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Formation and healing of defects at the Si(111) 7×7 surface under low-energy ion bombardment

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We studied the formation and healing of adatom defects on a Si(111)7×7 surface bombarded by 0.5-keV Ar ions. Scanning tunneling microscopy showed that adatoms were missing from the Si(111)7×7 surface. Increasing the temperature during the bombardment increased the percentage of missing adatom sites. However, the percentage saturated at 400 K, then decreased with temperature. This temperature dependence was due to competition between the formation and healing of adatom defects; defect formation dominated at low temperatures, but was overcome by healing at high temperatures. We analyzed the temperature dependence using a rate equation for missing adatoms which included the temperature-independent sputtering and other temperature-dependent formation and healing processes. Activation energies of 0.29 and 0.39 eV were obtained for the temperature-dependent formation and the healing of adatom defects. The temperature-dependent formation was attributed to vacancy-adatom recombination, and the temperature-dependent healing was attributed to the interstitial atom–missing adatom site recombination. These vacancy and interstitial atoms were generated in the collision cascade under the surface. Some of them migrated to the surface and contributed to the temperature-dependent formation and healing of missing adatoms. [S0163-1829(98)03512-7]

I. INTRODUCTION

The interaction of low-energy (below several keV) ions with surfaces has been intensively studied because of the importance of materials processing.[1] The interaction with Si surfaces in particular has been studied in detail, using a scanning tunneling microscope (STM).[2–7] On a Si(111)7×7 surface, bombardment of rare-gas ions causes missing surface adatoms in the low-energy range.[2–4] It has also been reported that adatom defects, introduced to the surface by ion bombardment at room temperature, are healed by subsequent annealing at high temperatures.[4,5] Based on these reports, the formation of adatom defects and their healing would compete at the surface under ion bombardment at high temperatures. In this study, we investigated this competition on a Si(111)7×7 surface under bombardment of 500-eV Ar ions as a function of the temperature during bombardment.

We first explain the experimental apparatus. Next, we describe the results and related discussions. In the results and discussion, we show typical STM images of the bombarded surface, and the characteristics of these images are qualitatively discussed. We then examine the recent suggestion that a defect at the corner adatom site is recovered faster than that at the center adatom site.[5] Based on the STM images, the site of missing adatoms is quantitatively analyzed with respect to their relative positions in the unit cell of the Si(111)7×7 reconstruction; the results of this analysis contradict the recent suggestion. In the bombardment at room temperature, the center adatom site is slightly favored over the corner adatom site by missing adatoms. However, no preference is observed in the healing by annealing up to 900 K subsequent to the bombardment. From this viewpoint, we investigated the competition from the formation with the healing in the bombardment at high temperatures. We counted the number of missing adatoms regardless of the center or corner site, and obtained the percentage of missing adatom sites as a function of the temperature during the bombardment. The missing adatom percentage initially increased with the temperature, but decreased above 400 K. The formation and healing activation energies were quantitatively obtained by analyzing the temperature dependence. We will discuss the elementary processes of the formation and healing that cause the temperature dependence.

II. EXPERIMENTAL APPARATUS

The experiments were performed in an ultrahigh-vacuum (UHV) apparatus consisting of a loading chamber, a preparation chamber with the Ar-ion gun, and a main chamber with the STM unit (JEOL JSTM 4000XV). The base pressure of the preparation and the main chamber was less than 1×10^{-8} Pa. The samples, with dimensions of $1\times7\times0.2\ \mathrm{mm}^3$, were cut out from n-type Si(111) wafers. They were preheated in the preparation chamber at 500 °C for 12 h. The sample was then flashed at 1200 °C and slowly cooled to room temperature. The surface cleanliness was confirmed by STM observation of the 7×7 reconstruction.[8,9]

The 7×7 surface was bombarded by Ar ions. For the bombardment, Ar gas was introduced up to 1×10^{-3} Pa into the preparation chamber. The 500-eV Ar ions hit the surface from a 30° off-normal direction. The ion current was measured at 0.1 $\mu\mathrm{A/cm}^2$ by a Faraday cup. After the bombardment, the preparation chamber was evacuated to UHV, and the sample was then transferred to the main chamber. The STM images of the bombarded surface were observed with a sample bias voltage of $+0.1-+3.0$ V and a tunneling current of 0.3 nA. Images are shown with a conventional gray scale keyed to the surface height.

