Influence of 1×1 defects on Schottky barrier height at the Ag/Si(111)7×7 interface

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We examined the influence of 1×1 defects at the Si(111)7×7 surface on the Schottky barrier height (SBH) of the Ag/Si interface. By quenching samples from high temperatures, we intentionally introduced 1×1 defects on Si(111) 7×7 surfaces. After characterizing the area of the 1×1 defects by scanning tunneling microscope, we deposited Ag films *in situ* at room temperature on the surfaces and measured the SBH. As the 1×1 area increased from 0 to 50 %, SBH increased from 0.60 eV to 0.66 eV. The 1×1 area dependence of the SBH was caused by a locally high SBH in the 1×1 area with the pinch-off area extending around it.

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I. INTRODUCTION

The Ag/Si interface is abrupt, and has no silicide phase.[1] Furthermore, recent x-ray diffraction studies have shown that the 7×7 long-range ordering is preserved at the interface when the Ag film is deposited at room temperature on the Si(111)7×7 surface.[2–4] In addition, a close correlation between the interface structure and Schottky barrier height (SBH) was pointed out.[5] We thus expect the Ag/Si(111)7×7 interface to exhibit a reproducible SBH. However, the previously reported SBH of the Ag/Si(111)7×7 interface has scattered,[6–10] though the Ag films were deposited on Si(111) surfaces that had been confirmed to exhibit the 7×7 reconstruction by electron diffraction.

Surface segregation of the dopants in thermal cleaning has been pointed out as a possible origin of the scattering in SBH.[7,8] Besides the dopant segregation, the 1×1 defects at the Si(111)7×7 surface could cause scattering in SBH. In preparing the Si(111)7×7 surfaces, the sample is usually flashed at high temperature above 1000 °C in ultra-high vacuum (UHV). The surface has a perfect 7×7 reconstruction when the sample is cooled slowly enough after the flash, while the 1×1 patchy domains appear in the 7×7 reconstruction when the sample is quenched after the flash.[11–13] However, the surface including the 1×1 domains also exhibits the 7×7 diffraction pattern. The inclusion of the 1×1 defects is not observed in the electron diffraction pattern. The 1×1 defects could affect the growth of Ag and the interface structure to give different SBHs from the 7×7 surface. However, the effect of the 1×1 defects on SBH has not received much attention. In this study, we introduced the 1×1 defect at the Si(111)7×7 surface intentionally, and investigated its effect on SBH.

II. EXPERIMENT

Our experiments were conducted in an UHV apparatus consisting of the loading chamber, the treatment chamber with an Ag Knudsen cell, and the main chamber with a scanning tunneling microscope (STM) unit.[14,15] The base pressure of the treatment and main chambers was less than 2×10^{-8} Pa. The samples, with dimensions of 2.5 mm ×7.0 mm×0.2 mm, were cut from a low doped *n*-type Si(111) wafer ($\rho=1.5\ \Omega$ cm). We made ohmic contacts on the backside of the samples by depositing Sb and Au for dc current heating and *I-V* characteristic measurement.

In the UHV apparatus, the samples were cleaned by 1200 °C flash heating to expose 7×7 reconstruction at the surface. The samples were then cooled to room temperature slowly (1 K/sec) to prepare the perfect 7×7 reconstructed surface or quickly to prepare the 7×7 surface with 1×1 defective domains. Since rapid cooling at around the transition temperature from high-temperature metastable 1×1 to stable 7×7 phase is necessary to freeze the 1×1 defect domains in the 7×7 reconstruction,[11,12,16–18] we quenched the samples by turning off the heat current at high temperatures to preserve 1×1 domains in this study. Although the appearance of 1×1 defects was stochastic, the appearance of the 1×1 domains was strongly affected by the temperature at which the heat current was turned off. By changing the heat-off temperature from 1200–880 °C, we were able to control the 1×1 area in the range of 0 to 50 % at the Si(111)7×7 surfaces. The 1×1 area was characterized as an average of the local 1×1 areas observed in more than 100 scanning tunneling microscopy images taken randomly at various points on the surface.

