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Quenched Si(111)-DAS (dimer-adatom-stacking fault) structures studied by scanning tunneling microscopy

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Abstract

Stacking-fault (SF) half-units of $N \times N$ ($N = 5$ to 11) DAS (dimer–adatom-stacking fault) structures were observed to be quenched on the Si(111) surface, and to be surrounded by disordered 1×1 phase. From analysis by bias dependent scanning tunneling microscopy, which reflects charge transfer between top-layer adatoms and underlayers, Si dimers were found to remain at the boundary between the SF half-units of the DAS structures and the disordered 1×1 phase.

Keywords: Low index single crystal surfaces; Scanning tunneling microscopy; Semiconducting surfaces; Silicon; Surface structure, morphology, roughness, and topography

1. Introduction

The Si(111)-7×7 reconstructed surface has been extensively studied, and the DAS (dimer–adatom-stacking fault) model proposed by Takayanagi et al. [1] is widely accepted to explain the structure. However, the determination of its formation mechanism still remains as an important problem to be solved. Since DAS structures consist of three atomic layers, information on the underlayer structures is necessary to understand the formation mechanism. Recently, the Si(111)-7×7 phase boundary was analyzed by scanning tunneling microscopy (STM) with consideration of the charge transfer between the topmost adatom layer and underlayers [2], and dimers were found to be formed at the boundary of the stacking-fault (SF) half-unit of 7×7 structure and a disordered area. A similar dimer structure was also observed for the boundary of SF half-unit of 5×5 structure surrounded by 7×7 structure, and for the boundary between the SF half-unit of 7×7 structure and a disordered 1×1 structure [2]. Recently, Hoshino et al. [3] observed a quenched Si(111) surface, and pointed out the importance of the SF half-unit in the formation of DAS structures. According to their model, the SF half-unit was stabilized by the formation of dimer chains and corner holes. However, only the atomic structure of the topmost adatom layer was analyzed in their work.

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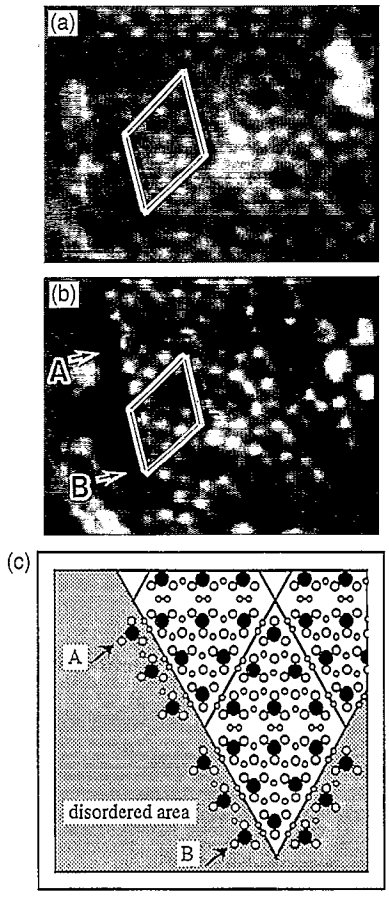

Fig. 1. STM images of the 7×7 units with disordered 1×1 area: (a) $V_s = 2.0$ V, $I_t = 300$ pA, (b) $V_s = -2.0$ V, $I_t = 300$ pA, and (c) schematic structural model.

In this paper, we present the results of structures of the DAS family remaining on the quenched surface, with consideration of the electronic charge transfer described above.

2. Experimental and results

Phosphorus-doped (1 Ω cm) Si(111) sample surfaces were subjected to flash heating, and cooled down to room temperature. The base pressure was about 1.0×10^{-8} Pa, and pressure during the heat treatment was kept below about 5×10^{-8} Pa. STM was performed at room temperature using an electrochemically etched W tip, and all STM images shown in this paper were obtained in the constant current mode.

As has been described in Section 1, it is possible to analyze the atomic structure of the DAS family including underlayers, by measuring bias-voltage-dependent STM images [2]. On the basis of the DAS model, since the energy level of the dangling bond state is lower than that of the adatom state, electronic charge is transferred from adatoms to dangling bonds [4–6]. Therefore, charge density of the adatoms depends on the number of the dangling bonds surrounding each adatom. When dimers are formed in the underlayer, the number of dangling bonds is reduced, thereby the amount of charge transfer becomes less.

Fig. 1a and Fig. 1b show an empty-state and a filled-state image of the 7×7 phase obtained at (a) a sample voltage V_s of 2.0 V and tunneling current I_t of 300 pA, and (b) a V_s of -2 V and I_t of 300 pA. There is a 7×7 unit in Fig. 1a and Fig. 1b which is surrounded by the disordered 1×1 phase. If dimers exist at the boundary between the SF half-unit of the 7×7 structure and the disordered 1×1 area, adatoms at the edge of the 7×7 structure should be bright even in the filled-state STM image [2]. In fact, as shown in Fig. 1b, the adatoms are as bright as those observed in the normal 7×7 structure. Fig. 1c shows a schematic model to explain the electronic structure, brightness of adatoms, shown in Fig. 1b. As was pointed out previously [3], adatom chains exist at the boundary, as indicated by arrows A and B in Fig. 1b and Fig. 1c.

