Scanning-tunneling-microscope observation of 2×1 structure on a homoepitaxially grown Si(111) surface

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We have used scanning tunneling microscopy to study molecular-beam epitaxial growth on Si(111)7×7 surface. On the homoepitaxially grown surface at 500 °C, we find the small domains of non-DAS (dimer adatom stacking fault) rowlike ordered structures, the periodic rows of which run along the $[01\bar{1}]$ and $[\bar{1}10]$ directions. The atomic configuration of these structures seems to be consistent with Pandey's π-bonded chain model for Si(111)2×1 structure. We discuss two kinds of π-bonded chains, and the boundaries along the atomic rows between the 2×1 and DAS domains.

It is well known that the cleaved Si(111) surface exhibits 2×1 structure, which is described by Pandey's π-bonded chain model.[1] After thermal annealing, this 2×1 structure changes irreversibly into the more stable 5×5 and 7×7 structures, which are explained by the dimer adatom stacking-fault (DAS) model proposed by Takayanagi *et al.*[2] The transition of Si(111)2×1 to 7×7 structure has been studied by scanning tunneling microscopy (STM).[3] Besides the cleavage on Si(111), small domains of 2×1 reconstructed structures have also been observed on sputtered, and subsequently thermally annealed and quenched surfaces,[4,5] as well as atomic hydrogen desorption from Si(111):H-1×1.[6] Concerning the origin of the formation of the quenched 2×1 structures, Becker, Klitsner, and Vickers suspected that a microcleave due to a thermal stress during the rapid cooling caused this 2×1 reconstruction.[4] Pashley, Haberern, and Friday concluded that if the cooling rate from the high-temperature 1×1 phase to the room-temperature phase is sufficiently high, the surface is unable to overcome the potential barrier to the formation of the stable 7×7 reconstruction. In this case, the most easily formed structure is the 2×1.[5]

In this paper, we report the STM observation of the small regions of non-DAS rowlike ordered structures on a homoepitaxially grown Si(111) surface. It is shown that the rowlike structures are consistent with Pandey's π-bonded model for Si(111)2×1 structure.[1] Moreover, we discuss two kinds of π-bonded chains, as well as the boundaries along the atomic rows between the 2×1 and DAS domains.

The experiment was performed in an ultrahigh-vacuum (UHV) chamber[7] with a base pressure of $<7\times10^{-9}$ Pa. The sample wafer was a B-doped Si(111) with the resistivity of 1.3–3.0 Ω cm, misoriented towards $[11\bar{2}]$ by 4°.[8] By using the molecular-beam-epitaxy (MBE) technique, silicon atoms were deposited, with the rate of about 0.3 monolayers (ML)/min (1 ML = 1.57×10^{15} atoms/cm^2), from a resistively heated Si bar, the size of which was about 0.5×1×5 mm^3. The distance between the Si bar and the sample was about 25 cm. The coverage was calibrated using a sensitive quartz-crystal monitor. The sample was heated by direct current, while the temperature was measured by an infrared pyrometer. In order to avoid an unexpected step flow, the current was made to pass through the sample in the $[\bar{1}10]$ direction, i.e., along the step edge's direction.

We prepared a sample surface as follows. The sample was carried into the UHV chamber, outgassed by heating up to about 700 °C for 20 h, and then flashed up to 1200 °C. After these heat treatments, the deposition was performed at 500 °C in UHV ($<2\times10^{-8}$ Pa), and then the sample was cooled down with an initial rate of 3 °C/s. STM images were obtained at room temperature in the constant-current mode with a tunneling current of 50 pA. We estimated the atomic distance of the 2×1 structure by comparing them with those of the 7×7 ones.

Figure 1 shows a STM image after deposition of 6.5

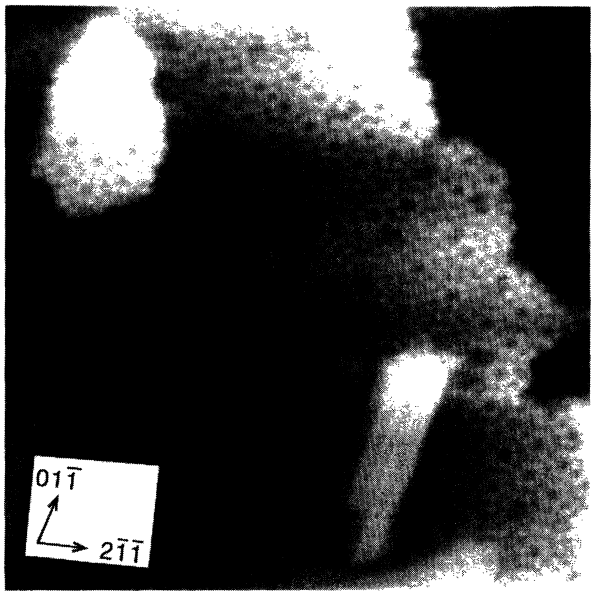


FIG. 1. STM images after deposition of 6.5 ML Si at 500 °C on Si(111) surface. The image extends over 380×380 Å^2, acquired at a sample voltage of +2.0 V. The 2×1 structure can be seen in the lower right-hand corner of the image, as the periodic rows running in the $[01\bar{1}]$ direction with an area of about 120×35 Å^2.

