Extended Abstracts of the 1996 International Conference on Solid State Devices and Materials, Yokohama, 1996, pp. 377-379



# Boron-Induced $\sqrt{3} \times \sqrt{3}$ Reconstruction on Si(111) Surface

M. Umekawa, S. Ohara, S. Tatsukawa, H. Kuriyama and S. Matsumoto
*Faculty of Science and Technology, Keio University,*
*Hiyoshi, Yokohama 223, Japan*

**Abstract**

The boron-induced $\sqrt{3} \times \sqrt{3}$ reconstruction on Si(111)7×7 surface has been studied by evaporating elemental B on Si surface with the scanning tunneling microscope. In case of the room temperature boron evaporation on Si, 7×7 reconstructed surface is preserved. When boron is evaporated on Si elevated at high temperatures, $\sqrt{3} \times \sqrt{3}$ B reconstructed surface structures develop from the step edge to the adjacent lower terrace. The $\sqrt{3}$ B reconstruction emerges at temperatures between 800°C and 900°C, suggesting an important role of phase transition from 7×7 to 1×1 surface structure. The phase boundary between 7×7 and $\sqrt{3} \times \sqrt{3}$ regions is a straight line with the termination of the faulted halves of the 7×7 unit cells.

## 1 Introduction

Controlled adsorption of dopant atoms on semiconductor surfaces is of much interest both from scientific and technological points of view. The dopant atoms can change the character of surface electronic states and form new two dimensional structure that differ from the clean surface.

It has been reported that boron causes the surface to favor a $\sqrt{3} \times \sqrt{3}$R30° reconstruction over the Si(111)7×7 surface, occupying a subsurface substitutional site directly below a Si adatom at a $T_4$ position [1–4]. This unique $\sqrt{3} \times \sqrt{3}$ B reconstruction enables to deposit additional Si layers on top of the $\sqrt{3}$ surface without breaking the ordered structure, leading to possibilities for new metastable materials and interesting two dimensional phenomenon. Moreover, negative differential resistance (NDR) has been reported in the scanning tunneling spectroscopy (STS) of the Si(111)$\sqrt{3} \times \sqrt{3}$-B surface [5,6]. NDR is also observed in Si/$\sqrt{3} \times \sqrt{3}$B/Si(111) diode structures [7].

So far the $\sqrt{3} \times \sqrt{3}$ B surface reconstruction has been prepared either by surface segregation from highly boron doped silicon, or by deposition of boron from compound source ($HBO_2$, $B_{10}H_{14}$), since elemental B is not easy to evaporate with a usual Knudsen cell. These ways, however, include complex segregation reactions or surface reactions besides the essential reconstruction phenomenon.

In this work, we manage to evaporate elemental B as a source with an electron gun evaporator to avoid the interfering with above unnecessary phenomena and examine the boron-induced $\sqrt{3} \times \sqrt{3}$ reconstruction on Si(111)7×7 surface at the atomic scale using scanning tunneling microscopy (STM).

## 2 Experimental

Experiments were performed in ultra-high vacuum chambers equipped with XPS, STM and electron gun evaporators with a base pressure of $1 \times 10^{-10}$ Torr.

A degreased Si(111) wafers (*n*-type, 0.7 ~ 1.3Ω· cm) were degassed overnight at 600°C. A few cycles of flashing up to 1250°C of the sample yielded a ordered clean 7×7 surface. Boron deposition on the clean surface was accomplished by evaporation from a chunk of elemental boron (99.9% purity) with an electron gun evaporator. All STM images presented here were acquired at room temperature with a constant current mode.

## 3 Results and Discussion

### A RT boron evaporation followed by annealing

It has been reported that Ag clusters not having a characteristic structure at RT gradually form $\sqrt{3} \times \sqrt{3}$ reconstruction from cluster edge during annealing process. In order to investigate such possibility for boron, samples were annealed in vacuum. Figure 1 shows the STM image of the sample annealed at 750°C for 5 min. immediately after the evaporation of boron at RT.

