The geometry of Bi nanolines on Si(001)

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Abstract

A study of the Bi nanoline geometry on Si(001) has been performed using a combination of an \textit{ab initio} theoretical technique and scanning tunnelling microscopy (STM). Our calculations demonstrate decisively that the recently proposed Haiku geometry is a lower energy configuration than any of the previously proposed line geometries. Furthermore, we have made comparisons between STM constant-current topographs of the lines and Tersoff-Haman STM simulations. Although Haiku and the Miki geometries both reproduce the main features of the constant-current topographs, the simulated STM images of the Miki geometry have a dark stripe between the dimer rows that does not correspond well with experiment.

\textit{Key words:} Silicon surface; Ab-initio calculations; nanolines; scanning tunneling microscopy; semiconductor hetero-epitaxy.  
PACS: 73.20.-r, 73.20.At, 73.21.Hb

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Bismuth has been found to exhibit two distinct structural patterns of adsorption on the Si(001) surface. When it is deposited onto a room temperature Si(001) surface and the surface is subsequently annealed at 350 °C, the Bi adsorbates form an ordered \((2 \times n)\) surface mesh where the value of \(n\) depends upon the duration of the annealing cycle \([1]\). The \(2 \times n\) superlattice period is produced by the formation of Bi-dimers and the \(n \times \) superlattice period arises from ordered rows of Bi-dimer vacancies that relieve strain in the Bi overlayer. By raising the substrate temperature above the Bi desorption temperature, the Bi atoms can be coerced into a self-organised nanoline (hereafter line) structure with a high degree of order. The lines are grown either by (1) depositing Bi onto a room temperature Si(001) surface and annealing it above the Bi desorption temperature \((T_d \approx 500 ^\circ C)\), or (2) by depositing Bi onto a surface that is maintained at a temperature that is above \(T_d\) \([2,3]\). This is an unusual growth methodology and the lines are of particular interest because of their high structural quality. Clearly understanding why line structures with a width of only 1.5 nm and lengths of up to 500 nm form on Si(001) will have important implications for patterning other line structures on semiconductor surfaces. Although the Bi lines are semiconducting and their electronic structure is very similar to that of the Si(001) surface, line structures like this may serve as interconnects in either nanoelectronic or spintronic devices if their electronic properties can be tailored. Consequently, these lines have been the subject of a number of careful experimental and theoretical studies and a detailed understanding of the line geometry and electronic structure is now emerging.

In this paper we present the results of a study of the Bi line geometry using a combination of an \textit{ab initio} theoretical technique and scanning tunnelling microscopy (STM). In order to examine the atomic geometry and electronic structure of a single line, \textit{ab initio} calculations were performed in the framework of the density functional theory, within the local density approximation (LDA) \([4]\). To simulate the Bi-covered Si(001) surface, a repeated slab method was used, with a supercell containing ten atomic layers of Si and a vacuum region equivalent to twice the cubic lattice constant. The electron-ion interaction was treated by using norm-conserving, \textit{ab initio}, fully separable pseudopotentials \([5]\). The wave functions were expanded in a plane wave basis up to the kinetic energy cutoff of 12 Ry (see Ref. \([6]\)).

Figure 1 shows an STM image, acquired at room temperature, with ten parallel Bi lines running from bottom-left to top-right. This surface was prepared by depositing \(\approx 2.0\) ML of Bi, over 30-minutes, onto a two-domain Si(001)\(2 \times 1\) surface that was maintained at temperature of 590 °C; the surface was subsequently annealed for an additional 30 minutes at the same temperature.

The building block of the line structure is a Bi-dimer. To date there have been three different proposals for the arrangement of the Bi dimers and the neighbouring Si dimers. Miki et al.\([3]\) interpreted their STM images in terms of two parallel Bi dimers in phase with the surrounding Si dimers, with a missing dimer row between them. On the other hand, Naitoh et al. \([2]\) suggested that the Bi lines are formed by two parallel and adjacent Bi dimers substituting for four Si dimers, with a missing dimer row next to each Bi dimer.
Previous calculations [6] suggest that the Miki model is energetically more favourable than the Naitoh model, by 0.45 eV/Bi-dimer. Another structural model, the Haiku structure, has recently been proposed by Owen et al.[7]. In the Haiku geometry the Bi dimers are separated by a missing Si dimer line, and the substrate is reconstructed to form five- and seven-membered rings of Si. The Bi line width for this structure is \( \approx 1.5 \) nm, equivalent to four unreconstructed substrate surface unit cells (1.536 nm). The structure of the Miki and the Haiku line geometries are shown in Fig. 2. Our calculations suggest that the Haiku model is energetically more stable than the Miki model by 0.37 eV/Bi-dimer.

Figure 3 shows a comparison of an STM image taken at a sample bias of -2.09 V with a simulation calculated using the Tersoff-Hamann method [8] at an energy that lies 1.5 eV below the valence band maximum. This energy is \((-1.72 \pm 0.06)\) eV below the calculated Fermi level position. We find that both the Miki and Haiku line geometries reproduce the main features of the experimental STM images extremely well. However, the simulated image of the Miki geometry has a dark stripe separating the Bi-dimer rows that is not observed experimentally.

The Bi line height, defined to be the height of the Bi atoms above the average position of the up and down Si-dimer atoms, is 1.35 Å for the Haiku geometry. For the Miki geometry this quantity is smaller and closer to 0.55 Å. The experimentally determined ‘apparent’ height (the STM is probing the local density of states and not simply the atomic position) is 1.2 Å. Although caution has to be exercised in comparing the theoretical and experimental linescans, it is intriguing that the line heights for the two theoretical models differ by more than a factor of 2 and the Haiku line height is much closer to the experimental estimate. Moreover, our experimental estimate of the line height is in good agreement with a published experimental linescan obtained from a H-terminated line surface [9]. A line height of 1.4 Å, that is close to our experimental value, can be extracted from this linescan.

A study of the Bi nanoline system using \textit{ab initio} calculations and STM has been described. Although, simulated STM images for both the Haiku and Miki line structures agree well experiment, the simulated image of the Miki geometry has a dark stripe separating the Bi-dimer rows that is not in accord with experiment. Our calculations suggest that the recently proposed Haiku structure is the most stable line structure and a comparison of line heights obtained from experiment and Tersoff-Haman simulations also favors the Haiku model.

Acknowledgements

This work is supported by EPSRC (UK), NSERC (Canada) and CNPq and FAPEMIG (Brazil).
References


Fig. 1. Ten Bi lines grown on Si(001). Bias voltage $V_{\text{sample}} = -2.47$ V (full states). Image size $47$ nm $\times$ $47$ nm.
Fig. 2. The line models considered in the text: (a) The Miki ad-dimer model comprises two parallel Bi-dimers separated by a missing dimer line. (b) The Haiku model.
Fig. 3. Simulated STM images, calculated for a bias of $V_{\text{sample}} = -1.72$ V (full states), and the corresponding simulated linescans are shown for the Miki model in (a) and (b), and for the Haiku model in (c) and (d), respectively. (e) Filled state STM image of the Bi lines for a bias $V_{\text{sample}} = -2.09$ V and (f) the corresponding linescan.