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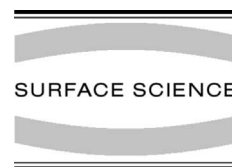
# Surface roughness and electrical resistance on Si(1 0 0)2 × 3-Na surface

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## Abstract

Using scanning tunneling microscopy, reflection-high-energy-electron diffraction and in situ electrical-resistance measurements, we studied the relation between surface morphology and electrical resistance of a Si(1 0 0)2 × 3-Na surface phase. It was found that the step density and domain size of the 2 × 3-Na phase depended on Si coverages deposited prior to Na deposition, because the amount of Si atoms incorporated in the 2 × 3-Na phase is a definite value, 1/3 monolayer (ML). The evolution of surface morphology was found to influence the transport properties dramatically. The resistance was reduced for smoother surfaces with larger domains with the pre-deposited Si of around 1/3 or 4/3 ML, while it increased for rougher surfaces with the intermediate amounts of Si pre-deposition. These phenomena directly associate with carrier scattering due to surface roughness. © 2001 Published by Elsevier Science B.V.

## 1. Introduction

Among other submonolayer-metal-on-silicon systems, alkali-metal-adsorbed Si surfaces are one of the most extensively studied systems [1–7]. This is partly because such surfaces exhibit extraordinary chemical and electronic properties that show promise for possible device applications [8–10],

and partly because alkali-metal atoms have simple electronic structures and do not form silicides so that they are considered to be a handy prototype for study of atom adsorption on solid surfaces in general.

Formation of the Si(1 0 0)2 × 3-Na surface phase has been found to involve a substantial redistribution in the top layer Si atoms of Si(1 0 0) substrate (i.e. surface Si mass transport) because the Si atom concentration in the 2 × 3-Na phase is 1/3 monolayer (ML), rather than 1 ML [11]. Consequently, a flat terrace of the 2 × 1 clean surface converts to a rough surface which contains numerous small domains dividing by monoatomic

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steps [12] when the $2 \times 3$-Na phase is formed. Using this phenomenon, reversibly, the surface morphology can be controlled by adding small amount of Si atoms prior to making the $2 \times 3$-Na phase. For example, if one provides additional 1/3 ML of Si on the initial Si(1 0 0)$2 \times 1$ clean substrate, which is exactly the amount of Si necessary for the $2 \times 3$-Na phase, the substrate Si atoms do not need to be incorporated, resulting in the step-terrace configuration kept unchanged at the $2 \times 3$-Na phase formation.

Recently, on the other hand, it has been found that the surface conductivity is reduced in the $2 \times 3$-Na phase compared with the $2 \times 1$ clean surface [13], when the $2 \times 3$-Na phase was made on the pristine $2 \times 1$ clean surface without pre-deposition of Si. As a possible reason of such behavior, the above-mentioned change in surface roughness accompanied with the $2 \times 3$-Na phase formation was proposed.

In the present paper, we report results of in situ measurements of surface resistance and reflection-high-energy-electron diffraction–scanning tunneling microscopy (RHEED–STM) studies of the Si(1 0 0)$2 \times 3$-Na phase formation. Pre-deposition of controlled amounts of Si atoms led to changes in surface roughness and domain size of the $2 \times 3$-Na phase, which correlated to the change in surface resistance; the rough surfaces showed higher resistance. Although it is not yet known whether the surface conductivity of this phase is due to the surface-state bands or surface-space-charge layer, the present results directly demonstrate that the surface steps and domain boundaries actually scatter the carriers flowing at/near the surface.

## 2. Experiments

Experiments were carried out in separate ultrahigh vacuum chambers with base pressure of less than $2 \times 10^{-10}$ Torr, one of which was for in situ electrical resistance measurements at low temperatures combined with RHEED, and other was for STM with RHEED. The substrates used were P-doped Si(1 0 0) wafers of 35–40 $\Omega$ cm resistivity. An atomically clean Si(1 0 0) surface was prepared in situ by direct heating up to 1250°C.

After this treatment, a sharp $2 \times 1$ RHEED pattern was observed at room temperature (RT), and STM images corresponded to a well-ordered $2 \times 1$ surface. Sodium atoms were deposited from thermal cell (from SAES Getters Inc.) onto the $2 \times 1$ substrate kept at 250°C with direct heating to make the $2 \times 3$-Na phase. The deposited Na coverage was estimated by assuming a saturation coverage of the $2 \times 3$-Na phase to be 1/3 ML in accordance with the data of Ref. [11], and its deposition rate was about 0.1 ML/min. Before making the $2 \times 3$-Na surface phase, controlled amounts of Si were deposited on the $2 \times 1$ clean substrate at RT. The deposition rate of Si was about 0.4 ML/min, which was determined in the separate measurements by using the intensity oscillation of RHEED specular spot during homo-epitaxy at a substrate temperature of 600°C. The important parameter in the present study is the pre-deposited Si coverage $\theta_{Si}$, rather than the Na coverage. The Na coverage was always the same ($\theta_{Na} = 1/3$ ML) to make the $2 \times 3$-Na phase.

