Tunneling Images of Biatomic Steps on Si(001)

P. E. Wierenga,[a] J. A. Kubby, and J. E. Griffith
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
(Received 27 July 1987)

Tunneling images of vicinal Si(001) tilted 4° about the [1$\bar{1}$0] direction have been obtained. Straight double steps running along the [1$\bar{1}$0] direction, separated by terraces of relatively uniform width, dominate the topography of the surface. The structure of the biatomic steps is best described by a model that involves a rebonded geometry with buckling.

PACS numbers: 61.16.Di, 68.35.Bs

One of the most intriguing semiconductor surfaces, from both a scientific and a technological point of view, is vicinal Si(001). Scientifically, its propensity to form double steps is particularly interesting.[1-6] Two structural models have recently been proposed for the biatomic steps.[7,8] Aspnes and Ihm[7] explained the tendency for this surface to become primitive upon annealing with a π-bonded step reconstruction. They determined that the formation of a π-bonded chain along the step edge lowered the total energy per step atom by 0.04 eV relative to step edges that are not reconstructed. Moreover, the formation of other types of steps was found to be suppressed because of correlation, freezing out the step configurational entropy. Chadi[8] calculated the formation energies per unit length for different configurations of single- (S) and double- (D) layer steps where the dimerization axes on the upper terrace are perpendicular (subscript A) or parallel (subscript B) to the step edge. The energetically most favorable biatomic step configuration was found for a D_B type of step, where the atoms forming the lower step edge are rebonded. This type of double step essentially consists of the most closely spaced combination of single steps S_A and S_B. Because of the rebonding, however, its formation energy is lower than that of two regular single steps S_A and S_B.

Technologically, the tendency to form double steps has important implications for heteroepitaxy on Si(001).[9] In the growth of a zincblende crystal, such as GaAs, on silicon's diamond lattice, a monatomic step on the substrate causes disorder in the zincblende overlayer, whereas a biatomic step allows the growth of coherent Ga and As layers. The effects of the antiphase domains generated by single steps have recently been reviewed by Kroemer.[10] Until now, however, the discussion of the effects of steps has been limited by a lack of direct experimental information about their structure. We have obtained the first real-space images of biatomic steps on a vicinal Si(001) surface. The structure of the double steps has been determined with tunneling images that show transitions from a double-step edge to a single-step edge.

Our sample was boron-doped 0.025-Ω-cm vicinal Si(001), cut 4° ± 15′ from the (001) plane about the [1$\bar{1}$0] direction. The tunneling tip employed was an etched tungsten wire. To obtain a clean surface, the sample was argon-ion sputtered and then annealed at 875 °C for a few minutes in a UHV chamber with a base pressure of 5×10^{-11} Torr. Bright 2×1 and faint 1×2 diffraction spots were observed by LEED. Spot splitting in the 2×1 pattern indicated the presence of regularly spaced steps in the [1$\bar{1}$0] direction.

Figure 1 shows a tunneling image of the vicinal Si(001) surface in a perspective view. The image is displayed as a curvature-keyed gray-scale plot: white areas correspond to regions of high downward curvature ("hills"), and dark areas correspond to regions of high upward curvature ("holes"). Four type-B double steps can be seen running straight along the [1$\bar{1}$0] direction. The adjacent terraces are clearly reconstructed. Aside from some defects, regions of local (2×1), $c(4\times2)$, and $p(2\times2)$ symmetry are present with the dimer rows running along the [110] direction, perpendicular to the step edges. Similar surface reconstructions have been ob-

