -2.25 V, (b) -2.00 V, (c) -1.75 V and (d) -1.50 V. The arrowed lines in the images indicate the location for the line profiles presented beneath the images. The profiles clearly show a decrease in apparent line height with decreasing bias voltage magnitude.
FIG. 12: (a) STM constant-current image of a single line; approximate area 30 Å × 80 Å, bias voltage $V_{\text{sample}} = -2.09$ V. The dashed and solid lines indicate the position of the profiles showing topography between and on top of surface dimers, respectively. The profiles indicate that the Bi-line occupies 4 surface unit cells (shaded region); $4a_o = 15.4$ Å where $a_o = a_c/\sqrt{2} = 3.84$ Å and $a_c$ is the lattice constant of Si (5.43 Å). The $1\times$ periodicity of the unit cell is inferred from the region to the left that lies along a Si dimer row.
FIG. 13: Simulated STM images (a) and (c), and the vertica position of the “tip” (b) and (d), for the Bi–lines on hydrogenated Si(001) surface. The energy interval is equal to 1.7 eV below the ν1 (occupied states). M model (a)–(b), and H model (c)–(d). The vertical and horizontal positions are in Å.