The resistance near the surface region of the Si wafers having the $2 \times 3$-Na structure was measured under isothermal conditions at 180 K by a kind of macroscopic four-probe method; a voltage drop between a pair of Mo wire contacts (0.3 mm in diameter) about 5 mm apart was measured, with small direct currents supplied through the clamp electrodes of both ends of the Si wafer. The ohmic relation between the voltage signal and current was confirmed from 0 to 100 μA range.

For STM observation at RT, electrochemically etched tungsten tips cleaned by in situ heating were employed. The sample surfaces were prepared in the same ways with aid of RHEED as in the chamber for the resistance measurements.

## 3. Results and discussion

In order to characterize the surface morphology first, line profiles of specular and fractional-order RHEED spots along lines perpendicular to the shadow edge were measured at the $2 \times 3$-Na phase. Fig. 1a and b shows typical profiles of such spots, indicating that the spots are sharp at the pre-deposited Si coverage $\theta_{Si}$ around 0.2–0.4 ML,
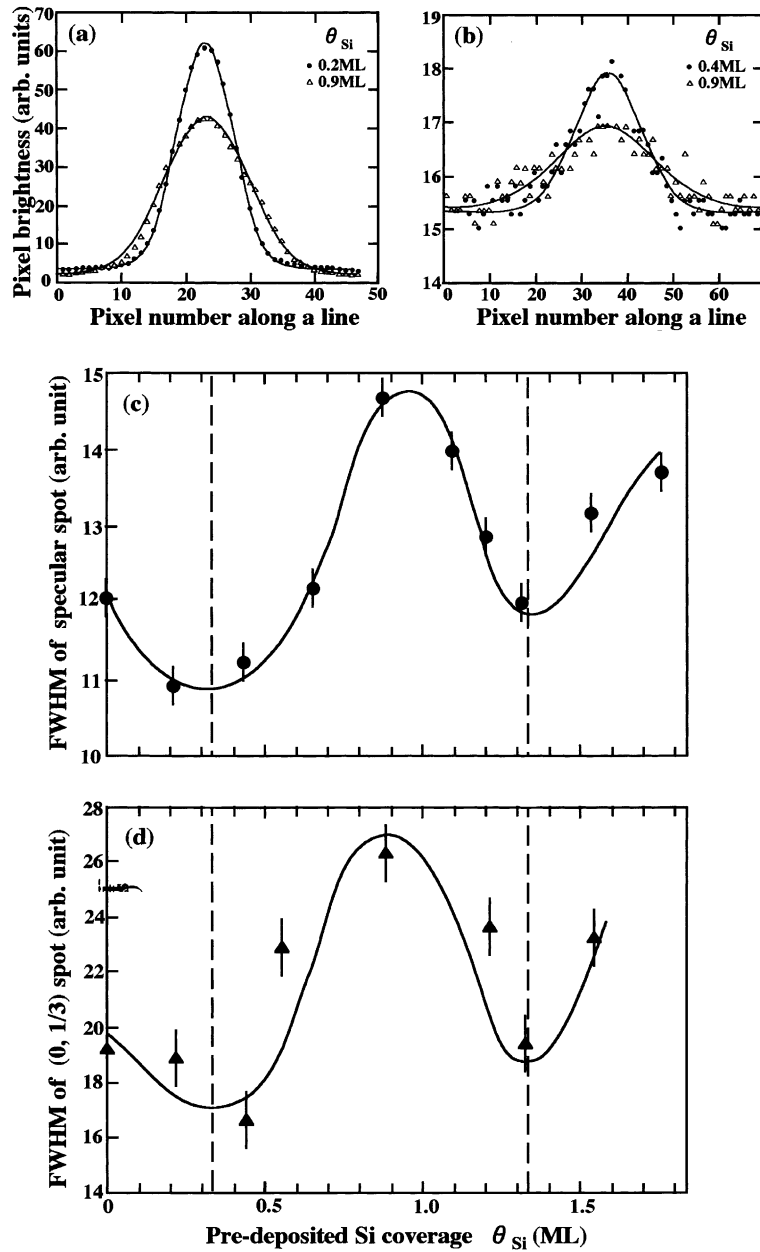
Fig. 1. Line profiles of (a) specular and (b) (0,1/3)th RHEED spots of Si(1 0 0)2 × 3-Na surfaces that were prepared on the substrates with different pre-deposited Si coverages. The variation of FWHM of (c) specular and (d) (0,1/3)th RHEED spots of Si(1 0 0)2 × 3-Na surfaces as a function of the pre-deposited Si coverage.