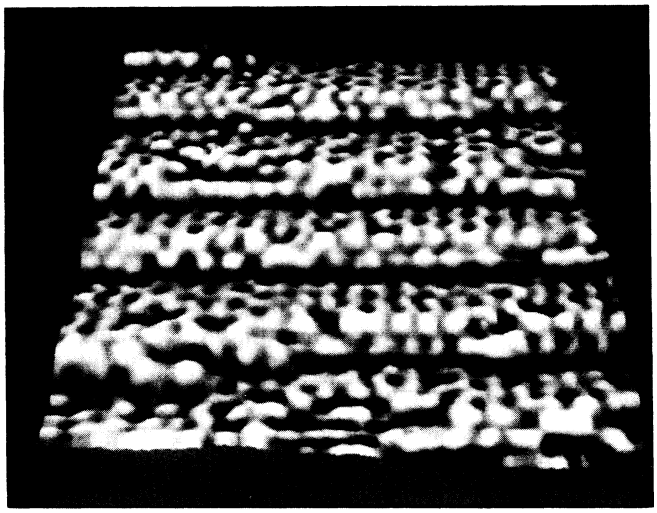


FIG. 1. Tunneling image of biatomic steps on the vicinal Si(001) surface. The image shows a 150×150-Å^2 area and was obtained with a demanded tunneling current of 0.1 nA and a tip bias of 2.0 V, tunneling from sample to tip.

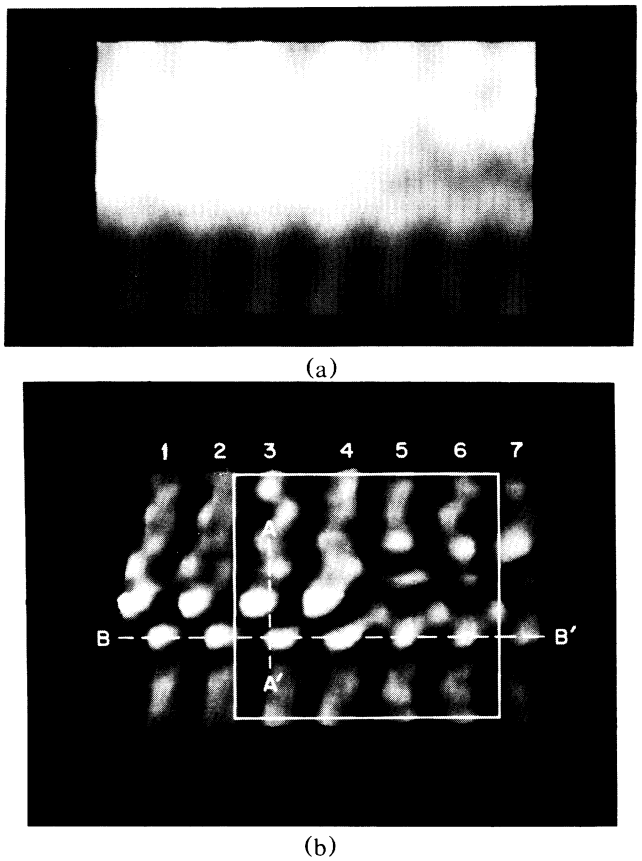


FIG. 2. Tunneling image of a step edge on vicinal Si(001) showing a transition from a double step (rows 1 to 4) to a pair of single steps (rows 5 to 7), in (a) height and (b) curvature mapping. This image was obtained with a demanded tunneling current of 1 nA and a tip bias of 1.2 V, tunneling from sample to tip. The z scale was expanded by a factor of 5.

