Non-Contact Atomic Force Microscopy and Scanning Tunneling Microscopy of Coexisting Reconstructions on Si(111)†

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The coexisting metastable reconstructions of the Si(111) surface have been investigated by non contact-atomic force microscopy (NC-AFM). True atomic resolution has been achieved in the NC-AFM imaging of the 7 × 7, c(2 × 8), 2 × 2, c(2 × 4), and $\sqrt{3} \times \sqrt{3}$ coexisting reconstructions of the same quenched surface sample. A simple comparison with scanning tunneling microscopy (STM) results is given, and imaging of 2 × 1 π-bonded chains island is also reported. [DOI: 10.1380/ejssnt.2005.258]

Keywords: Non-Contact Atomic Force Microscopy; Scanning Tunneling Microscopy; Si(111); Surface Reconstruction

I. INTRODUCTION

Non contact-atomic force microscopy (NC-AFM) has become a new powerful tool for surface science studies such as topography mapping [1], atomic manipulation [2], surface modification [3], dissipation [4] and Kelvin force measurements [5]. Obtaining real atomic resolution [6] on a surface with NC-AFM is a rather complicated and difficult experiment in comparison with scanning tunneling microscopy (STM). A review and detailed explanation of the technical challenges faced by atomic force microscopy with respect to scanning tunneling microscopy have been reported by F. Giessibl [7]. Furthermore, difficulties in achieving stable NC-AFM imaging can be due to the presence of disordered areas, defects, adsorbed species and contaminant, or of different topological features exhibiting very different shapes and dimensions on a surface. One particular example is the NC-AFM imaging of coexisting surface reconstructions with atomic resolution. Restricted to the case of semiconductor surfaces, NC-AFM observations with atomic resolution of different phases coexisting on the same semiconductor surface have only been reported for the case of GaAs(100)-n × 6 and -4 × 1 [8]. On the other hand, NC-AFM has been proven to be a convenient tool for probing different semiconductor surface reconstructions. In the case of silicon, the 7 × 7 reconstruction [1] of the Si(111) surface, and the c(4 × 2), p(2 × 2), and 2 × 1 reconstructions on the Si(100) surface [9] have been atomically imaged. Observation of Ge(111)-c(2 × 8) [10], InP(110)-1 × 1 [11], InAs(110)-1 × 1 [12], InSb(100)-c(2 × 8) [13], GaAs(110)-2 × 1 [14], GaAs(100)-c(2 × 8) [13] and GaAs(100)-c(8 × 2/4 × 6) [15] have also been reported.

In the present study, we achieved atomic resolution in the NC-AFM topography of the coexisting reconstructions of the quenched Si(111) surface, namely, the 7 × 7, c(2 × 8), 2 × 2, c(2 × 4), and $\sqrt{3} \times \sqrt{3}$ reconstructions. We also observed on the very same quenched silicon sample 2 × 1 π-bonded chains islands. For the sake of comparison, two separated sets of observations were performed, one with a NC-AFM, the other with a STM.

II. EXPERIMENTAL

NC-AFM experiments were carried out by using a JSPM4500-A NC-AFM by JEOL, and STM measurements were taken with a JSPM-4500S STM by JEOL. Both equipments were operated at room temperature (RT) in an ultra-high vacuum (UHV) system with a base pressure of 8 × 10⁻¹⁰ Pa. A highly doped conductive Si
ber to be degased at 600 °C acetone for 30 min, then transferred to the UHV chamber.

0.1 Ω from RT to 900 °C, frequency shift -41 Hz, 0 V).

Metastable reconstructed areas appear in the form of triangular shaped regions (see Figs. 3b, 3c, and 4a) and the domain size for each metastable reconstruction is quite small, on the order of 10 × 10 nm² (see Fig. 1). These small metastable domains can be routinely imaged with NC-AFM, even when topological defects (disordered atomic arrangements, dislocations, and adatom vacancies) and Si clusters are present [17].

The most stable of all the metastable phases is the c(2×8) reconstruction, and the manifestation of its higher stability is that domains with relatively larger sizes, on the order of 50 × 50 nm² for the largest, can be observed. This is shown in the atomically resolved NC-AFM topographs of Figs. 2 and 3 (a), where c(2×8) double rows as long as 10 adatoms in size are measured. In Fig. 2, the c(2×8) adatoms double rows running in the three equivalent [110] directions reveal the threefold symmetry of the reconstruction. A domain boundary between the metastable c(2×8) and stable 7×7 phases is displayed in Fig. 3 (a), and it can be remarked here, that even if the Si(111)-7×7 reconstruction described by the dimer-adatom-stacking-fault (DAS) model [18] is the most stable reconstruction of this surface, its topology is more complicated than the c(2×8) one [19]. In the case of Si(111)-c(2×8), only the topmost layer reconstructs whereas four layers are involved in the 7×7 reconstruction. As seen in the c(2×8) model of Fig. 5(d), the adatoms of the c(2×8) reconstruction occupy the T₄ sites (three out of four of the original bulk dangling bonds are saturated by these adatoms) and can be surrounded by 3 or for 4

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**FIG. 1:** Atomically resolved NC-AFM scan (4 × 45.3 nm², frequency shift -41 Hz, 0 V) of the coexisting 7×7, c(2×8), 2×2, c(2×4), and, √3×√3 reconstructions of the same quenched Si(111) surface sample.

**FIG. 2:** Si(111)-c(2×8) adatoms double rows running in the three equivalent [110] directions (NC-AFM scan, 23.3 × 17.4 nm², frequency shift -41 Hz, 0 V).

