Atomic Manipulation and Atomic scale Experiment on Si(111) Surface with STM

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Abstract

We manipulated Si atoms on Si(111)-7x7 surfaces by approaching a biased W STM-tip to the surface until a point contact and consecutively retracting to the original tunneling region. The adatom layer and the double layers were controllably removed by tuning sample bias voltages and clear atomic images were obtained in the created holes. The current flowing through nanoscale contacts between the tip and substrate were also measured during the tip excursion, exhibiting characteristic structures (the saturation at the point contact region and the staircase reductions during the tip excursion) which are closely related to both the atom removal process and the nature of the Si nanoscale contacts. Especially, the height of staircase reductions in the currents exhibited rectification characteristics originated by the nanoscale Schottky effects.

1. Introduction

Scanning probe microscopy (SPM) can provide us good opportunities to do various atomic scale experiments in our office. Typical examples are of course to observe an atomic arrangement of solid surfaces and to measure their local electronic and chemical properties. In addition, since Eigler demonstrated the manipulation of individual atoms by STM tip [1], many people has tried to use SPM technique as a new experimental tool for fabricating new atomic (nanoscale) structures and simultaneously characterizing them [2]. The manipulation of Si atoms on Si(111)-7x7 surfaces is one of the best studied cases where the removal of single atom from the top layer has been carried out by applying pulse biases between tip and substrate [3,4]. However, the surface atomic structures after removing the top or surface layers have not been well studied so far. In addition, there are few reports on the current variation during the atom removal from the surface [5]. We have been attempting to manipulate silicon atoms and fabricate atomic scale structures on clean Si(111)-7x7 surfaces by approaching a biased W STM-tip to the surface until a point contact and consecutively retracting to the original tunneling region [6]. At the same time, the current flowing between the tip and substrate was measured during tip excursion to characterize the electrical properties of the nanoscale contact as many papers have been published in the case of metals [6]. Here we shall summarize our recent results by stressing the relationship between the atom removal process and the electrical conduction on Si(111)-7x7 surface.

2. Experimental

The Si substrates used in this experiment were p-type (B-doped, 1 Ω cm) and the clean Si(111)-7x7 surfaces were prepared by flashing them at 1,100 C. Electrochemically etched W tip was cleaned in UHV condition repetitively by heating in the presence of high electric field, since the existence of contamination on the surface had a large effect on the reproducibility of the atom removal and the variation of the current in the whole process. Prior to the whole indentation experiments, the tip was positioned at a position (a set-point) at the tunneling current of 0.5 nA and the sample bias of +1.5 V. Then the feedback loop was turned off and additional voltages were applied to the z-piezo to approach and retract the tip to and from the surface at a speed of 320 nm/sec. The tip displacement was varied from 0.52 - 0.94 nm in the present experiment. The bias voltages were set to certain values between -3.0 and +3.0 V before the tip movement and the preamplifier was switched to a lower gain type one to measure high currents up to 100 mA. The resulting surface atomic structure was checked by the STM observation immediately after each indentation.

3. Results and Discussion

First, we describe the change in the atomic structures obtained by this technique with the bias voltage between -3 and 3 V, where the tip was approached to the surface by 0.8 nm from the set-point for all cases. There appeared two types of structures after removing atoms, which were dependent on the bias voltages. The first type corresponds to the removal of only adatoms of the DAS structure for Si(111)-7x7 surface with leaving the rest layer atoms behind as shown in Fig.1 (a), where the depth of the hole created is measured as ~0.12 nm. The second type corresponds to the removal of double layers from Si(111)-7x7 surface with clear atomic structures characterized by 2x2, c(2x4) and 3x3 structures in the hole with the depth of ~0.3 nm as shown in Fig. 1(b).