while they are broader at $\theta_{Si} \sim 0.9$ ML. The full width at half maximum (FWHM) of the specular spot thus obtained shows a periodic change as a function of $\theta_{Si}$ as shown in Fig. 1c, which corre-sponds to a periodic change in the surface rough-ness. The surface is smooth, corresponding to the minimal FWHM, at $\theta_{Si} \sim 1/3$ or $4/3$ ML, while the surface is rougher with higher step densities at

intermediate $\theta_{Si}$. Similar behaviors were also observed for the $(0, 1/3)$th-order spot for the $2 \times 3$-Na superstructure (Fig. 1d), indicating a change in domain size. The minimal and maximal values of FWHM for both of the specular and fractional-order spots occurred at the same coverages $\theta_{Si}$.

The direct STM observations revealed such an evolution of surface morphology of the $2 \times 3$-Na phase as a function of $\theta_{Si}$. Fig. 2a shows a filled-state STM images of a fresh Si(1 0 0)$2 \times 1$ clean surface before the Na deposition. The surface consists of flat terraces of about 350 Å in width separated by monoatomic steps, containing also a modest number of surface defects. Formation of the $2 \times 3$-Na phase on this original substrate upon the Na deposition resulted in a surface like that shown in Fig. 2b. One can see the $2 \times 3$ reconstructed islands of different sizes with basically rectangular shapes at different height levels. In this

way, the surface becomes rougher at the structural conversion to the $2 \times 3$-Na from the $2 \times 1$ clean surface, due to the different concentrations of Si atoms between the two phases. This is the case for $\theta_{Si} = 0$ ML, i.e., without pre-deposition of Si. When Si of about 0.3 ML coverage was deposited on the initial $2 \times 1$ clean surface prior to the Na deposition ($\theta_{Si} \sim 0.3$ ML), the $2 \times 3$-Na surface became smoother with terrace widths comparable to those on the original $2 \times 1$ clean surface (Fig. 2c). In case of $\theta_{Si} \sim 0.8$ ML, the $2 \times 3$-Na surface became rougher again as shown in Fig. 2d. Closer inspection in this image reveals that small $2 \times 3$-Na domains are divided by monoatomic steps, resulting in a very rough surface. At $\theta_{Si} \sim 1.3$ ML, the $2 \times 3$-Na surface returned to be smoother as shown in Fig. 2e, consisting of larger $2 \times 3$-Na domains. Thus the surface roughness actually changes periodically with $\theta_{Si}$.
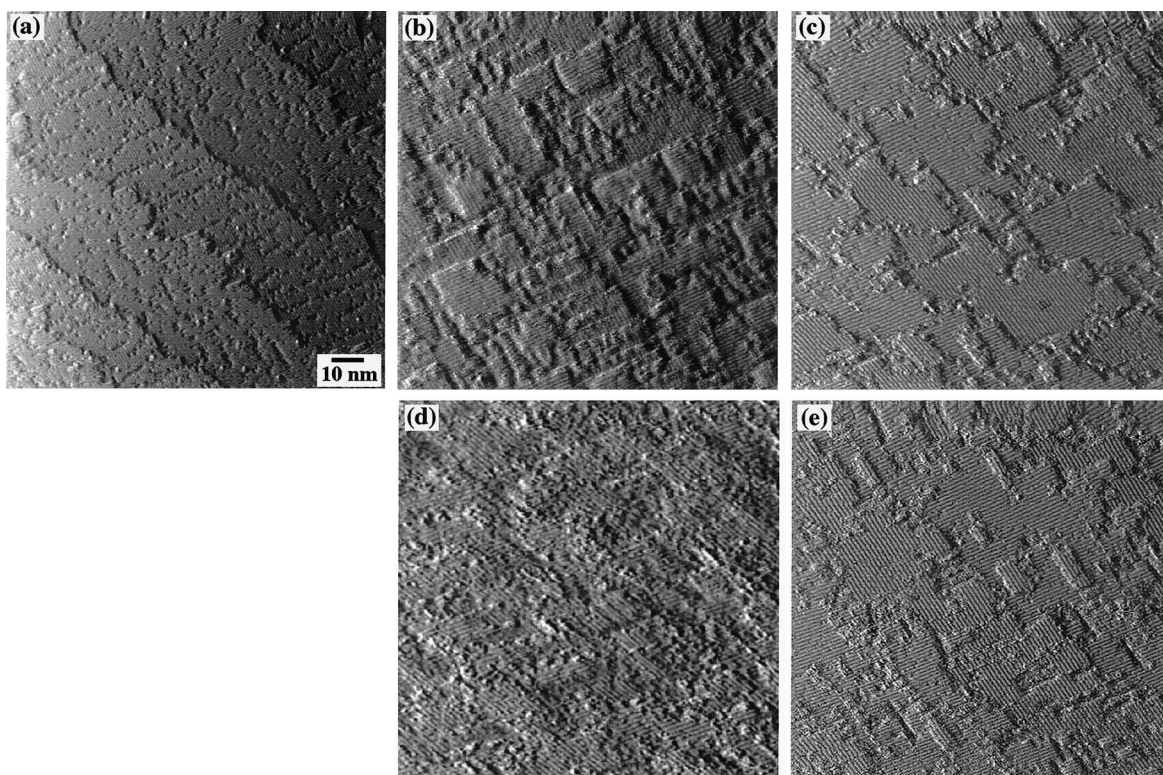