III. RESULTS AND DISCUSSION

A. STM observation

We studied the formation and healing of adatom defects at the surface by obtaining STM images with atomic resolu-

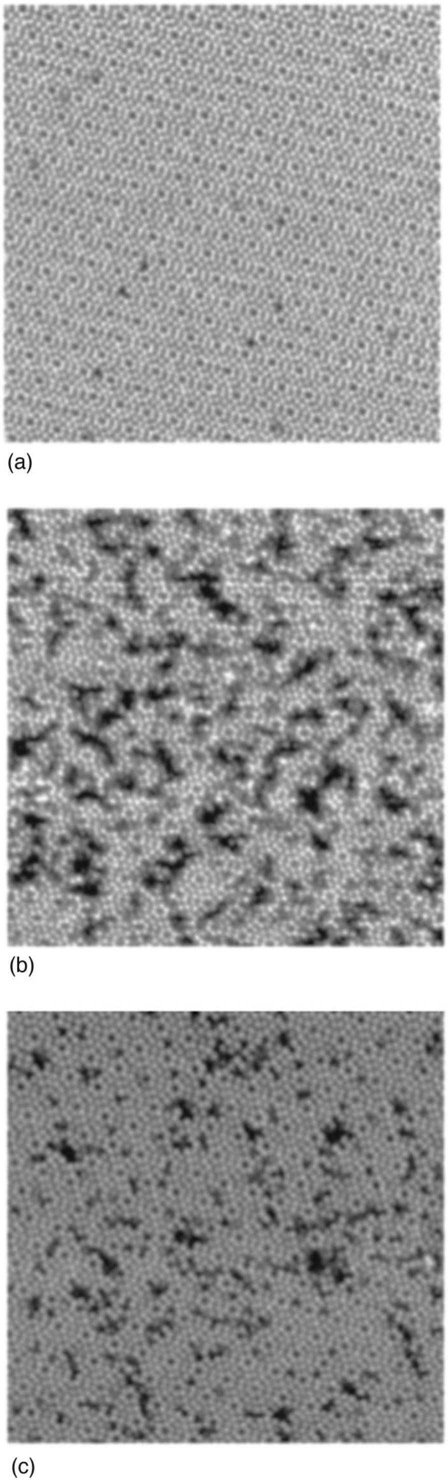

FIG. 1. STM images of the Si(111) surface; (a) before bombardment, (b) after bombardment for 16 s at room temperature, and (c) after annealing for 16 s at 1020 K subsequent to the bombardment for 16 s at room temperature. All these images were taken with a tunneling current of 0.3 nA at a sample bias voltage of 0.2 V.

tion. Typical examples of the STM images are shown in Fig. 1. Figure 1(a) is the image of the clean surface. At this surface, most of the adatom sites of the 7×7 reconstruction were imaged as bright protrusions.[9] However, a considerable number of adatom sites were not imaged brightly after bombardment at room temperature for 16 s [Fig. 1(b)]. The dark site is attributed to the missing adatoms.[2] After annealing at 1020 K for 16 s, the surface in Fig. 1(b) changed to that in Fig. 1(c); many of the adatom defects were recovered by annealing. These images clearly show that the bombardment caused adatom defect formation, and that these defects were healed by annealing at high temperatures.

In the bombardment at room temperature [Fig. 1(b)], the impact of one Ar ion caused the loss of several adatoms.[10] The random introduction of a defect composed of several missing adatoms and their occasional overlap generated the adatom defects distribution shown in Fig. 1(b). However, even at the edges of the defect, the remaining bright protrusions still occupy the adatom sites of the original 7×7 reconstruction. These defect distribution characteristics were also commonly observed at a surface bombarded at high temperatures, though the number of adatom defect sites changed with the temperature (as described below).