The probabilities of the removal process for adatoms (a) and double-layer (b) are also shown in Fig. 2. The adatom removal probability increases almost linearly with the increase of the bias voltage for both polarities (a), and the slopes are less steep for the negative bias. The minimum point of the probability is slightly shifted to the positive bias. It is interesting

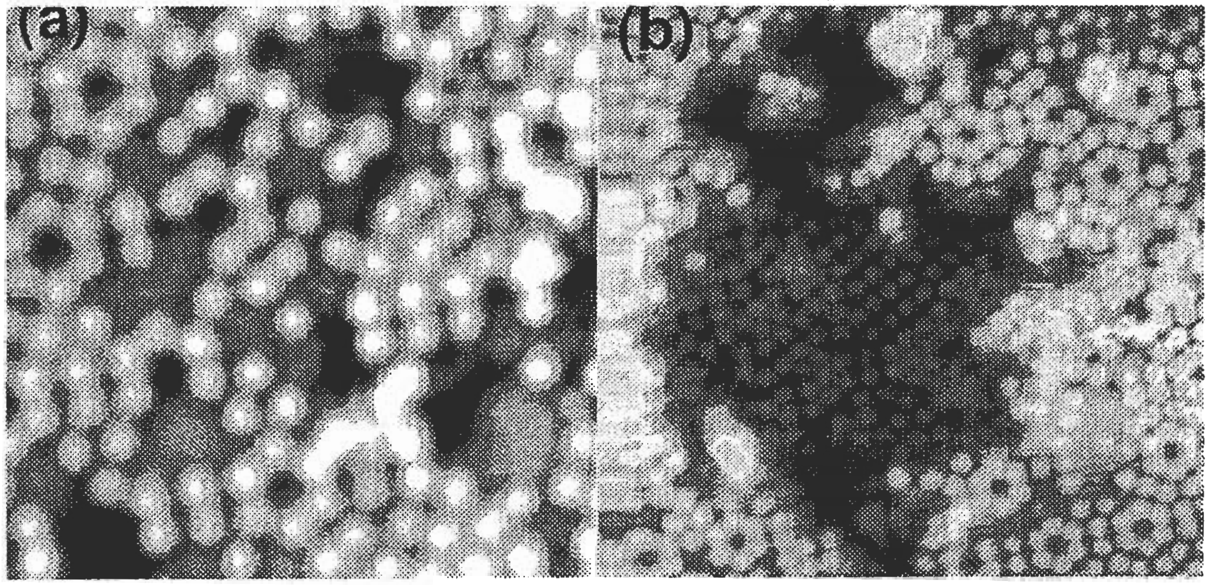

Fig.1 The atomic structures after indenting (0.8 nm) STM tip with sample biases at 1.5 V (a) and 2.0 V (b). In (a), adatoms were mainly removed after indenting STM tip for a few times and the rest layer atoms were observed. In (b), double layers were removed and several atomic strucutres were clearly observed in the hole after indenting STM tip for 10 times for widening the hole.