ML Si at 500 °C. A small domain of the non-DAS-ordered structure can be seen in the lower right-hand corner of the image. This structure has periodic atomic rows running in the $[01\bar{1}]$ direction with an area of about 120×35 Å^2. A similar structure is observed on the same sample, as shown in Fig. 2. The latter has periodic atomic rows running in the $[\bar{1}10]$ direction with an area of about 120×35 Å^2. Figure 3(a) is the magnified image of the non-DAS structure in Fig. 1. Cross-sectional cuts along k-k' and l-l' in Fig. 3(a) are shown in Fig. 3(b). From these, the lateral periodicity between the rows is estimated to be about 7.0 Å, while the peak-to-valley corrugation amplitude of the periodic rows is about 0.3 Å. These values are consistent with the prior STM results of the cleaved 2×1 structure[3,9,10] within an accuracy of a few percent. Thus the atomic configuration of the non-DAS structures seem to be that of the cleaved 2×1 structure, which is described by Pandey's π-bonded chain model.[1]

In Fig. 3(a), the two left chains run straight, whereas the two right chains do not. Namely, the latter two chains break their strings between k-k' and l-l'. The value of the larger spacing α, denoted by A in Fig. 3, is about 10.9 Å, compared with the previously measured value of 7.0 Å. By first-principles calculations, Takeuchi and co-workers found two differently tilted π-bonded structures for a Ge(111)2×1 surface, which they called "chain right" and "chain left" structures.[11,12] Based on their results, the larger spacing α is explained to be due to the difference between these two structures. Similar structure has also been reported by Feenstra, Thompson, and Fein on a cleaved Si(111) surface.[9]

From the cross-sectional cuts in Fig. 3(b), the 2×1 domains are about 1.8 Å higher than the nearby DAS structures. The boundaries between the higher (2×1) and the lower (DAS) domains are well ordered along the π-bonded chains of the 2×1 structures. The left boundary of the 2×1 structure has an extra atomic row between 2×1 and DAS domains, denoted by B in Fig. 3. In the opposite (right) boundary, this extra row of atoms is absent. The peak-to-peak height difference between the periodic rows of the 2×1 domain and the extra atomic

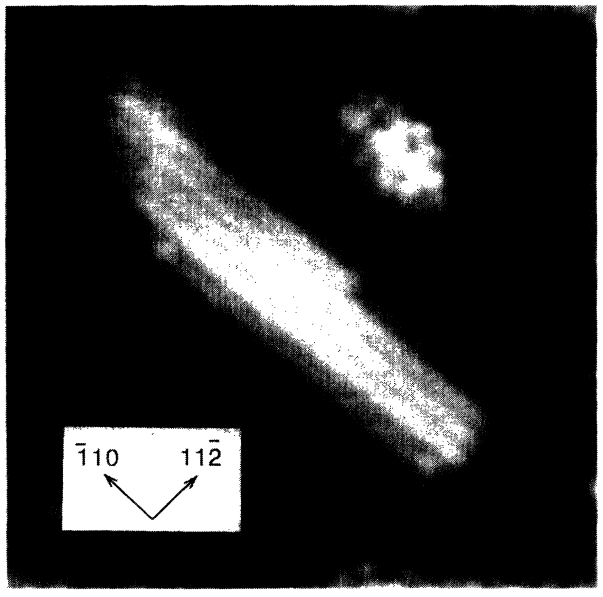
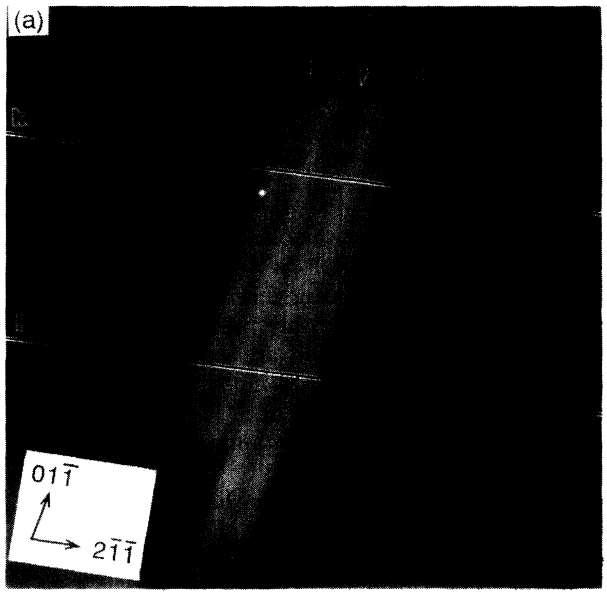