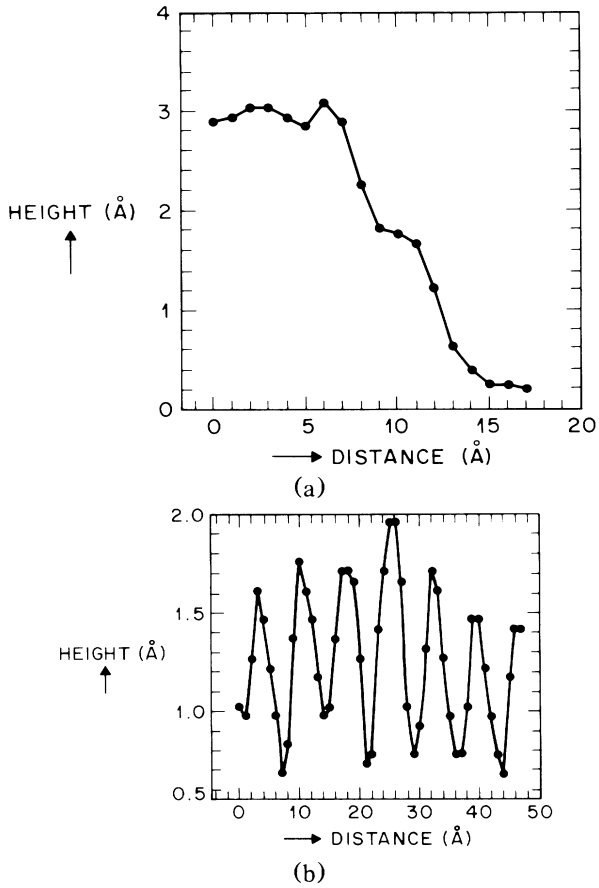
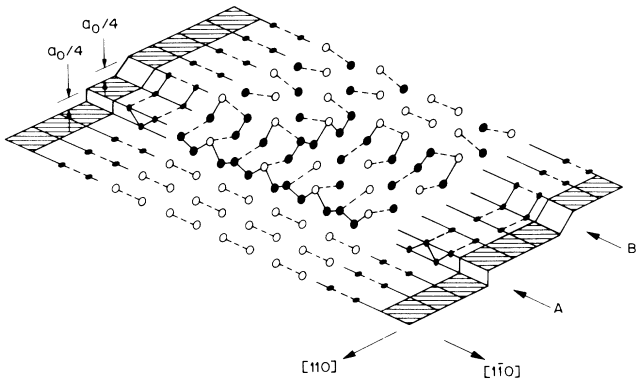


FIG. 3. Sectional cuts along lines (a) AA' and (b) BB' of Fig. 2(b).

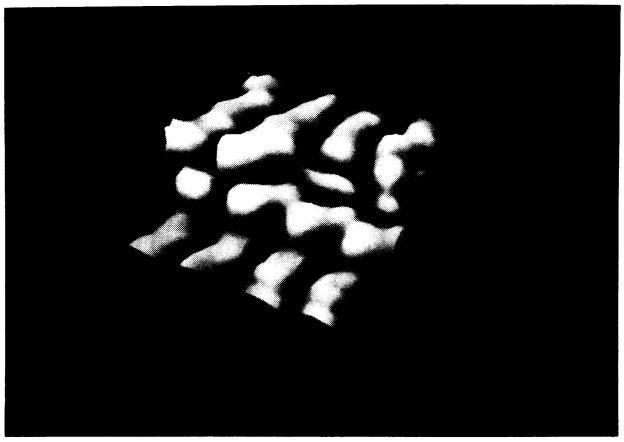
served with the tunneling microscope on nonvicinal Si(001)[11] and Ge(001).[12] Since the wafers were not perfectly flat, the terrace widths varied, and in many areas the double steps had kinks in them. At those kinks, the steps usually split into single steps to avoid forming a type-D_A segment, which Chadi found to have high energy.[8]

Figure 2 shows tunneling images of a step edge on the vicinal Si(001) surface in a plan view. The upper image [Fig. 2(a)] is a height mapping; the lower image [Fig. 2(b)] is a curvature-keyed gray-tone plot of the same area. In both pictures surface protrusions are white, whereas depressions are black. The tip bias was +1.2 V relative to the sample tunneling from sample to tip. Under this condition, the main contribution to the tunneling current originates from the π_b dimer bonds in case of a symmetric dimer[13] and from the almost filled dangling bonds localized on the upper atoms in case of a buckled asymmetric dimer.[11] In Fig. 2, rows 3, 4, and 5 of the upper terrace clearly show a zigzag pattern implying that they consist of asymmetric dimers. The other rows of the upper terrace as well as the rows of the lower terrace are apparently formed from symmetric dimers.