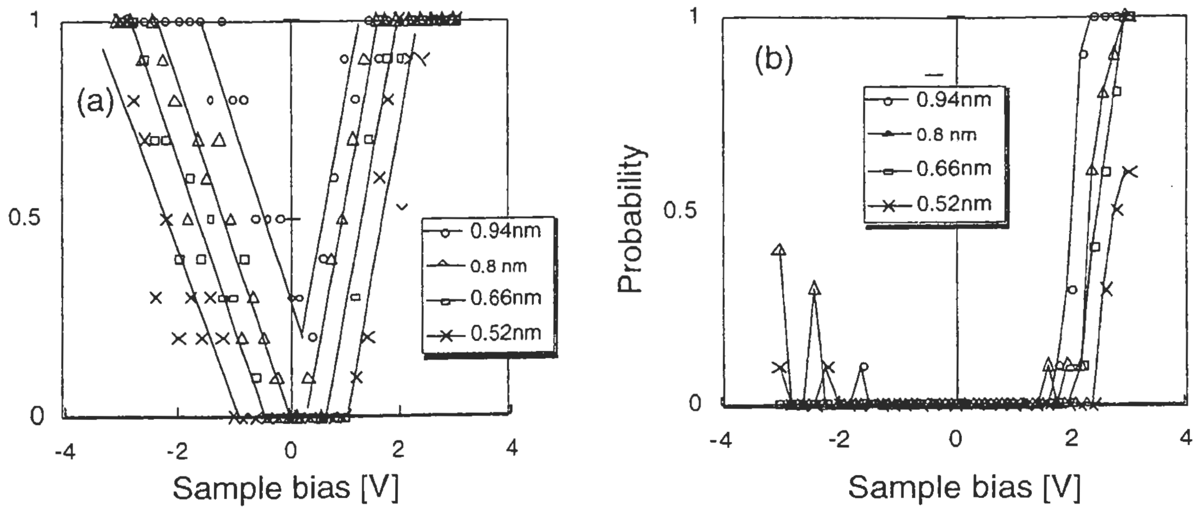

Fig.2 The removal probability of Si atoms from the adatom layer (a) and from the double-layer (b) at various sample bias voltages.

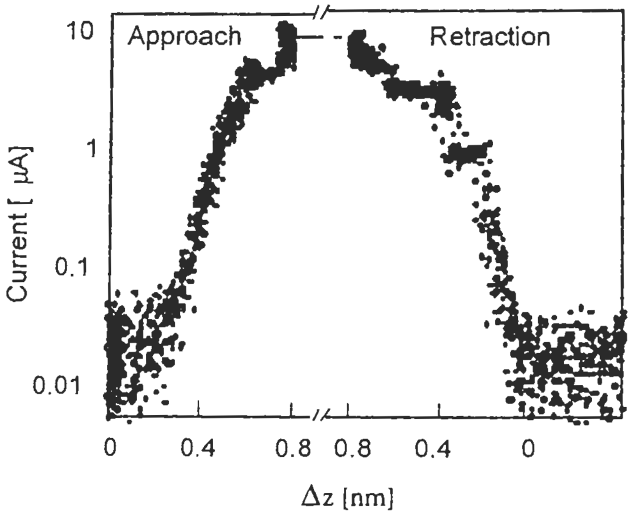

Fig.3 A current (log scale)-tip displacement (Δ z) cureve at a sample bias of +0.8 V.

that the adatoms can be removed even at 0V when the tip displacement is 0.94 nm. On the other hand, in the case of double-layer removal (b), there exists remarkable polarity dependence where the double-layer was preferably removed at the positive bias above a certain threshold value of the voltage (~2 V). The currents flowing between the tip and surface exhibited the characteristic behavior as shown in Fig. 3. During approaching the tip, the current increases logarithmically and starts to saturate (a maximum current) at a certain distance. In contrast, during retracting process, the stair-case decrease is appeared in the current before its final drop to the tunneling region. The periodicity of the stair-cases is ~0.12 nm. The atom-removal proceeds atom-by-atom manner as shown in the image of Fig. 2(a) which can be due to the more brittle bulk property of Si compared with the metal. So the mechanism of the appearance of stair-case structures in the current variation can be attributed to the removal of Si atoms in the bonding between W and Si substrate atom-by-atom manner.

When we plot the maximum current (a) and height of the staircase (b) at various sample bias, we can see the Schottky type rectification for both cases as seen in Figs. 4. Among the electric properties involved in the present experiment such as the Schottky contact, spreading resistance, nanoscale Si wire between the tip and substrate, and surface conductance, only the Schottky contact can be affected by the biases. It means that the staircase current drops can be attributed to the reduction of the Schottky contact area in an atom-by-atom manner. The appearance of a quantized conductance have been reported in metal surfaces, where the staircase drops were expressed as the multiple of the quantified conductance $2e^2/h$ due to the quantum interference effect with decreasing the width of the wires. However, it is not the present case, since the size of the Si wires is limited to an atomic scale.