Fig. 2. Filled-state STM images of Si(1 0 0) surfaces with tip-bias voltage $V_t = 2$ V ($135 \times 135$ nm$^2$). (a) The initial $2 \times 1$ clean surface. The $2 \times 3$-Na surfaces were formed (b) on the pristine $2 \times 1$ surface ($\theta_{Si} = 0$ ML), and on the surfaces with pre-deposited Si coverage (c) $\theta_{Si} = 0.3$ ML, (d) $\theta_{Si} = 0.8$ ML and (e) $\theta_{Si} = 1.3$ ML, respectively.
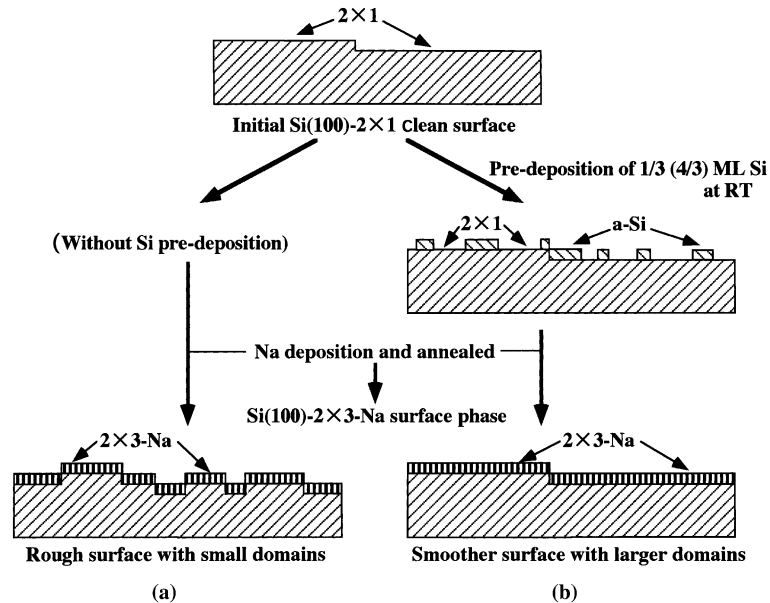
Fig. 3. Schematic illustrations of the Si(1 0 0)2 × 3-Na phase formation: (a) on the pristine 2 × 1 surface, and (b) on the 2 × 1 surface with pre-deposited Si of 1/3 ML.

Fig. 3 summarizes the difference in the $2 \times 3$-Na phase formation, revealed by the RHEED and STM studies mentioned above, between that on the pristine Si(1 0 0)$2 \times 1$ clean substrate and that on the clean substrate with pre-deposition of an optimal amount of Si. On the former substrate, since the concentration of Si atoms in the $2 \times 3$-Na phase is 1/3 ML, in contrast to 1ML in the $2 \times 1$ clean phase, Si atoms of 2/3 ML should be utilized to make the islands of one-atomic level higher. Thus, flat terraces of the $2 \times 1$ structure convert to rough terraces with numerous small domains of the $2 \times 3$-Na phase separated by monoatomic steps, because the diffusion length of Si atoms is not so long at the substrate temperature used (a). On other hand, if 1/3 ML of Si (or 4/3 ML) was deposited on the pristine Si(1 0 0)$2 \times 1$ substrate before the $2 \times 3$-Na phase formation, the substrate Si atoms are not needed to be incorporated in the $2 \times 3$-Na phase formation, so that the terraces remain flat without formation of islands (b).