Judging from the bright protrusions which remained at the adatom sites of the original 7×7 reconstruction, the second layer of the 7×7 dimer-adatom-stacking fault (DAS) reconstruction[11] is thought to be conserved even at the darkly imaged area. In the 7×7 reconstruction, adatoms aligned over the template of the rest atoms, which aligned with the order in the second layer.[8] Therefore, the adatoms would lose the correlation of the 7×7 reconstruction across the dark region if the second layer was destroyed at the dark region. Thus the surface defect is one monolayer deep; i.e., only the adatoms of the top layer were missed at the surface. This is consistent with the result of a previous scanning tunneling spectroscopy study on defects on an Si(111)7×7 surface bombarded by 3-keV Ar ions.[3]

In addition to the dark and bright sites, a small number of protrusions imaged gray at the bombarded surfaces. These three classes of contrast were previously reported for a Si(111)7×7 surface bombarded by 225-eV Xe ions.[2] In that study, the gray site was tentatively attributed to the site where the adatom was displaced. We found that some gray protrusions appeared at sites slightly shifted from the adatom site of the 7×7 DAS reconstruction; however, a majority of the gray protrusions appeared at the 7×7 adatom site. The origin of the gray protrusions is not presently clear. The adatom was not missed at the site with the gray protrusion; therefore, the gray protrusion was not included in the counting of missing adatoms in the following analysis.

B. Site analysis of adatom defects

Adatom sites on the Si(111) surface can be classified by their position in the unit cell of the 7×7 reconstruction. The unit cell of the 7×7 DAS reconstruction[8] is illustrated in Fig. 2(a). It includes 12 adatoms. These are classified into corner adatoms (Nos. 1, 4, 6, 7, 9, and 12) and center adatoms (Nos. 2, 3, 5, 8, 10, and 11) with respect to their positions relative to the corner hole. They are also classified into the adatoms in the faulted half unit (Nos. 1–6) and in the unfaulted half unit (Nos. 7–12).

Yoneyama and Ogawa recently suggested that the defects at the corner adatom site are recovered faster than those at the center adatom site during annealing of the bombarded Si(111) surface.[5] They also proposed that the healing rate