FIG. 2. STM image obtained from the same sample as Fig. 1. The image extends over 155×155 Å^2, acquired at a sample voltage of -2.0 V. The 2×1 structure has the periodic atomic rows running in the $[\bar{1}10]$ direction with an area of about 120×35 Å^2.



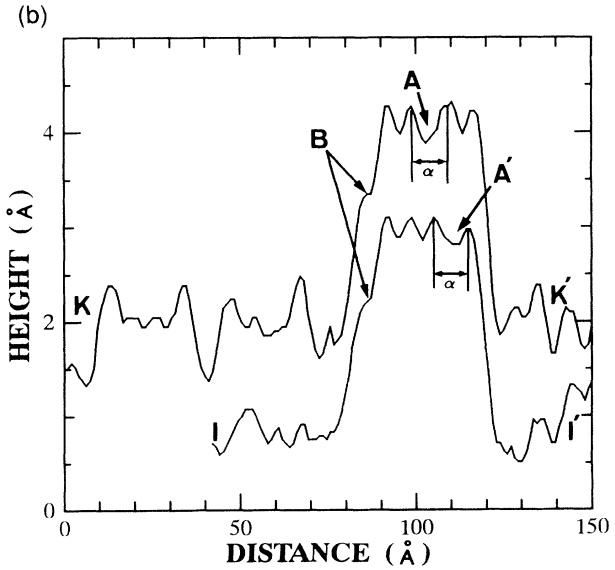


FIG. 3. Expanded image of the 2×1 structure in Fig. 1. (a) The STM image has an area of about 155×155 Å^2. Four π-bonded chains (denoted by 1, 2, 3, and 4), a larger lateral spacing of π-bonded chains (denoted by A), and an extra atomic row (denoted by B) can be seen in the image. The left two chains, denoted by 1 and 2, run straight, while the right two, denoted by 3 and 4, break their strings between k-k' and l-l'. (b) Cross-sectional cuts along k-k' and l-l' in (a). A and A′ denote the larger lateral spacing of the π-bonded chains, and B denotes an extra atomic row. The value of the larger lateral value α is about 10.9 Å, compared with the lateral periodicity of 7.0 Å.

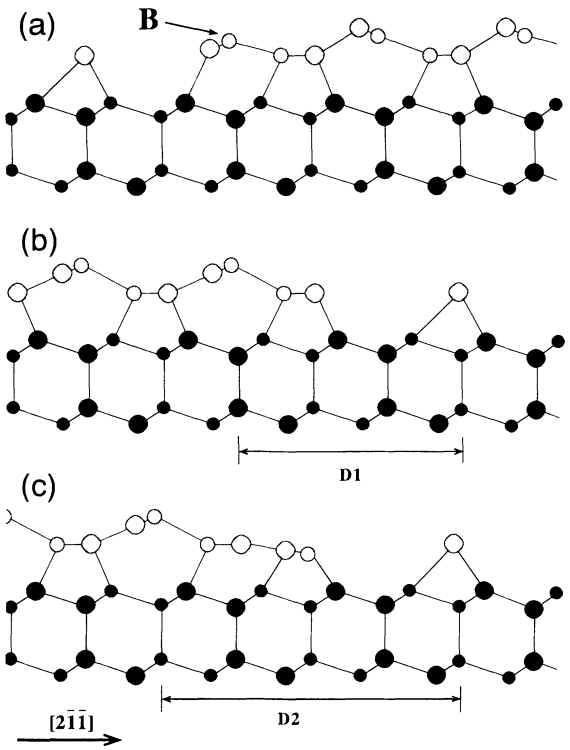


FIG. 4. Side view of models for the boundaries between the 2×1 and the DAS structures. (a) The left boundary between the π-bonded 2×1 and the DAS structures. B denotes the extra atomic row as shown in Fig. 3. (b) and (c) The right boundaries between the π-bonded 2×1 and the DAS structures. The value D1 and D2 of the distance between π-bonded chains and the nearest adatoms is $\frac{3}{2}$ double unit cells (9.98 Å) in (b), and 2 double unit cells (13.30 Å) in (c).