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**III. RESULTS AND DISCUSSION**

Figure 1 shows an atomically resolved NC-AFM topograph of the coexisting stable 7×7, and metastable c(2×8), 2×2, c(2×4), and √3×√3 reconstructions of the quenched Si(111) surface. Metastable reconstructed areas appear in the form of triangular shaped regions (see Figs. 3b, 3c, and 4a) and the domain size for each metastable reconstruction is quite small, on the order of 10 × 10 nm² (see Fig. 1). These small metastable domains can be routinely imaged with NC-AFM, even when topological defects (disordered atomic arrangements, dislocations, and adatom vacancies) and Si clusters are present [17].

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FIG. 3: Domain boundaries between Si(111)-c(2 × 8) and Si(111)-7 × 7 reconstructions. (a) Atomically resolved NC-AFM topography of the black squared area in (b), showing on the left hand side a Si(111)-c(2 × 8) domain, and on the right hand side a Si(111)-7 × 7 domain (26 × 26 nm², 0 V, frequency shift -41 Hz). √3 × √3 structures are also observed. Between (b) -0.6 V and (c) +0.6 V, a clear contrast reversal is observed (600×600 nm², frequency shift -26 Hz). 7 × 7 domains appears darker in (b) and brighter in (c).

restatoms. The quality of the NC-AFM scans of Figs. 2 and 3 (a) is good since true atomic resolution of the reconstructed areas, dislocations, and Si clusters can be routinely performed. Observation of the restatoms of a c(2 × 8) structure has been reported in the case of NC-AFM imaging of Ge(111)-c(2 × 8) [10]. In the present case of Si(111)-c(2 × 8), we notice that atomic resolution of the restatoms could not be successfully achieved.

The domain boundary of Fig. 3a corresponds to the squared area in Fig 3b. Due to the large difference of surface contact potential (SCP) between the 7 × 7 and '1 × 1' triangles, these two phases are clearly resolved in the large scale NC-AFM images of Figs. 3 (b) and (c), taken with different sample voltages $V_s$. We measured that with applied voltages $V_s$ ranging from 0 V (Fig. 4 (a)) to -0.6 V (Fig. 3 (b)), the 7 × 7 and '1 × 1' triangles appear as dark and bright features respectively. At $V_s = +0.6$ V (Fig. 3 (c)) a contrast reversal occurs resulting in bright 7 × 7 and dark '1 × 1' triangles. These results are in good agreement with scanning Kelvin probe microscopy experiments that have already measured SCP differences between 7 × 7 and '1 × 1' domains [20]. Considerable discussion and detailed description related to SCP in the dynamic force microscopy of quenched silicon reconstructions will be reported in a future communication [21].

In the constant frequency shift scan of Fig. 4 (a), a large area of the quenched Si(111) surface is displayed, showing large dark and bright triangles, and three bright islands, corresponding to Si(111)-7 × 7 reconstructed regions, '1 × 1' areas, and 2 × 1 π-bonded chains islands respectively. The corners of the triangles formed by the 7 × 7 and '1 × 1' areas point in the [11̅2] directions. Figure 4(b) (NC-AFM) and (c) (STM) give a close up view of a 2 × 1 island with π-
FIG. 5: Atomic diagrams ((a), (d), and (g)), NC-AFM scans ((b): 0 V, frequency shift -264 Hz; (e) and (h): 0 V, frequency shift -41 Hz), and constant current STM images ((c), (f), and (i): +2 V, 0.2 nA) of the Si(111)-2 × 1 ((a), (b), and (c)), Si(111)-c(2 × 8) ((d), (e), and (f)), and Si(111)-7 × 7 ((g), (h), and (i)) reconstructions. (a) Representation of the π-bonded chains with the 2 × 1 unit cell drawn. Large and small filled circles stand respectively for ‘up’ and ‘down’ atoms of the ‘zig-zag’ chains. (d) Adatom-restatom (respectively large-small filled circles) model of the c(2 × 8) reconstruction. The rectangular unit cell is drawn. (g) Adatoms of a 7 × 7 unit cell: filled circles represent the unfaulted half (U), and open circles the faulted half (F). All scans are 7 × 7 nm².

Comparison between NC-AFM and STM topography experiments is given in Fig. 5 for the three main reconstructions of the Si(111) surface. NC-AFM and STM scans have been recorded with the same cantilever and STM tip respectively. From the imaging point of view, the quality and resolution of Fig. 4 (b) (NC-AFM) and (c) (STM) are in stark contrast. We experienced that obtaining atomic resolution of the Si(111)-2 × 1 and Si(111)-7 × 7 reconstructions is well known and respectively described by the π-bonded chains model [22, 23], a simple adatom restatom model [19], and the dimer-adatom-stacking-fault (DAS) model [18]. Nevertheless, experimental results are still needed in order to unveil the band structure of the Si(111)-c(2 × 8) or the differences in the chemical reactivity of these reconstructions. In the case of group IV semiconductors, reconstruction, surface stabilization, electronic band structure, nature of the surface atoms and chemical reactivity are related to each other in a complex way. In order to study this complex interplay in the case of Si(111), it is thus an advantage to be able to probe directly on the same surface its three main reconstructions. In this report we have actually shown that it is possible to study concomitantly with the same
surface science tool (NC-AFM or STM) the coexisting Si(111)-2 × 1, Si(111)-c(2 × 8), and Si(111)-7 × 7 reconstructions of the same quenched surface sample, opening the way for further direct comparison of the electronic spectroscopy or reactivity of these reconstructions [24]. In conclusion, we have broadened the scope of NC-AFM imaging on the Si(111) surface by achieving true atomic resolution on 7 × 7, c(2 × 8), 2 × 2, c(2 × 4), and, √3 × √3 coexisting reconstructions, and imaging 2 × 1 π-bonded chains island on the same quenched surface sample. We also confirmed that the SCP of 7 × 7 and c(2 × 8) are different.

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