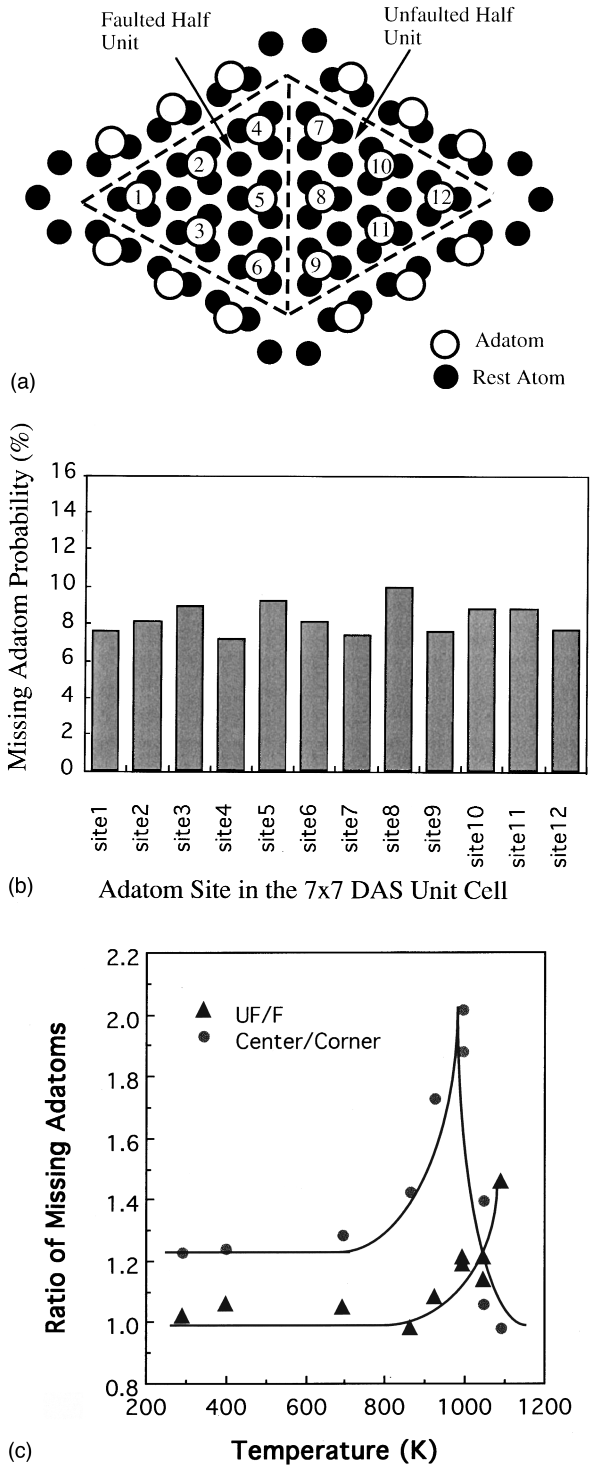

FIG. 2. Site-specific analysis of missing adatoms; (a) the specific sites of the Si(111)7×7 reconstruction. The unequivalent adatoms are numbered from 1 to 12 in the unit cell. (b) The site dependence of missing adatoms at the surface bombarded for 16 s at room temperature. (c) The temperature dependence in the center/corner and unfaulted/faulted ratio of missing adatoms at the surface annealed for 16 s after bombardment for 16 s at room temperature. Solid lines represent visual guides only.

changes with the completion of the corner sites recovery. This makes it complicated to analyze the competition between the formation and the healing. Their proposition implies that the healing preferentially decreases the number of missing adatoms at the corner sites, while the preferential recovery increases the number of target atoms at the corner site for the formation of missing adatoms. If this proposal is valid, we should consider the corner site as distinct from the center site. However, the preferential recovery of the corner site has never been confirmed experimentally. Therefore, we examine the site preference in the formation and healing of missing adatoms before discussing the competition in Sec. III C.

First, we will describe the site analysis of missing adatoms at the surface bombarded at room temperatures. In the analysis, we counted the number of missing atoms over 5000 sites. They were classified into the 12 adatom sites in the 7×7 unit cell, and were normalized as the probability of finding missing adatoms at each site. The result is expressed as the histogram in Fig. 2(b). Figure 2(b) shows the result of the surface bombarded for 16 s at room temperature. Thirty percent of the adatoms were lost from the surface by the bombardment. As the figure indicates, the missing adatom event favors the center site slightly over the corner site. The center-to-corner ratio of missing adatoms was ~ 1.2. The density of missing adatoms increased with the bombardment time. However, since the total number of missing adatoms was less than 60%, the results were similar to that in Fig. 2(b); the center site was always favored slightly over the corner site for missing adatoms. When more than 60% of the adatoms were missed, the site assignment became difficult. This is due to the large reduction of the remaining corner holes which we used as the signpost for the site assignment.

The center site preference in the formation of missing adatoms at room temperature occurs because, at room temperature, the adatom is displaced by the sputtering with the incident ions. Generally stated, its probability is inversely proportional to the binding energy of the atoms at the surface.[13] Thus our result demonstrates that the center adatom bonds to the surface more weakly than the corner adatom. The weaker bond of the center adatoms is due to the atomic configuration of the underlayers. Both the center and corner adatoms bond with the three rest atoms in the second layer. However, all three rest atoms under the corner adatom bond to the Si dimers, whereas only two rest atoms bond to the dimer under the center adatom.[8] The binding energy can be modified on the order of 0.1 eV through the second-neighbor overlap integrals.[14] We suggest that this makes the center site favorable for the missing adatom event.