After the STM characterization of the 1×1 domains, we deposited 200 nm thick Ag films *in situ* on the surface at room temperature. By using a hard mask, we deposited Ag on the 1 mm^2 area in the center of the sample surface. The *I-V* characteristics of the Ag/Si(111) samples were measured *ex situ*. SBH and the ideal factor were deduced by fitting *I-V* characteristics with the thermoionic emission theory[19] after subtracting the voltage drop at the backside ohmic contact. To rule out any effect of dopant segregation, we prepared the surfaces with 1×1 defects of smaller and larger thermal budgets than the standard 7×7 surfaces with no defects. The 1×1 surfaces of smaller thermal budget were prepared by quenching just after the flashing (omitting the slow cooling necessary to obtain the perfect 7×7 surface). The 1×1 surfaces with larger thermal budgets were prepared by quenching the perfect 7×7 surfaces that were made by the standard flashing and subsequent slow cooling processes. No systematic difference was found in SBH and the ideality factor between the 1×1 samples prepared in these two ways. The

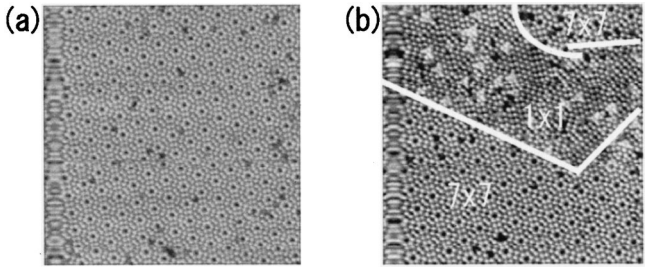

FIG. 1. STM images of the slowly cooled (a) and quenched Si(111) surfaces (b).

scatterings were less than 0.01 eV and 0.05. Thus, the changes in SBH we report here are regarded to be caused purely by the inclusion of the 1×1' defects at the Si(111)7×7 surface.

III. RESULTS

Typical STM images of the slowly cooled and quenched Si(111) surfaces are shown in Figs. 1(a) and 1(b). The slowly cooled samples exhibited a perfect 7×7 reconstruction over all the surface. The quenched samples included 1×1 domains in the 7×7 reconstruction. In the 1×1 domains, adatoms were arranged with 2×2 or $c(2\times4)$ short-range ordering, though they did not hold any long-range ordering.[11,12] In the Ag growth on the 7×7 surface, small Ag islands nucleated and were confined in the half unit cell of the 7×7 reconstruction.[14,20,21] With the coverage, the two-dimensional (2D) Ag islands became larger in each half unit cell and percolated to form the 2D wetting layer keeping the 7×7 long-range ordering. In further deposition, the 3D Ag islands nucleated on the 2D wetting layer incoherently with the ordering of the underlying wetting layer. However, the 7×7 ordering in the wetting layer was preserved even after the 3D island nucleation. Thus, the Ag/Si(111) interface grown on the perfect 7×7 reconstruction maintained the 7×7 ordering as has been confirmed by x-ray diffraction experiments.[3,4] In contrast, no long-range ordering was preserved in the growth on the 1×1 domains. Therefore, the 7×7 interfacial ordering was broken locally at the interface grown on the sample including the 1×1 domains.

Figure 2 shows the 1×1 area dependence of SBH. The Ag/Si(111) interface on the prefect 7×7 reconstruction had an SBH of 0.60 ± 0.005 eV. The 1×1 area at the Si(111) surface caused an increase in SBH. Roughly, SBH increased linearly with the 1×1 area as illustrated by the dotted line. The 40% 1×1 area at the 7×7 surface raised SBH to ~0.65 eV. The ideality factor (n) also increased from less than 1.05 to ~1.6 with the inclusion of the 1×1 area (not shown).

