# Direct observation of the $c(8\times8)$ defect structure on Si(001) using scanning tunneling microscopy

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An unusual defect structure occurring on the Si(001) surface has been studied using scanning tunneling microscopy (STM). The structure has $c(8\times8)$ periodicity, as evidenced by both STM and low-energy electron diffraction (LEED). Although Auger electron spectroscopy (AES) shows no contamination, secondary ion mass spectroscopy data indicate the presence of trace amounts of Cu. This impurity is implicated in the reconstruction, being related to a similar mechanism for Ni-induced defect structures previously found on Si(001). The $c(8\times8)$ structure is seen to consist of rows of raised rectangular structures formed by added dimers perpendicular to dimer rows on the terrace with alternate rows shifted out of phase. [S0163-1829(96)05044-8]

Scanning tunneling microscopy (STM) studies have yielded a great deal of information on the subject of defects on surfaces, which play an important role in the physical and chemical properties. Many studies have focused on semiconductor surfaces, in particular the Si(001) surface due to its technological importance. On the clean surface a $(2\times1)$ reconstruction is observed at room temperature (RT). It is well established that this reconstruction is caused by the dimerization of atoms in the top layer. In addition, a number of defect structures have been reported for Si(001). In particular, the $(2\times n)$ reconstruction has been studied by a number of groups.[1–5] They are formed by defect rows (vacancy channels) running perpendicular to every $n$th dimer row. However, no consensus has been reached regarding the mechanisms of formation. Some studies have claimed that the $2\times n$ reconstruction can be formed by quenching from high temperature[1–4] while others have suggested that they may be induced by trace amounts of Ni below the limits of Auger electron spectroscopy (AES) detection.[5] Niehus *et al.*[6] carried out STM studies on the $2\times8$ reconstruction that they formed by controlled Ni evaporation onto the surface. They found it impossible to form the $2\times8$ by annealing alone. Similar structures were more recently seen by Koo and coworkers upon Ni contamination.[7]

In addition to the $2\times n$ reconstructions a higher-order $c(4\times4)$ defect structure has been observed.[8–12] As with the $2\times n$ structures, the sample preparation required to obtain such a structure remains unclear. Wang, Lin, and Wang[9] formed the $c(4\times4)$ by annealing alone and found that the transition between the $2\times1$ and $c(4\times4)$ phases was reversible. Other studies have formed a metastable $c(4\times4)$ reconstruction by hydrogen exposure and annealing.[10] The use of either $p$-type (P doped) or $n$-type (B doped) samples appeared to have no effect on the reconstructions.[9] Proposed structural models for the $c(4\times4)$ structure have included a $\pi$-bonded defect model (missing dimer),[8] an alternative missing dimer model,[9] and a parallel ad-dimers and mixed ad-dimer model.[12]

In this paper we image a higher-order reconstruction of Si(001) using STM. The $c(8\times8)$ reconstruction has been previously reported by Müller *et al.*[1] based on low-energy electron diffraction (LEED) patterns. Our results indicate a structure composed of parallel rows of rectangular structures, which are shifted out of phase with each other. The data indicate that the structures consist of added dimer rows one step height above the surface resulting in a larger scale version of the $c(4\times4)$ structure proposed by Wang, Lin, and Wang.[9] Although AES shows a clean sample, secondary ion mass spectroscopy (SIMS) studies carried out on the samples after imaging in STM showed evidence for Cu present on the surface. This tentatively suggests that the formation of the $c(8\times8)$ structure is related to the trace contamination. However, as in the case of Ni contamination, a detailed explanation of the driving mechanism remains unclear.

The experiments were carried out using an Omicron STM operated at RT in ultrahigh vacuum with a base pressure of $\leqslant10^{-10}$ mbar. The chamber was also equipped with a four-grid rear view LEED and Auger analyzer. In this instrument the (tungsten) tip is held at ground potential and the sample biased. A number of samples were cut from a Si(100) wafer ($n$ type) and mounted on Ta holders by Ta clips, which were spot welded to the holder. The samples were washed in methanol, dried in nitrogen gas, and then inserted into the vacuum chamber via a fast entry lock and outgassed at 600 °C for approximately 14 h. They were then flashed to 1325 K using an $e$ beam heater with electrons striking the

 