Next we analyzed the site occupation of missing adatoms after healing. The number of adatoms were counted on the surface, annealed at various temperatures after the bombardment. Before annealing, adatom defects were introduced to the surface by bombardment for 16 s at room temperature. This made 30% of the adatom sites defective. The surface was then annealed for 16 s at various temperatures. As a function of the annealing temperature, we obtained the ratios of missing adatoms at the center-corner sites and in the unfaulted-faulted half unit. The results are shown in Fig. 2(c). With in an error bar of $\pm10\%$, we found that neither the center-corner nor unfaulted-faulted ratios changed during annealing below 800 K. However, this lack of change is not due to a lack of healing progress at low temperatures. The healing of adatom defects was clearly observed in the STM images from the healing above 600 K. At 700 K, half of the adatom defects were healed in annealing for 16 s. Therefore, the healing proceeded with no preference towards the corner site at temperatures below 800 K.

The ratios changed with temperatures above 800 K. In this temperature range, the center-corner ratio increased, showed a maximum at 1000 K, and then decreased. The unfaulted-faulted ratio increased monotonically. These changes were caused by a process other than healing, since healing proceeds with no site preference. We suggest that the changes are due to the site exchange between the adatom and adatom defect. As discussed above, the corner site is energetically favored by adatoms over the center site, and therefore an exchange between the center adatom and the defect at the corner site is energetically favorable. This exchange process is thermally activated at high temperatures, and results in an increase of the missing adatoms at the center sites and a decrease in the missing adatoms at the corner sites. The center-corner ratio of the missing adatoms increased. Therefore, the ratio increases at 900 K was attributed to the temperature, above which the exchange process is highly activated.

The center-corner ratio decreased again at temperatures above 1000 K. In counting the missing adatoms, we found that most of the defects at the corner site were recovered at healing above 1000 K. The number of remaining defects reduced by a percentage at the corner site, making it similar to the clean surface. The center site had a few more defects than the clean surface. Although the number of missing adatoms depends on the way the surface is cleaned, we regard several percent as the equilibrium density of the missing adatoms at room temperature. Therefore, the healing rate may cease at a missing adatom density around several percent. In this case, the healing proceeds only at the center site above 1000 K. We tentatively propose that this is the reason for the decrease of the ratio above 1000 K.

The increase in the unfaulted-faulted ratio is also attributed to the exchange between the adatom and the defect. The ratio increase suggests that the site in the faulted half unit is preferable for the adatom over the site in the unfaulted half unit. However, the preference for the unfaulted site over the faulted site was not clearly observed in the formation of missing adatoms [Fig. 2(b)]. Therefore, the difference in the binding energy is considered to be subtle, causing the preference for the faulted site to be weaker than that for the corner site in the healing. The unfaulted-faulted ratio increased more slowly than the center-corner ratio. Because of the weaker preference, the number of missing adatoms in the faulted half unit was still larger than in equilibrium. Thus, the unfaulted-faulted ratio increased continuously even at temperatures above 1000 K.

C. Bombardment at high temperatures: Competition between the formation and healing of missing adtoms

In high-temperature bombardment, the formation of missing adatom sites competes with their healing, which is thermally activated at high temperatures. To study the competition, the Si(111)7×7 surface was bombarded at various temperatures. After bombardment for 16 s, the surface was cooled to room temperature and observed by the STM. As described in Sec. III B, the preference for the corner site was slight in the formation and negligible in the healing at temperatures below 800 K. Thus we can safely assume that the site preference is negligible at temperatures below 800 K. Based on this assumption, we counted the number of missing adatoms over 5000 adatom sites in STM images, regardless of their relative sites in the 7×7 unit cell. From these data, we calculated the percentage of missing adatom sites at the surface as a function of the bombardment temperature. The result is shown in Fig. 3.[12] We found that the missing adatom percentage increased with the temperature up to 400 K. At 400 K, 60% of the adatoms were displaced from the surface; at higher temperatures, the percentage decreased.