IV. DISCUSSION

Figure 2 suggests that SBH is locally large on the 1×1 domains at the Ag/Si(111) interface. Schmidtdorf *et al.*[22] proposed that the stacking fault half unit of the 7×7 reconstruction has a dipole to lower the SBH at the Ag/Si(111) interface. They suggested that the 1×1 interface has a higher

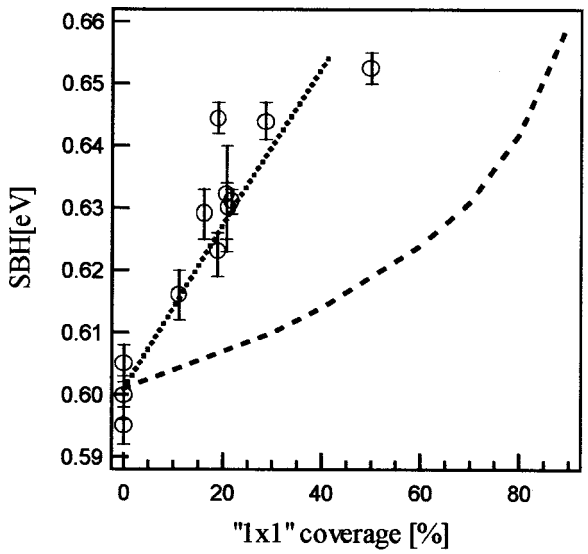

FIG. 2. SBH vs 1×1 area. Experimental data, circle+error bar. Dashed line, a calculation assuming that the experimentally observed 1×1 area did not pass the current. Dashed line, a calculation by extending the 1×1 area to fit the data.

SBH because the characteristic dipole of the 7×7 reconstruction disappears. However, more detail is not available about the reason for the large SBH on the 1×1 area, though it is reasonable to expect that the breaking of the 7×7 interface ordering at the 1×1 domains could yield specific interfacial electronic states that modify SBH locally. In the following, we assume *a priori* that the 1×1 area has a high SBH locally, and discuss its effect on the 1×1 area dependence of SBH we measured. In this respect, we regard the measured forward current as consisting of two components, the current through the 7×7 area and the current through the 1×1 area. Thus, the measured current (I) is given by the following equation in the framework of the thermoionic-emission theory:[19]

$$I=AST^2\{\exp(\beta V-1)\}\{(1-X_{1x1})\exp(-\beta\Phi_{7x7}) + X_{1x1}\exp(-\beta\Phi_{1x1})\}.$$

Here, A is the Rechardson constant for an n-type Si(111) interface, S is the interface area, T is the temperature, $\beta=1/(kT)$, and k is the Boltzmann constant. $X_{1\times1}$ is the area occupation of the 1×1 domain. $\Phi_{7\times7}$ and $\Phi_{1\times1}$ are the SBH on the 7×7 and 1×1 local domains, respectively. At $\Phi=0.60$ eV, a local increase in SBH by 0.10 eV reduces the current through the area by a factor of two. Thus, in the simplest approximation, we assume that the local SBH on the 1×1 increased over 0.10 eV and that the forward current on the 1×1 is negligible. In this case, only the current through the remaining 7×7 area (i.e., the first term in the last parentheses on the right-hand side of the above equation) contributes to the measured current. However, SBH was evaluated as the current flowing uniformly through all the area under the Ag dot in our experiment. Thus, the decrease in the current at the 1×1 local area results in an increase of the *apparent* SBH in this study. In Fig. 2, the dashed line

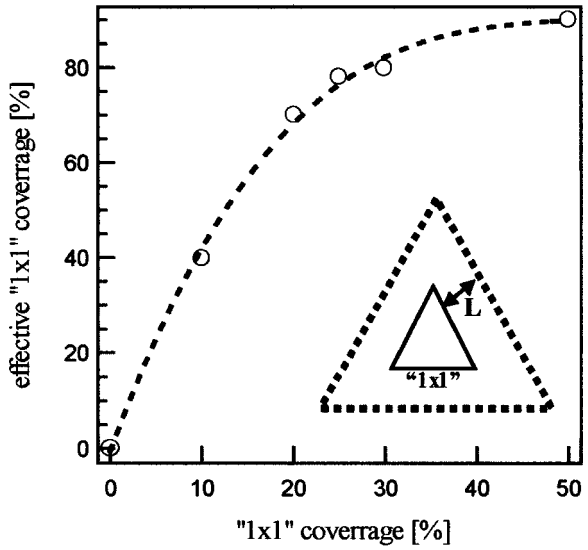

FIG. 3. Effective 1×1 area vs experimentally observed 1×1 area. Effective 1×1 area fits the experimental data better as indicated by the dotted line in Fig. 2. Inset, exudation of the pinch-off area of the width L around the 1×1 domain.

represents the *apparent* SBH calculated with the above assumption as a function of the 1×1 area measured experimentally. As shown in the figure, this assumption qualitatively explains the increase of the SBH with the 1×1 area. However, the quantitative agreement is not satisfactory.