Large islandlike clusters are observed both at the step edge and on the terrace, and any indication of $\sqrt{3} \times \sqrt{3}$ B reconstruction was not observed. Such large clusters are formed by diffusion and coalescence of small boron clusters without causing the $\sqrt{3} \times \sqrt{3}$ reconstruction. It is added that such agglomeration was observed even at very short annealing time of 10 seconds at lower temperature of 500°C.

I. -W. Lyo et. al.[8] reported that $\sqrt{3} \times \sqrt{3}$ B reconstruction was formed on Si(111) surface by the RT evaporation of $B_{10}H_{14}$ followed by annealing to temperatures above that of hydrogen desorption (> 500°C). In this case, hydrogen desorption reaction of $B_{10}H_{14}$ is strongly associated with the $\sqrt{3} \times \sqrt{3}$ B reconstruction.

### B Boron evaporation on high temperature substrate

When B was evaporated with 0.6L on the Si(111) elevated at 800°C, large clusters are observed in STM image, similar to the case of RT B evaporation followed by annealing of Fig. 1.

Figure 2 shows the STM image of the step-terrace region after exposure of 1.2L B evaporation on Si(111) elevated at 1000°C. It is clearly shown that $\sqrt{3} \times \sqrt{3}$ B structures develop from the step edge to the adjacent lower terrace. Similar surface phenomenon is also observed in case of 0.6L boron exposure at 900°C.

The fact that $\sqrt{3}\times\sqrt{3}$ B reconstruction occurs at temperatures between 800°C and 900°C suggests an important role of phase transition of 7×7 surface structure for the formation of $\sqrt{3}\times\sqrt{3}$ B reconstructed surface. It is well known that Si(111)7×7 reconstructed surface structures convert into high temperature 1×1 phases at about 830°C. At the temperatures existing 7×7 surface structures, boron terminates the dangling bonds only and does not bring about the $\sqrt{3}\times\sqrt{3}$ reconstruction because 7×7 structures are the most stable as compared with the other structures.

On the other hand, at temperatures of 900°C and 1000°C, 1×1 surface structures emerge instead of 7×7 structures. During the cooling period from high temperatures, 1×1 surface structures will convert to $\sqrt{3}\times\sqrt{3}$ B surface structures instead of 7×7 structures under the presence of B on Si surface.

### C Phase boundary between 7×7 and $\sqrt{3}\times\sqrt{3}$

The phase boundary between 7×7 and $\sqrt{3}\times\sqrt{3}$ regions is shown in Fig.3, which is the expanded image of Fig.2. In the local region, the boundary is a straight line with the termination of the faulted halves of the 7×7 unit cells. It was confirmed from the difference in brightness of the occupied STM image of 7×7 surface. This result disagrees with that of T.M.H.Wong[9] who concluded that the boundary between 7×7 and $\sqrt{3}\times\sqrt{3}$ was terminated with the unfaulted halves of the 7×7 unit cells.

It is also found that $\sqrt{3}\times\sqrt{3}$ regions don't change to 7×7 region continuously, but an additional dimer row is inserted at the boundary between the faulted halves of the 7×7 unit cells and the $\sqrt{3}\times\sqrt{3}$ regions. This is already pointed out by H. Wong et al. It suggests that the dimer row structure is a characteristic structures minimizing the energy in combining the long period structure (7×7) and short period structures (1×1 or $\sqrt{3}\times\sqrt{3}$). Figure 4 shows a schematic diagram indicating with the additional dimer now between 7×7 and $\sqrt{3}\times\sqrt{3}$ regions and the termination of the faulted halves of the 7×7 unit cell.

The other interesting characteristics is shown in Fig.5. Narrow $\sqrt{3}\times\sqrt{3}$ regions extend along the domain boundary of 7×7 surface structures. It should be noted that the phase of 7×7 domain of both sides differs as shown from the point indicated by arrows. It is expected that there are excess dangling bonds at the domain boundary, triggering the $\sqrt{3}\times\sqrt{3}$ reconstruction.