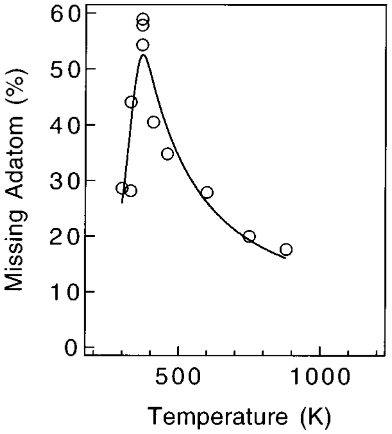

FIG. 3. The temperature dependence of the percentage of missing adatoms at the surface bombarded for 16 s at high temperatures. The fitting with the rate equation is indicated by the solid line.

The temperature dependence shown in Fig. 3 is understood as follows. In high-temperature bombardment, the formation of missing adatoms is thermally activated, as well as healing. The thermal activation of formation causes the initial increase in the missing adatom probability. However, healing is also activated by the temperature. If the healing process exhibits a larger activation energy than defect formation, healing will be suppressed by the formation at low temperatures, but will overcome formation at high temperatures. The competition between the formation and healing processes causes the temperature dependence shown in Fig. 3.

This temperature dependence is odd because of the following two points. (1) The missing adatom is usually caused by the sputtering of adatoms from the incident energetic ions. This phenomenon is independent of the substrate temperature.[13] The healing is activated by the temperature. Thus the number of missing adatoms should decrease monotonically with the temperature in the competition between formation by temperature-independent sputtering and thermally activated healing. However, this is inconsistent with our result. To make it consistent, not only the sputtering but also some thermally activated processes must contribute to the formation of the missing adatoms. (2) Our result suggests that the healing starts to be highly activated at 400 K. To heal the missing adatom site, an additional adatom must be supplied. The step edge at the surface is the most probable source for additional adatoms. However, 400 K is too low to cause the adatom's detachment from the step.[15]

To understand this result, we analyzed the temperature dependence with a rate equation using the surface density of adatoms n. (1) Sputtering of the surface adatoms with the incident ions and (2) the supply of additional adatoms from the step edge can contribute to the change of adatom density n. In addition to these processes, (3) thermal desorption of adatoms and (4) absorption of adatoms into the step edge can change the surface adatom density. During bombardment, vacancy and interstitial Si atoms are generated by the collision cascade under the surface.[13,16] Some of these migrate to the surface and recombine with the adatom or adatom defect at the surface.[4] (5) The vacancy-adatom and (6) interstitial Si atom-adatom defect recombination can also contribute to the change of adatom density n.

These processes contribute to the temporal decrease of the adatoms $-dn/dt$ as follows. (1) Sputtering causes a decrease of adatoms. With the sputtering cross section σ, the decrease rate is described by σnJ,[17] where J is the flux of incident ions. (2) An adatom supply from the step edge increases n. However, its contribution is negligible in our temperature range, as described above. (3) Thermal desorption decreases the number of adatoms, but has been reported to be active only at temperatures above 1000 K.[18,19] Thus this contribution is also negligible. (4) Adsorption of adatoms into the step edge decreases the number of adatoms. This process has been reported to be active in the homoepitaxial growth of Si on a (111) surface at temperatures below 1000 K, and therefore this contribution should be included in the rate equation. The decrease rate of adatoms is proportional both to the density of adatoms n and adsorption sites (i.e., kink sites) m. Therefore, its contribution is described as P_1nm. Here the rate coefficient P_1 has the temperature dependence of $P_1=p_1\exp(-E_{p1}/kT)$. E_{p1} is the activation energy of this process. (5) The vacancy-adatom recombination contributes to the decrease of adatoms. The decrease rate is proportional to the density of adatoms n and the vacancy N_V under the surface. Thus, with the rate coefficient of the recombination $P_2=p_2\exp(-E_{p2}/kT)$, its contribution is described as P_2nN_V. (6) The interstitial atom–missing adatom site recombination increases the number of adatoms. Its contribution is proportional to the density of missing adatoms sites $(N-n)$ and interstitial atoms under the surface N_i. Here N is the surface density of adatoms at a perfect Si(111)7×7 surface. With the rate coefficient of recombination $Q=q\exp(-E_q/kT)$, its contribution is described as $-Q(N-n)N_i$. Both N_V and N_i change in the competition progress. However, we assume that both are independent of n, because sufficient vacancy-interstitial atom pairs continued to be generated under the surface[13,16] during the bombardment.