row is about 0.9 Å, while the lateral spacing is about 7.0 Å, which is equal to those of the periodic atomic rows for the 2×1 structure. On the right boundary, the distance between chains and the nearest adatoms is about 10.9 Å from the result of the cross-sectional cut k-k' in Fig. 3(b). On the cleaved Si(111)2×1 surface, Feenstra and Stroscio have found such an extra atomic row along the [2$\bar{1}\,\bar{1}$]-oriented steps.[13] They proposed three variants of Pandey's models[1] for the [2$\bar{1}\,\bar{1}$]-oriented steps. Based on them, we present similar models for the boundaries between the 2×1 and the DAS structures in Fig. 4. On the left boundary, a possible structure is depicted in Fig. 4(a), which should be compared with Fig. 5(a) in Ref. [13]. On the right boundary, there are two possible classes of atomic configurations, as shown in Figs. 4(b) and 4(c). The distance between chains and the nearest adatoms is about $\frac{3}{2}$ double unit cells (9.98 Å) in Fig. 4(b) and 2 double unit cells (13.30 Å) in Fig. 4(c). We measured the distance as 10.9 Å from the cross-sectional cut. Therefore we concluded the structure of the right boundary to be the model in Fig. 4(b).

From the results of our observations, we deduce the origin and the process of the formation of the structures as follows. As shown in Fig. 1, a 5×5 island exists near the 2×1 domain, and the 2×1 structure is reconstructed in the local area surrounded with many domain boundaries; the reconstruction of the 2×1 structures seems to concern the existence of these domain boundaries. The 2×1 structures take the shape of narrow phase boundaries along the direction of the periodic atomic rows. The effects of diffusion and desorption or reevaporation should be negligible at low temperature. Then, gathered atoms in the narrow area, bounded with distinct domains along the direction of the periodic atomic rows, may form narrow hills. At this time, however, the atomic configuration of the narrow area can no longer change into a DAS structure. Thereby, the 2×1 structure, which has been known to be metastable, may have become the most easily formed structure in this case.

In summary, we have used STM to study the homoepitaxially grown Si(111) surface. We found 2×1 structures, the periodic rows of which run along the [01$\bar{1}$] and the [$\bar{1}$10] directions. From the measured cross sections of the STM images, the 2×1 structures were found to be consistent with the π-bounded structure. In the [01$\bar{1}$]-directed 2×1 structure, we observed the broken chains, which were explained as being due to the difference between the "chain right" and "chain left" structures. Furthermore, based on the model in Ref. [13], we presented models for the boundaries between the π-bonded 2×1 and the DAS structures.

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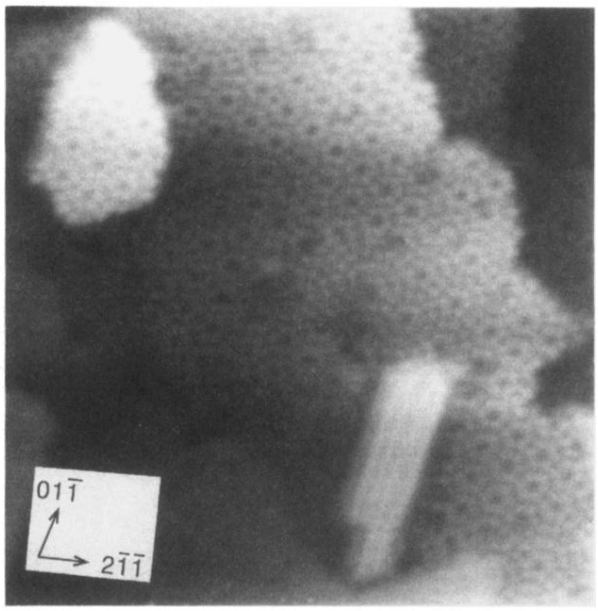

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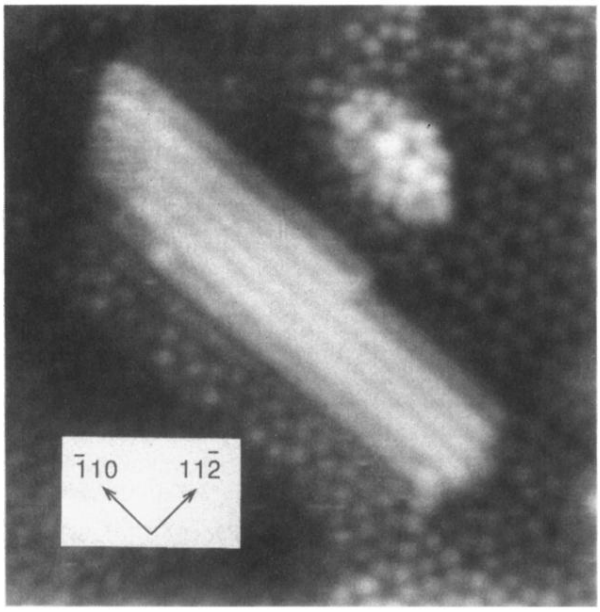