The images of Fig. 2 are particularly interesting since they show a transition from a double step D_B (rows 1 to 4) to a pair of single steps (rows 5 to 7) separated by a very small type-A terrace. Along the upper edge of the single step S_A, we clearly see a zigzag row of buckled dimers. The double-step area is characterized by two rows of bright dots. The dots along the upper step edge represent the "up" atoms of the first dimers on the upper terrace. This is illustrated by Fig. 3(a) which is a sectional cut along line AA' in Fig. 2(b). The upper terrace evidently extends up to about 7 Å on the relative distance scale given in Fig. 3(a). It can also be seen that the apparent height of the dots along the lower edge of the double step, positioned around 10 Å on the distance scale, is approximately half the total step height of about 2.7 Å. The lateral spacing of these dots is equal to approximately 7.6 Å, the spacing of the "up" atoms of the zigzag row along the edge of single step S_A. Moreover, there is no change in apparent height of the dots in going through the transition from double step D_B to single step



(a)



(b)

FIG. 4. (a) Model representation and (b) perspective view of the area surrounded by the box in Fig. 2(b).

S_A. This is shown in Fig. 3(b), which is a sectional cut along line BB' in Fig. 2(b).

Comparing our data to the π-bonded chain model of Aspnes and Ihm,[7] we must conclude that these are not in agreement. First, the apparent height of a π-bonded chain along the step edge is expected to be closer to the height of the upper terrace. Second, and even more important, the period of approximately 7.6 Å in the row of dots along the lower step edge is twice as long as expected for a tunneling image of a π-bonded chain.[14] The position of the dots along the lower step edge about midway between lower and upper terrace [Fig. 3(a)] is more consistent with Chadi's rebonded geometry.[8] In addition, this model predicts a smooth transition from a double-layer step D_B to a single-layer step S_A, in agreement with the tunneling images in Fig. 2. Again, however, the period in the lower row of bright dots along the edge is twice as long as expected from the model. This inconsistency can be removed by introduction of buckling in the rebonded row running along the step edge. This is visualized in Fig. 4(a), which is a model representation of the area surrounded by the box in Fig. 2(b). For comparison, the same area is displayed in Fig. 4(b) as a curvature-keyed gray-tone mapping in a perspective view. In Fig. 4(a), only the atoms in the outermost surface planes are shown. The equivalent geometric planes are also given. Dimer bonds are indicated by dashed lines. The bright dots in the tunneling images occur over the atoms denoted by open circles. Symmetric dimers are visualized by open circles at both sides of the dimer bond. Figures 4(a) and 4(b) show that the "up" atoms in the buckled row along the double-step edge are always opposite "down" atoms at the upper terrace. From a purely mechanical point of view, keeping bond lengths the same and allowing bond angles to change, this is the most logical configuration. It is interesting to note that the same type of rebonding is seen along the edge of single step S_B. This single-step configuration was also observed on nonvicinal Si(001) by Hamers, Tromp, and Demuth.[15]

Sectional cut BB' [Fig. 3(b)] suggests that the "up" atoms in the row along the double-step edge are not only geometrically equivalent to those in the zigzag dimer row along the upper edge of single step S_A, but also electronically. Tunneling images obtained at opposite polarity support this conclusion. These images show a more or less continuous band of empty sample states along line BB'. These observations are somewhat surprising because the edge atoms involved in the rebonded geometry originally had only one dangling bond instead of two. As a consequence, the bonds connecting these edge atoms with the "up" and "down" atoms in the buckled row along the double-step edge are not real dimer bonds.

As an alternative, one might think of adatom structures to explain the data in the double-step region. Apart from the fact that such configurations seem to be energetically unfavorable, they are not in agreement with tunneling images obtained at opposite bias voltages showing a continuous band of empty states along the step edge.

In conclusion, we have obtained high-resolution tunneling images of biatomic steps on vicinal Si(001). The images are inconsistent with a π-bonded chain reconstruction of the step riser as proposed by Aspnes and Ihm. Observation of the transition from a single type-A step to a double step suggests a *buckled* rebonded geometry for the double step.

We are indebted to L. C. Feldman for bringing the biatomic step issue to our attention. We would like to thank R. S. Becker and M. S. Hybertsen for helpful discussions and we thank J. Bevk and J. P. Mannaerts for their generous assistance.