By summing up the above factors, we obtained the following rate equation:

$$-dn/dt=\sigma Jn+P_1nm+P_2nN_V-Q(N-n)N_i. \tag{1}$$

In this equation, the first, second, and third terms on the right side contribute to the formation of missing adatoms, whereas the last term contributes to the healing. Here both the second and third terms are temperature dependent and proportional to n. Therefore, we simplified the equation as follows:

$$-dn/dt=\sigma Jn+[\alpha_0\exp(-E_\alpha/kT)]n-[\beta_0\exp(-E_\beta/kT)](N-n). \tag{2}$$

We solved this equation using the condition of $n=N$ at $t=0$. The solution was used to calculate the percentage of missing adatom sites $(N-n)/n(\%)$ at $t=16$ s. We fitted the result with the calculated percentage by using the measured σ (Ref. 10) and J. The calculated percentage accorded well with the experiment for $E_\alpha=0.29$ eV, $E_\beta=0.39$ eV, $\alpha_0=392$, and $\beta_0=9290$, as shown by the solid curve in Fig. 3.

Regarding the activation energy $E_\alpha=0.29$ eV, we attribute the temperature-dependent formation of missing adatoms to the vacancy-adatom recombination. In the recombination, the activation energy is expected to be roughly equal to that for vacancy diffusion in the bulk. An activation energy of 0.33 eV was reported for vacancy migration in bulk Si.[20] 0.43 eV was used for the vacancy migration in a recent molecular-dynamics (MD) simulation of the Ar irradiation of Si crystals.[4] These are sufficiently close to our energy of 0.29 eV. However, 0.29 eV is too small to be attributed to the formation of missing adatoms by adatom adsorption into the step edge. For adsorption into the step edge, the adatom migrates on the terrace, then attaches to the kink site. The diffusion of Si atoms was reported to have an activation energy of 1.3 eV (Ref. 21) at the Si(111)7×7 surface. An activation energy of 1.4–1.6 eV was also reported for the attachment.[22] Thus we propose that the temperature dependence for defect formation is predominantly caused by the recombination of adatoms with vacancies migrating from below the surface.

An activation energy of 0.39 eV was obtained for the healing by the interstitial atom–missing adatom site recombination. This energy should be roughly equal to the migration energy of the interstitial Si atom in the bulk. For the self-interstitial atom diffusion in Ge, 0.3 eV was reported as the upper limit on the migration.[24] Since the chemical nature of Si is close to Ge, an energy around 0.3 eV is expected for Si. However, an energy of 0.80 eV was also reported for the n-type Si.[23] 0.90 eV was used in recent MD simulation of the diffusion of the interstitial atom in the bulk Si crystal.[4,16] Our obtained energy was half of these values. To examine which energy is realistic, we estimated the diffusion time of interstitial atoms. By a TRIM (transport of ions in matter) simulation[26] of the 500-eV Ar-ion bombardment of Si, the ion range is estimated to be ~50 Å.[27] Interstitial atoms distribute in this region. The migration length x in the diffusion time t is described by $\overline{x^2}\sim(t/\tau)l^2$ in the diffusion of interstitial atoms by random walk. Here $\tau=\tau_0\exp(E_d/kT)$, and l are the hopping interval and hopping length, respectively.[28] Assuming that $\tau_0=10^{-13}$ s and $l=1.5$ Å [a half of the spacing between two double layers along the Si(111) direction], we estimated t for $x=50$ Å at 400 K. For $E_d=0.4$ eV, t was $\sim10^{-5}$ s, whereas t was 1.7 and 22 s for $E_d=0.8$ and 0.9 eV, respectively. In this study, the surface was bombarded by Ar ions for 16 s. In this 16 s, healing progressed at 400 K. Thus t should be less than 16 s. In this respect, the diffusion energy of interstitial atoms is at least less than 0.8 eV. Thus 0.39 eV can probably be attributed to the diffusion energy of interstitial atoms. On the other hand, much larger activation energies have been reported for adatom surface diffusion