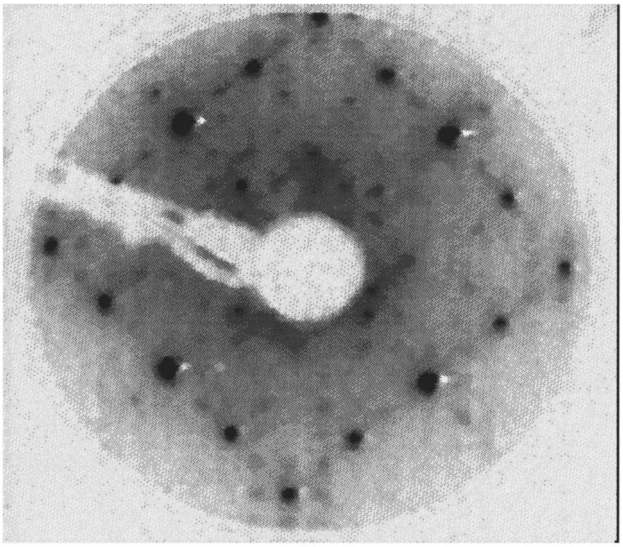

FIG. 1. Low-energy electron diffraction pattern recorded from Si(001) at 103 eV showing $c(8\times8)$ periodicity. This pattern was observed over the entire surface and was seen on several samples. (The contrast has been inverted in order to make the features in the LEED pattern clearer.)

back of the sample. No contamination was detected within the limits of AES recorded using a cylindrical mirror analyzer, although SIMS measurements taken after imaging on the same samples showed evidence for Cu. Given the AES showed no contamination indicates that only trace amounts of Cu were present. LEED was used to check the spatially averaged structure of the samples, which evidenced a $c(8\times8)$ structure. The LEED patterns were comparable with those obtained by Müller *et al.*[1] We were unable to obtain any other structure by annealing at different temperatures or by cooling the sample slowly. The STM images were taken using both positive and negative bias voltages in the constant current mode.

Figure 1 shows a LEED pattern obtained from the Si(001) surface at an energy of 103 eV. This LEED pattern was observed over the entire sample and was reproduced several times on different samples. An STM image of the corresponding surface is shown in Fig. 2. Features present in this image are typical of those seen in various images taken at different locations on a number of samples. Reconstructed areas of $2\times n$ having vacancy channels running perpendicular to the dimer rows can be seen in areas $A$. These are similar to the structures reported by Niehus *et al.*[6] and Kato *et al.*,[5] while rectangular structures ($B$) can be seen over a large proportion of the image. Steps can be seen running diagonally on the image with the dimer rows and $2\times n$ structures rotated by 90° on the lower (higher) terraces. We also note that the longer side of the rectangular structures are always perpendicular to the dimer rows of the adjacent $2\times n$ areas and that they appear brighter, possibly indicating a raised structure and neighboring rows of these rectangular structures are shifted out of phase. From the image in Fig. 2 the periodicity between these rectangular features along the larger side of the rectangle is approximately 30 Å, consistent with a distance of eight bulk unit cells (30.4 Å). In the perpendicular direction the distance between two in-phase rectangular units is also approximately 30 Å.

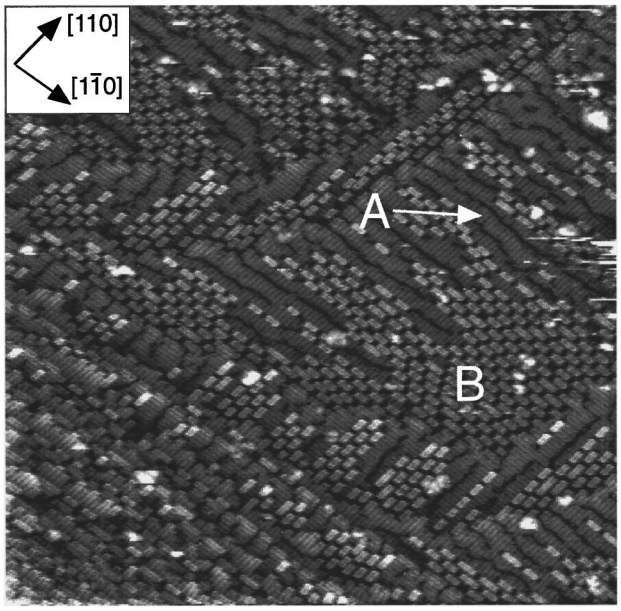


FIG. 2. A $1000\times1000$ Å$^2$ image of the Si(100)-$c(8\times8)$ surface taken at 2 V, 1.0 nA. $2\times n$ vacancy channels ($A$) together with rectangular structures ($B$) are observed on the terraces. Alternating rows of the rectangular structures are shifted out of phase. Both these features are rotated by 90° on neighboring terraces. In well-ordered areas the periodicity of the rectangular structures is $(8\times8)$.