---

[a]On leave from Philips Research Laboratories, Eindhoven, The Netherlands.

[1]M. Henzler and J. Clabes, Jpn. J. Appl. Phys., Suppl. **2**, pt. 2, 389 (1974).

[2]R. Kaplan, Surf. Sci. **93**, 145 (1980).

[3]T. Sakamoto and G. Hashiguchi, Jpn. J. Appl. Phys. **25**, L78 (1986).

[4]D. Saloner, J. A. Martin, M. C. Tringides, D. E. Savage, C. E. Aumann, and M. G. Lagally, J. Appl. Phys. **61**, 2884 (1987).

[5]T. Nakayama, Y. Tanishiro, and K. Takayanagi, Jpn. J. Appl. Phys. **26**, L280 (1987).

[6]R. D. Bringans, R. I. G. Uhrberg, M. A. Olmstead, and R. Z. Bachrach, Phys. Rev. B **34**, 7447 (1986).

[7]D. E. Aspnes and J. Ihm, Phys. Rev. Lett. **57**, 3054 (1986).

[8]D. J. Chadi, to be published.

[9]K. Mizuguchi, N. Hayafuji, S. Ochi, T. Murotani, and K. Fujikawa, J. Cryst. Growth **77**, 509 (1986).

[10]H. Kroemer, in *Heteroepitaxy on Silicon,* edited by J. C. C. Fan and J. M. Poate, MRS Symposia Proceedings No. 67 (Materials Research Society, Pittsburgh, PA, 1986).

[11]R. J. Hamers, R. M. Tromp, and J. E. Demuth, Surf. Sci. **181**, 346 (1987).

[12]J. A. Kubby, J. E. Griffith, R. S. Becker, and J. S. Vickers, Phys. Rev. B **36**, 6079 (1987).

[13]J. A. Appelbaum, G. A. Baraff, and D. R. Hamann, Phys. Rev. B **14**, 588 (1976).

[14]R. M. Feenstra, W. A. Thompson, and A. P. Fein, Phys. Rev. Lett. **56**, 608 (1986); J. A. Stroscio, R. M. Feenstra, and A. P. Fein, J. Vac. Sci. Technol. A **5**, 838 (1987).

[15]R. J. Hamers, R. M. Tromp, and J. E. Demuth, Phys. Rev. B **34**, 5343 (1986).

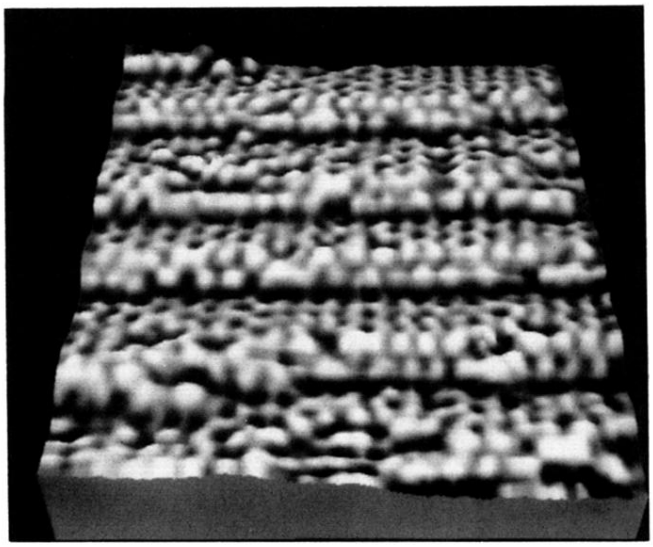
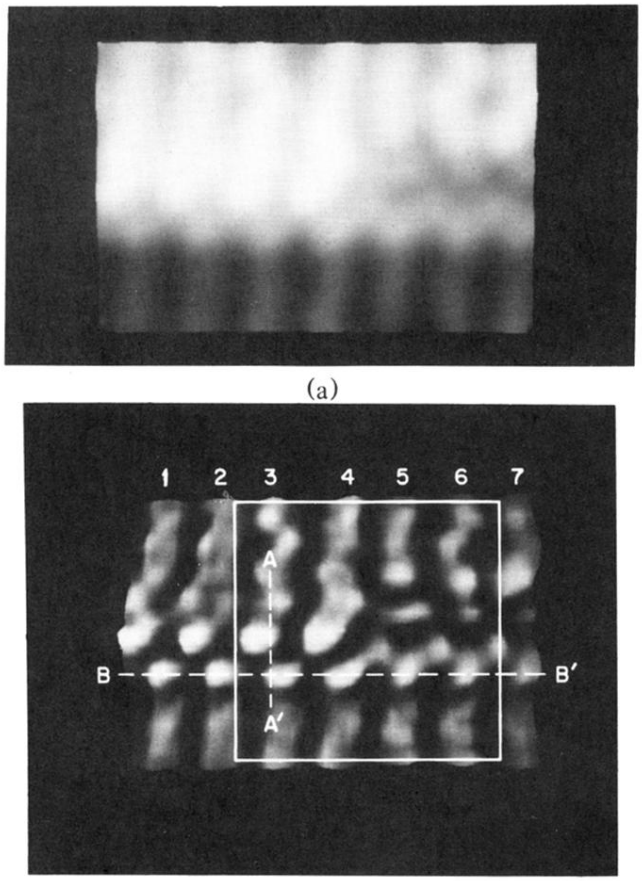