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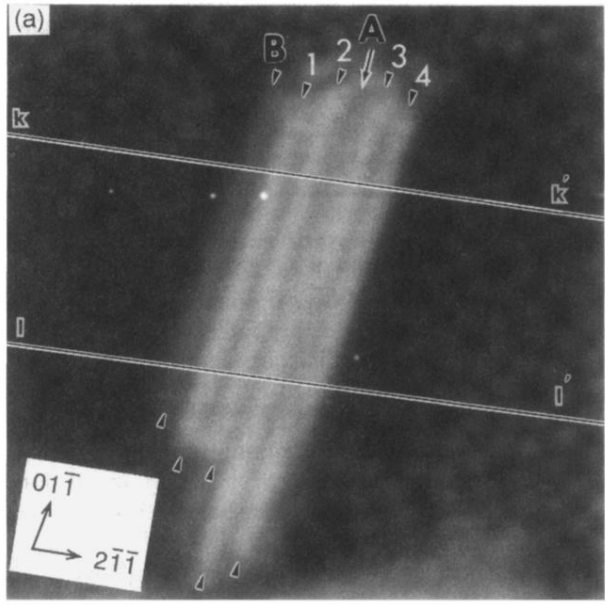

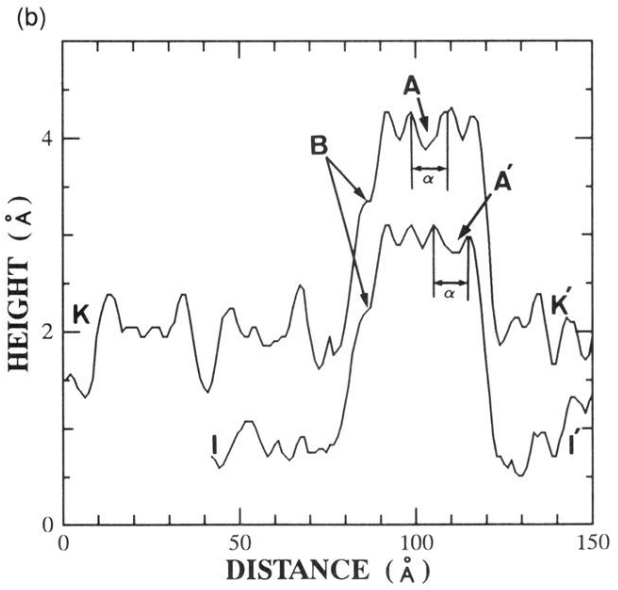

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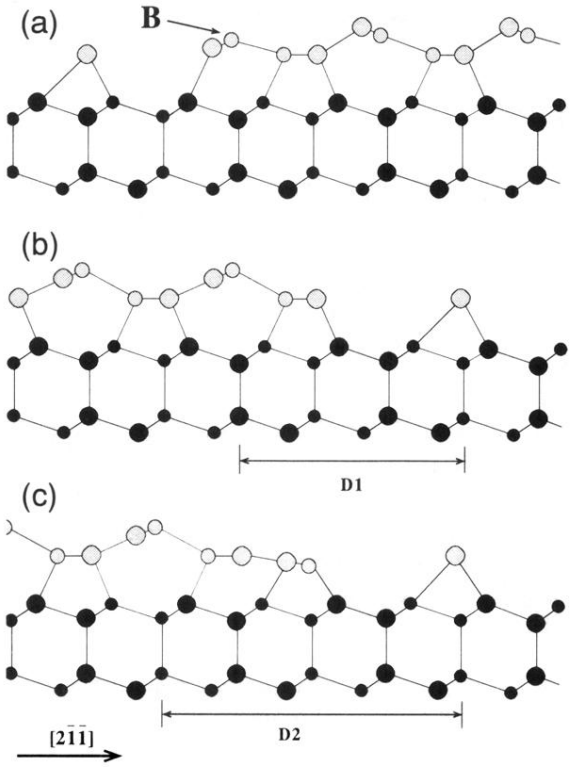

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