Such a change in surface morphology influences the resistance of the $2 \times 3$-Na surface measured at 180 K (Fig. 4). The $2 \times 3$-Na phase formed on the pristine Si(1 0 0)-$2 \times 1$ surface showed a resistance

higher than the initial $2 \times 1$ clean surface by about $12 \pm 2\%$, which is in accord with the previous measurements at RT [13]. With the pre-depositions of Si, however, the resistance changed oscillatory as a function of $\theta_{Si}$ as shown in Fig. 4. The $2 \times 3$-Na phase with $\theta_{Si} \sim 1/3$ ML shows a resistance lower than that of the $2 \times 3$-Na phase with $\theta_{Si} = 0$ ML, and even lower than that of the initial $2 \times 1$ clean surface. As $\theta_{Si}$ is increased, the resistance rises, making a maximum around $\theta_{Si} \sim 0.9$ ML, and then decreases again to take the second minimal value at $\theta_{Si} \sim 1.3$ ML. Such changes in resistance as a function of $\theta_{Si}$ correctly correspond to the surface roughness shown in Figs. 1 and 2.

We did similar measurements of resistance at RT, but the resistance change as a function of $\theta_{Si}$ was too small to recognize the oscillatory change. This may be due to a larger contribution of bulk conductivity that is not affected by the surface roughness. Cooling the sample reduces the bulk conductivity to highlight the surface conductivity more effectively (surface-state conductivity and/or surface-space-charge-layer conductivity). Actually, the raw values of measured resistance increased by
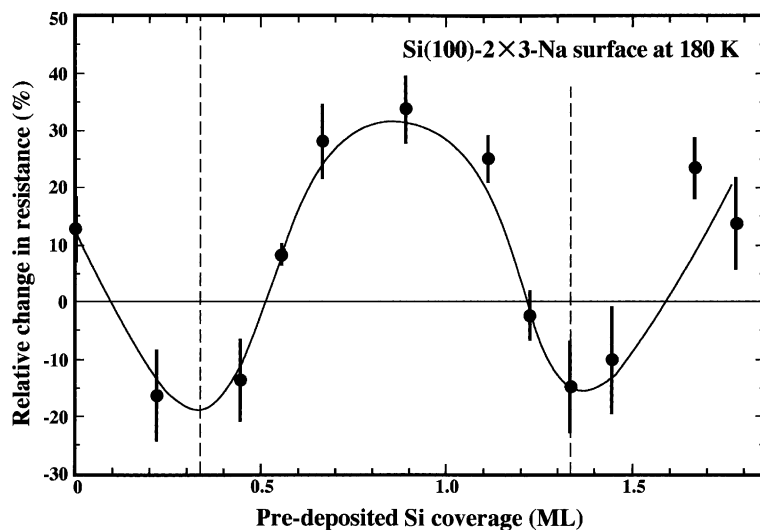
Fig. 4. Relative change in resistance of the Si(1 0 0)2 × 3-Na surface phase at 180 K with respect to the resistance of the initial Si(1 0 0)2 × 1 clean surface, as a function of the pre-deposited Si coverage.

about three times at 180 K compared to those at RT, due to a decrease of bulk conductivity.

Recently, it was shown that the diffuse scattering of conducting electrons at a rough surface has a significant contribution to the resistance of thin metal films, which is well known as the classical size effect [14]. In the present case, the carriers are scattered by surface steps and domain boundaries created at the 2 × 3-Na phase formation, although we do not know at the moment where the carriers of interest flow through, surface-state bands of the 2 × 3-Na phase or surface-space-charge-layer at the sub-surface region. The surface-state bands are interrupted at such boundaries, or the boundaries may have excess charges to make scattering potentials spreading at the space-charge layer, so that the surface-state carriers as well as sub-surface carriers can be scattered by surface steps and domain boundaries.

Another important issue to be addressed here is the intrinsic conductivity of surface phases. The previous paper reports a conductivity of the 2 × 3-Na phase apparently lower than that of the 2 × 1 clean phase [13]. But the present study shows this is incorrect; the apparent lower conductivity is due to the extrinsic reason (carrier scattering by surface roughness), not an intrinsic property to the

2 × 3-Na phase. Its intrinsic conductivity is higher than the 2 × 1 clean surface.

## 4. Conclusion

The morphology and resistance of the Si(1 0 0)2 × 3-Na surface have been studied by STM, RHEED and in situ resistance measurements at 180 K. Clear evidence has been shown that step density and domain size on the surface influence the electrical resistance dramatically. This is due to carrier scattering by such surface defects.

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