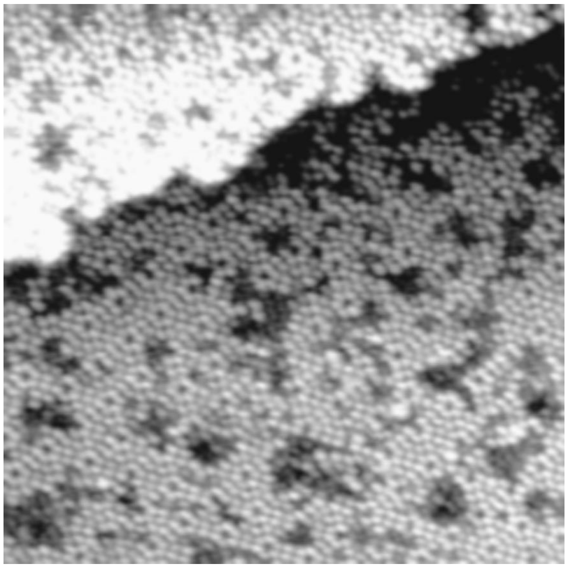

FIG. 4. The STM image of the surface bombarded at 900 K for 16 s. The image was taken with a tunneling current of 0.2 nA at a sample bias voltage of +0.2 V. No difference was observed between the near and far step regions in the distribution of missing adatoms.

(1.3 eV) (Ref. 21) and adatom detachment at the surface step (1.4–1.6 eV).[22] Moreover, as shown in Fig. 4, advanced recovery of the near step region was not observed at the bombarded surface. Thus the adatom supply from the step edge is negligible for healing. From this viewpoint, the interstitial atom–missing adatom site recombination is likely the origin of the temperature-dependent healing process.

The analysis of data in Fig. 3 indicates that the vacancy and the interstitial atom in the bulk make a significant contribution to the surface defect yield. The contribution of defects in the bulk was demonstrated in the low-energy ion bombardment on the Ge(001) (Ref. 24) and Pt(111) surfaces.[25] For Si(111) surfaces, a study was also reported in Ref. 4. Our results complement the study of Ref. 4 in showing the contribution of the vacancy and interstitial atoms to the formation and healing of missing adatoms at the Si(111) surface. In the study of Ref. 4 the Si(111) surface was bombarded by 5-keV Ar ions, followed by annealing at 350 and 500 °C. It was found that the number of missing adatoms increased at 350 °C and decreased at 500 °C. Since the surface was not bombarded in the annealing, the missing adatoms increase proceeded by some process other than sputtering. Although the activation energy was not obtained experimentally, the authors of Ref. 4 attributed the increase and decrease to the recombination of the vacancy-adatom and interstitial atom–missing adatom site in their MD simulation. We experimentally obtained the activation energy of the process other than sputtering in our study; we attribute it to the recombination of vacancy adatoms. Thus combining our results with the results of Ref. 4 strongly demonstrates that the vacancy under the surface contributes to the formation of missing adatoms at the surface.

IV. SUMMARY

In summary, we studied the formation and healing of missing adatoms on a Si(111)7×7 surface under 500-eV Ar-ion bombardment. The bombardment caused missing adatom defects that are healed by annealing after the bombardment. The formation of missing adatoms favored the center adatom site slightly over the corner adatom site. However, no preference was observed in the healing by annealing at temperatures below 800 K. In bombardment at high temperatures, the formation process competes with the healing process. By counting the number of missing adatoms, regardless of the site, we investigated the competition as a function of the temperature during bombardment. The percentage of missing adatoms increased with the temperature, showing a peak at 400 K, then decreased. In analyzing the result using a rate equation, we found that the formation of the adatoms was caused by temperature-independent sputtering with the incident ions and a temperature-dependent process with an activation energy of 0.29 eV. The healing was caused by a temperature-dependent process with an activation energy of 0.39 eV. The temperature-dependent formation and healing processes were attributed to the vacancy-adatom and interstitial atom–missing adatom site recombination.

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