Other DAS structures remain on the quenched Si(111) surface. Fig. 2a to Fig. 2(h) show empty-state (left column, $V_s = -2.0$ V, $I_t = 300$ pA) and filled-state (right column, $V_s = -0.5$ V, $I_t = 300$ pA) STM images of the DAS structures (Fig. 2a, b: 5×5; c, d: 7×7; e, f: 9×9; g, h: 11×11). There exist SF half-units of the DAS structure surrounded by a disordered area. Since adatoms of the half-unit cells in the filled-state images are as bright as those in the empty-state images, dimers exist at the boundaries of the SF half-unit cells according to our model. Therefore, as Hoshino et al. [3] pointed out, DAS units are considered to be stabilized together with the dimers formed at the boundary. Adatom chains are also observed at the boundary of the observed SF half-unit cells.

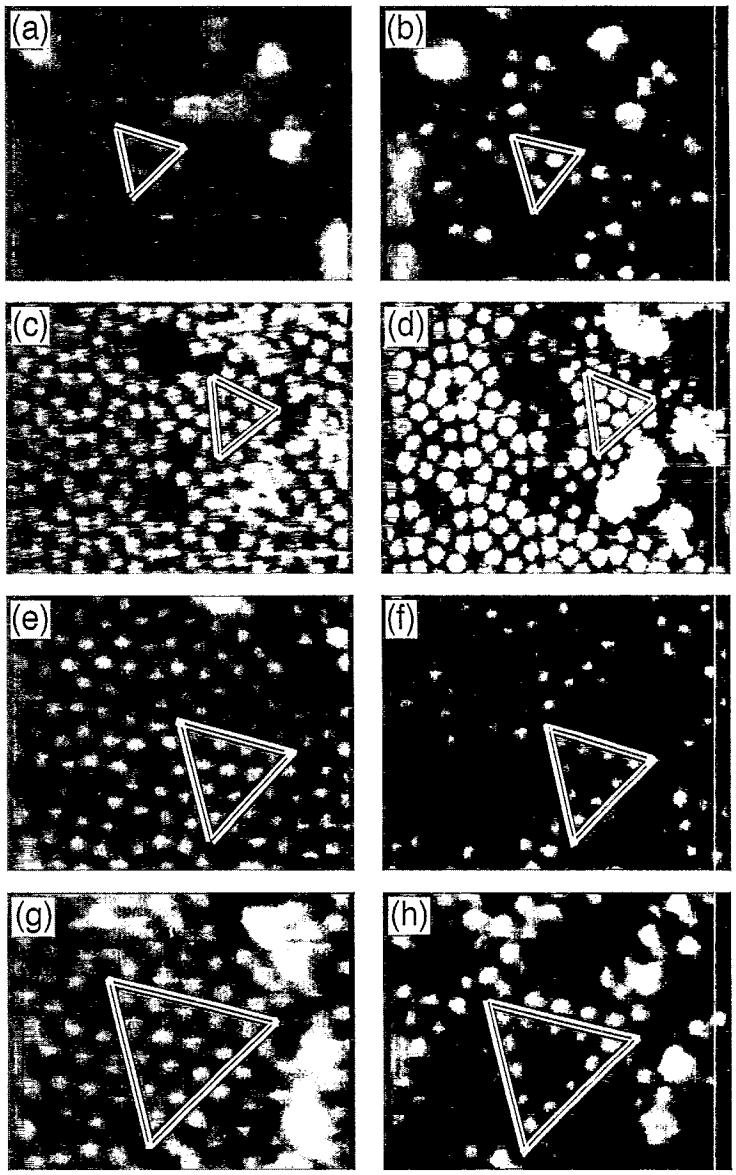

Fig. 2. Bias-voltage-dependent STM images of 5×5 ((a) $V_s = 2.0$ V, $I_t = 300$ pA, (b) $V_s = -0.5$ V, $I_t = 300$ pA), 7×7 ((c) $V_s = 2.0$ V, $I_t = 300$ pA, (d) $V_s = -0.5$ V, $I_t = 300$ pA), 9×9 ((e) $V_s = 2.0$ V, $I_t = 300$ pA, (f) $V_s = -0.5$ V, $I_t = 300$ pA), and 11×11 structures ((g) $V_s = 2.0$ V, $I_t = 300$ pA, (h) $V_s = -0.5$ V, $I_t = 300$ pA).

3. Conclusions

Structures of quenched Si(111) surface including underlayers were analyzed by bias-voltage-dependent STM with consideration of charge transfer from adatoms to rest atoms. Dimers were found to remain at the boundary between the $N \times N$ ($N = 5, 7, 9, 11$) SF half-units and the disordered area.

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