In order to investigate the Si atom removal processes, we estimated the size of the contact area by dividing the maximum current with the height of the staircase assuming that one staircase drop in the current is caused by reduction of the contact area which one adatom has, i.e. 0.53 nm^2. Then we found it as roughly ~6 nm^2 which is nearly equal to the unit cell of the 7x7 structure(6.3 nm^2). By considering these results, we discuss the mechanisms for the removal processes of the Si atoms. From the result that the probability increases for both polarities with the increase of the sample bias voltage, the adhesion is induced by chemical reaction between the tip and substrate as a result of the local heating by current. Indeed, the probability is less steep for the negative bias voltage, which is consistent with the Schottky-type rectification characteristics of the maximum current. Further, the adhesion is also assisted with the compressive stress applied to the substrate by indentation, since the adatoms can be removal at 0 V with the tip displacement of 0.94 nm. However, we should take account of the contact potential caused by difference in work function between W and Si. At the sample bias voltage of 0 V, there should exist the negative contact potential on Si, since the work function of W and Si in the present experiment

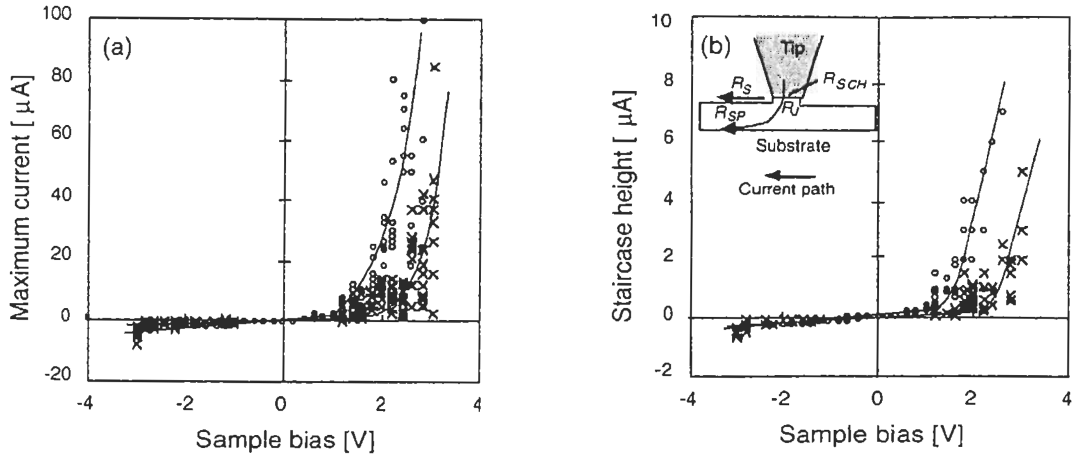

Fig.4 (a) The maximum current and (b) the height of the staircase as a function of the sample bias voltage with the tip displacement of 0.94 (circles) and 0.52 (crosses) nm.

can be estimated to be ~4.5 and ~5.0 eV, respectively. The electric field between the W tip and Si surface may play a role to assist the chemical adhesion in addition to the mechanical compression. Actually, the minimum point of the probability is slightly shifted to the positive bias, which can be explained in the sense of flatband voltage. Therefore, it can be said that the adatom removal occurs due to the chemical adhesion with the assist of 1) mechanical force, 2) contact potential, and 3) current induced heating.

On the other hand, the double-layer is removed with the assist of the electric field, since the probability has polarity dependence and the clear threshold. The positively charged Si atoms can jump up to the tip from the substrate by the field evaporation.

3. Conclusion

We examined the Si atom removal from Si(111)-7x7 surface by approaching and retracting the biased tip to and from the surface. The created holes were either the hole with only adatoms were removed or the hole where simple Si adatoms were formed structures like 2x2, c(2x4) and 3x3 on the exposed layer of Si(111) surface. The type of the holes was able to be controlled by tuning the bias. The mechanism for the Si adatom removal processes was considered as the chemical adhesion enhanced with the assist of the mechanical force, contact potential and current induced local heating of the Si surface during formation of a point contact between the biased tip and surface. The height of the staircase drop in current was attributed to the size reduction of the contact in an atom-by-atom manner. On the other hand, the double-layer was removed by the field evaporation with the assist of electromigration on the Si surface.

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