## 4 Conclusions

The boron-induced $\sqrt{3}\times\sqrt{3}$ reconstruction on Si(111) 7×7 surface has been studied by evaporating elemental B on Si surface with the scanning tunneling microscope.

In case of the room temperature boron evaporation on Si, 7×7 reconstructed surface is preserved and $\sqrt{3}\times\sqrt{3}$ B reconstruction is not observed. For the sample annealed at 750°C immediately after the evaporation of boron at room temperature, only large islandlike boron clusters are observed.

When boron is evaporated on Si elevated at high temperatures, $\sqrt{3}\times\sqrt{3}$ B reconstructed surface is observed. There is a threshold temperature for the emergence of the $\sqrt{3}\times\sqrt{3}$ B reconstruction, which is ranged between 800°C and 900°C. It suggests the important relationship between $\sqrt{3}\times\sqrt{3}$ B reconstruction and phase transition from 7×7 to 1×1 surface structure, which occurs at 830°C. It is found that the phase boundary between 7×7 and $\sqrt{3}\times\sqrt{3}$ regions is a straight line with the termination of the faulted halves of the 7×7 unit cells. An additional dimer row is also found to be inserted at the phase boundary between these regions.

## References


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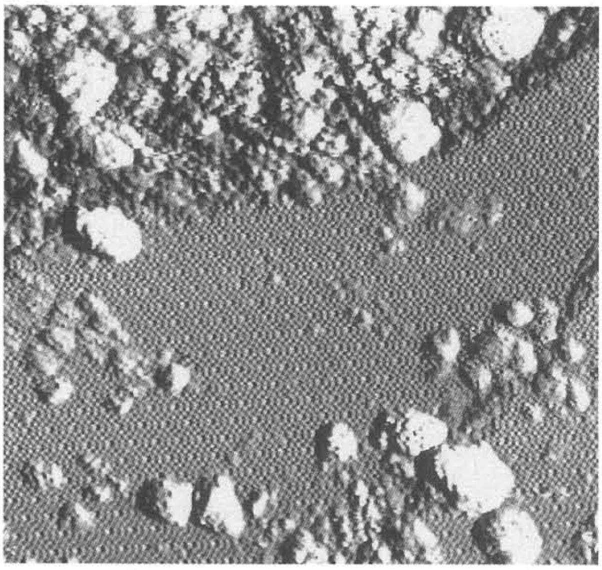

Fig.1: STM image of Si(111)7×7 surface after RT B evaporation followed by 750°C for 5min annealing. (sample bias=+2V)

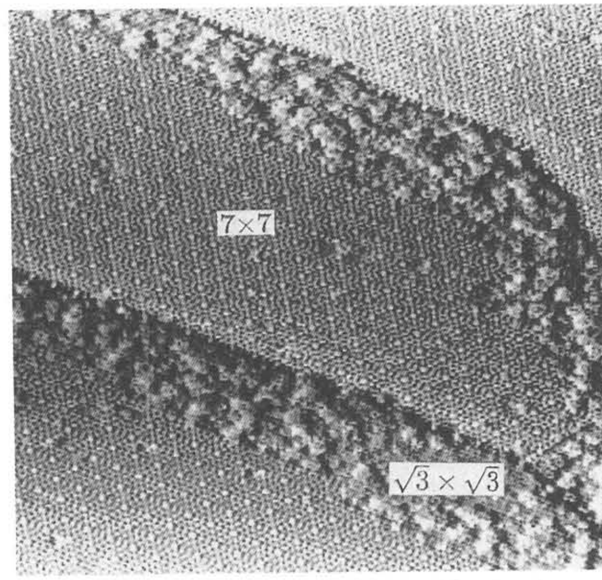


Fig.2: STM image of step-terrace after exposure at 1000°C to 1.2 L of boron. (sample bias=+2V)