A higher resolution 150 Å$^2$ dual bias image taken at $\pm2.0$ V and 1.0 nA is shown in Fig. 3. Figure 3(a) shows the image taken at positive bias (empty states) while Fig. 3(b) shows the image taken at negative bias (filled states). As in Fig. 2, areas of $2\times n$ structures are seen coexisting in the lower right-hand corner with the parallel rows of rectangular features. In Fig. 3(a) the rectangular structures appear to consist of two parallel rows. Furthermore, adjacent rows of rectangular structures are shifted out of phase as seen in the image of Fig. 1. Along the [110] direction, as indicated in Fig. 3(a), the ''raised'' rectangles appear to be separated by perpendicular rows of dimers ($\alpha$). The center to center separation of the rectangular units is $30\pm2$ Å. In places a few of the other rectangular structures are separated by a shorter distance ($\beta$) along [110].

Measurements indicate that the dimer rows that separate the rectangular structures in the image of Fig. 3(a) are 8 Å in length along [110], consistent with these rows containing two dimers. The height difference between the raised rectangular structures and the dimer rows is consistent with a single type $A$ step of 1.4 Å, using the step notation of Chadi[13] for the Si(001) surface. Thus, by adding the width of the rectangular structures, taking into account the steps and the length of the dimer rows between them, and continuing until the rectangular structures are again in phase leads to a periodicity of eight unit cells in the [110] direction. The morphology that this information suggests is at first sight similar to that proposed for the $c(4\times4)$ reconstruction.[9]

In Fig. 3(b), where the filled states are imaged, the rectangular structures appear to be formed from three features, each feature being a ''bean'' shape consistent with imaging the filled states of a dimer[14] (some of the rectangular structures are longer with four features as opposed to three). Given the fact that in negative bias images these appear to be

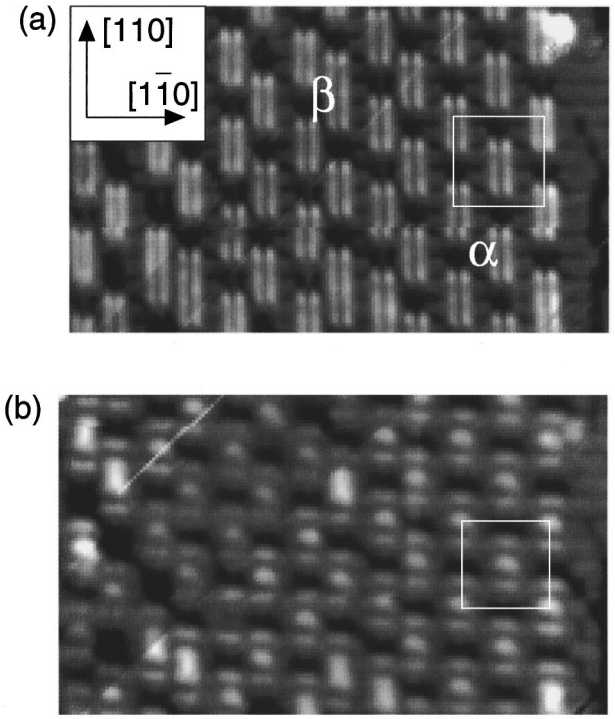


FIG. 3. A 200×100 Å$^2$ dual bias image recorded simultaneously on an area of Si(001)-$c(8\times8)$ at (a) +2 V, 1.0 nA showing empty states of the sample in which the rectangular features can be seen to consist of two parallel rows. (b) −2 V, 1.0 nA showing filled states of the sample. In both images the $c(8\times8)$ unit cell is outlined. The $2\times n$ vacancy structure can be in the lower right-hand corner of both images.

consistent with the bean shape associated with a dimer, while the positive bias image shows two parallel lines, we believe that we are imaging a dimer row under these conditions. That we can resolve the individual Si atoms along the [110] direction on the rectangular structures and not on the 2×1 dimer rows on the terrace may be caused by the different local environment in that the rectangular structures are raised from the surface and not surrounded by other dimers, which may lead to a lateral spread of the wave functions. This type of explanation was also used by Ide and Mizutani[10] to explain the larger size of imaged dimers for the $c(4\times4)$ reconstruction.