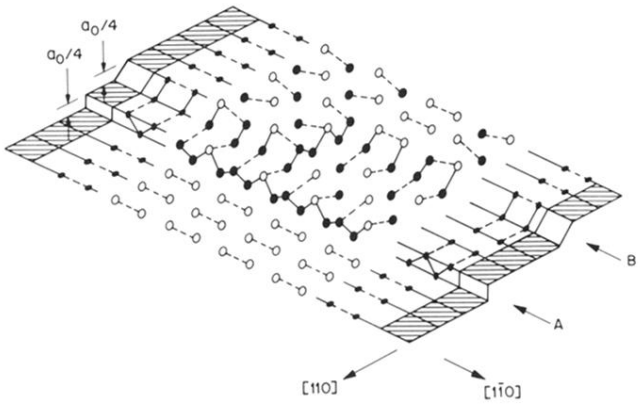
FIG. 1. Tunneling image of biatomic steps on the vicinal Si(001) surface. The image shows a 150×150-Å^2 area and was obtained with a demanded tunneling current of 0.1 nA and a tip bias of 2.0 V, tunneling from sample to tip.



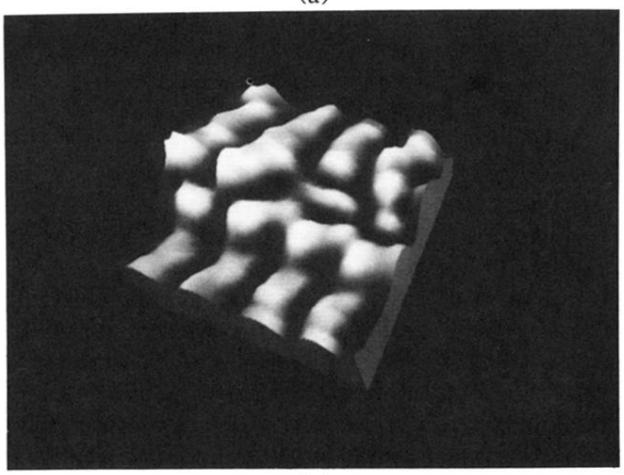
(a)

(b)

FIG. 2. Tunneling image of a step edge on vicinal Si(001) showing a transition from a double step (rows 1 to 4) to a pair of single steps (rows 5 to 7), in (a) height and (b) curvature mapping. This image was obtained with a demanded tunneling current of 1 nA and a tip bias of 1.2 V, tunneling from sample to tip. The z scale was expanded by a factor of 5.



(a)



(b)

FIG. 4. (a) Model representation and (b) perspective view of the area surrounded by the box in Fig. 2(b).