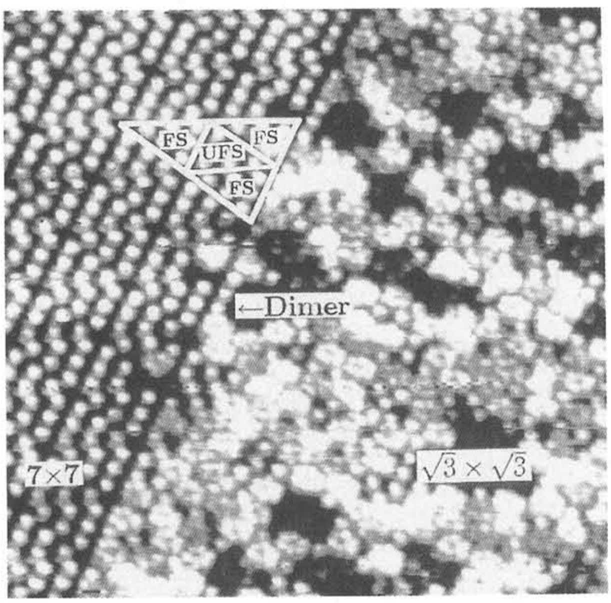


Fig.3: STM image of the phase boundary between the 7×7 and $\sqrt{3} \times \sqrt{3}$ regions. (sample bias=+2V)

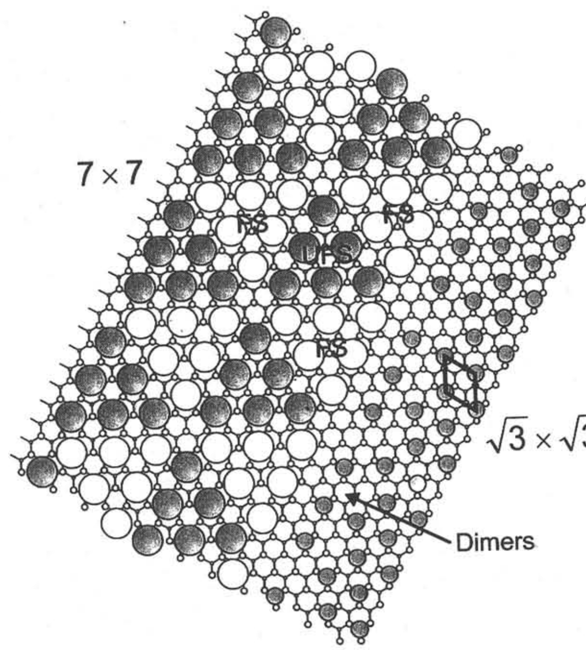


Fig.4: Schematic diagram of the phase boundary.

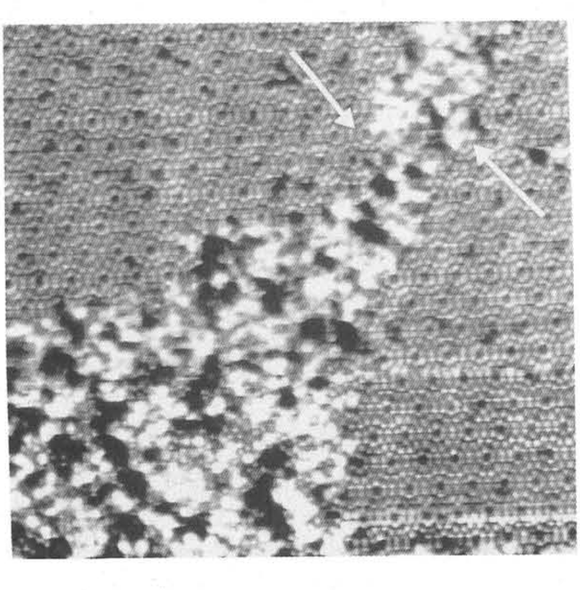

Fig.5: STM image of the domain boundary between unphased 7×7 regions. $\sqrt{3} \times \sqrt{3}$ region spreads to the narrow limited area. (sample bias=+2V)