To make the fitting better, we need more 1×1 area than was observed experimentally. Figure 3 shows the relation between the 1×1 area observed experimentally and the 1×1 area necessary to make the fit better as indicated by the dotted line in Fig. 2. The discrepancy between the observed 1×1 area and the area necessary for the better fitting could be solved by exuding the pinch-off area[22] of the high SBH around the 1×1 area. Based on Fig. 3, we estimated the size of the exuded pinch-off area assuming that the pinch-off area extended as a zone of width L around the 1×1 domains observed experimentally as illustrated in the inset of Fig. 3. As a result, L was roughly estimated to be 5–10 nm.

To examine the possibility of a pinch-off area of such a width, we calculated the potential around the 1×1 area. Here, the potential was assumed to be 1.00 and 0.60 eV on the 1×1 and 7×7 local domains at the Ag/Si(111) interface for simplicity. The effect of the local 1×1 area of high SBH was approximated by a dipole moment, and the Poisson equation was solved to obtain the spatial distribution of the potential[23] around the 1×1 domain. For the points 5, 10, and 20 nm apart from the 1×1 domain in the interface, we show the potential as a function of the depth from the interface (z)

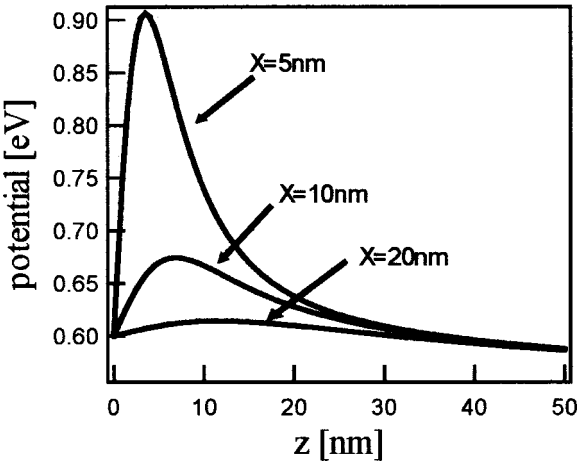

FIG. 4. Calculated depth profile of the potential barrier. Z, depth from the interface; X, distance from the edge of the 1×1 area in the interface plane.

in Fig. 4. Local maxima appear in the depth profile at $Z=5$–10 nm for points 5 and 10 nm apart from the 1×1 domain. The local maximum gives substantial SBH in the forward current transport. Thus, the depth profile means that the high SBH area exudes around the 1×1 domain. As mentioned in the preceding paragraph, the increase of 0.10 eV is enough to make the forward current pinchoff. Thus, the present calculation indicates the pinch-off area has a width of 5–10 nm. This width agrees with the experimentally estimated value. However, the width of the pinch-off area depends on the potential of the 1×1 area assumed in the calculation. The width becomes smaller as the potential assumed for the 1×1 domain decreases. In this respect, the local barrier height on the 1×1 domains should be determined experimentally. We are preparing to measure the local SBH distribution around the 1×1 area by ballistic electron emission microscope.[24] However, at present stage of our study, we attribute the necessity of a larger 1×1 area for the fitting to the high SBH area exuding around the 1×1 domains.

V. SUMMARY

In summary, we examined the effect of the 1×1 local domains at the Si(111)7×7 surface on SBH at the Ag/Si(111) interface. SBH was found to increase with the 1×1 area. The increase in SBH is qualitatively explained by the 1×1 area of high local SBH. However, a quantitative explanation needs the $5\sim10$ nm exudation of the high SBH pinch-off area from the 1×1 domains. A rough estimation supports the exudation of the pinch-off area of this width.

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