However, within each unit the periodicity of the three features (dimers) imaged in Fig. 3(b) in the [110] direction is about 8 Å, approximately double that expected for the 2×1 structure. Similar although less pronounced structures are also observed in Fig. 3(a). However, STM measurements and first-principles calculations based upon the local-density approximation by Bedrossian and Kaxiras[15] have shown that for solitary dimer rows on Si(001) the dimers are at two distinct heights with those located between the dimer rows on the underlying terrace being imaged lower. Thus on the basis of this we conclude that there are additional dimers between those seen on the raised features in Fig. 3(b). The separation of the rectangular structures along [110] is 11 Å. This together with the length of the rectangular features (three raised dimers plus two lowered dimers) also results in a periodicity of eight bulk unit cell lengths. Although the driving mechanism for such a structure is unclear, the fact

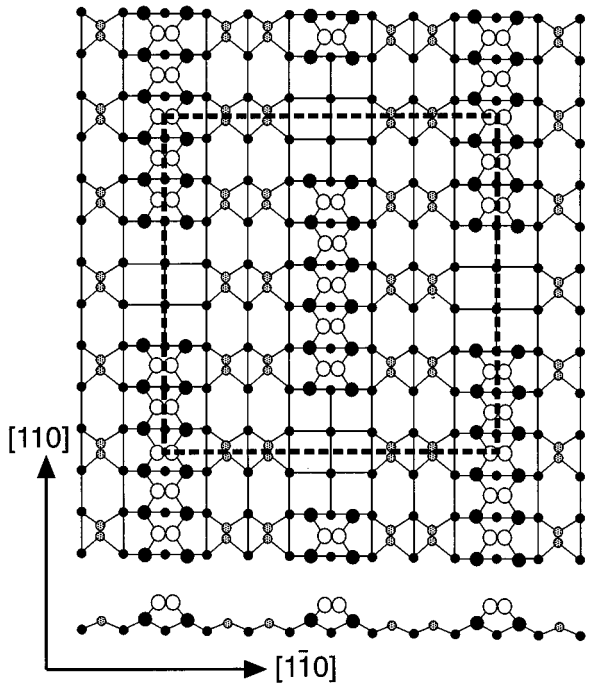


FIG. 4. Proposed model for the Si(100)-$c(8\times8)$ reconstruction. (a) Two-dimensional top view with black balls representing bulk Si atoms, shaded balls representing 2×1 reconstruction, and white balls the dimer rows forming the $c(8\times8)$ structure. The unit cell is outlined. (b) Two-dimensional side view.

that combined AES/SIMS data indicate trace amounts of Cu may suggest that this is related to the process. It has been shown by other studies that small amounts of metal contamination on Si(001) surfaces may be responsible for other defect structures, even when the scale of the reconstruction is far greater than the amount of contamination.[5–7] Therefore on the basis of the data presented we have proposed a structural model, shown in Fig. 4, for the $c(8\times8)$ structure in which the large rectangular structures consist of raised dimer rows. Alternate rectangular structures along [110] are separated from one another by a type-*B* down-up step,[13] while in the perpendicular [110] direction a short dimer row of two unit cells on the lower terrace is located between them. Such a model is essentially a larger version of the $c(4\times4)$ structure proposed by Wang, Lin, and Wang.[9]

In conclusion, we have reported the STM imaging of the Si(100)-$c(8\times8)$ reconstruction with SIMS data evidencing small amounts of Cu contamination. This suggests that the Cu may be related to the formation of the $c(8\times8)$ structure in a similar way to structures induced by Ni although the exact mechanism behind this remains unclear. Our results indicate that the reconstruction consists of rectangular structures containing dimer rows separated by dimer defects that are raised by a monoatomic step from the 2×1 surface. These are separated in the longer direction by a double type-*B* step while in the shorter direction they are shifted out of phase and separated by a row of two dimers one step below.

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