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Ordering of the vicinal Si(15 1 0) surface at low Au coverage

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Reflection high-energy electron diffraction (RHEED) and scanning tunnelling microscopy (STM) are used to investigate the ordering process of vicinal silicon surface. A vicinal Si(15 1 0) sample was cut from a Si(001) monocrystal and oriented by X-ray diffractometry techniques. At Au coverage within 1–2 ML and after the subsequent annealing at about 1000 K in UHV conditions this surface exhibits a rectangular imbricate step/terrace structure. The best surface ordering was found at 1.5–2 ML Au coverage where flat Si(001) terraces show 5×3.2 surface reconstruction. The edges of these rectangular terraces are parallel to the [011] and $[01\bar{1}]$ direction. Due to high density of corners formed by the rectangular terraces, this surface may be suitable for nucleation of quasi zero-dimensional structures.

1. Introduction

The control of semiconductor surface state in nano-scale is important because of its fundamental scientific aspect and also from the point of view of potential applications. Nucleation centres at steps are well recognised from experiments and theoretical investigation of epitaxial growth processes. In particular, the nucleation process is important during the growth of self assembled quantum dots and wires.

Standard surface sensitive techniques like scanning tunnelling microscopy (STM) [1], reflection high-energy electron diffraction (RHEED) [2] or low-energy electron diffraction (LEED) [3], [4] are frequently applied for examination of the distribution of atomic steps on vicinal surface.

Most of the resent studies are devoted to investigation of vicinal surfaces which are composed of linearly aligned terraces and steps. Annealing of the sample covered by ultra-thin layer of proper metal usually improves the order of the step distribution. The appropriate annealing temperature and metal thickness are determined experimentally. Si(111) based vicinal surfaces can be ordered when step spacing is reduced to the size of 7×7 surface unit cell. For example, a clean Si(557) sample forms atomically perfect grating structure [5] but for practical use it needs some passivation layer. Si(557) surface covered by 0.2 ML of gold was perfectly ordered after creation of single-atom chains of Au on each terrace [6]. Similar results were obtained on Si(533) surface [7], where the same mechanism occured as in the case of

Si(557) substrate. Step ordering of vicinal surfaces based on Si(100) is more difficult to achieve. Au/Si(100) system has been studied with LEED [4], [8] and its surface reconstruction phase diagram was established. It was found that a single reconstruction phase 8×2 exists for 0.3–0.5 ML Au coverage in a wide temperature range from 600 to 1000 K. Second stable phase 5×3.2 reconstruction was found in the temperature range 1000–1100 K for Au coverage from 0.6 to 2.5 ML.

The phase diagram of steps on Si(100) surfaces tilted to [110] direction was discussed by ALERHAND [9]. For the missorientation less than 0.4° the single atomic steps are formed. Neighbouring terraces show 2×1 or 1×2 reconstruction and dimers are oriented at right angles with respect to each other. For higher missorientation double atomic steps are formed and the dimers on neighbouring terraces are parallel. It was shown that the single and the double steps coexist in the wide 1–4° misscut range even at high temperatures [10]. In this work the ordering process of Si(15 1 0) surface upon thin gold films coverage is studied. Optimum Au coverage and temperature range for the best ordering of this vicinal surface is determined using RHEED. Detailed surface morphology after reconstruction is studied with UHV STM.

2. Experimental

The electron diffraction measurements were carried out in the UHV system with a base pressure below 2×10^{-10} mbar. The deposition chamber was equipped with a RHEED spectrometer, electron bombarded Au evaporator, and a quartz-crystal deposition monitor. RHEED patterns were recorded by a CCD camera with a 8-bit frame grabber. The Si(15 1 0) substrate was cut from a low resistivity (0.2 Ωcm), p-type boron doped Si(100) monocrystal, and was oriented by the standard X-ray diffraction technique with the error less than ± 0.03°. The tilt angle equal to 3.81° from [100] towards [010] direction was found by using X-ray reflection from Si(620) and Si(400) planes. Rectangular sample of dimensions $18\times4\times0.4$ mm^3 was cleaned several times with acetone, etched in 10:1 ethanol+HF solution for 1 minute and rinsed in deionized water. So prepared sample was loaded by transfer system into UHV chamber. The sample was slowly outgassed by keeping the pressure below 8×10^{-10} mbar. Direct heating of the substrate was applied by passing DC current through the sample. Flashing to about 1500 K for a few seconds was applied to remove surface contamination. Cleanness of the surface was confirmed by the observation of RHEED pattern where sharp Kikuchi line could be observed. All RHEED patterns presented in this paper were taken at 18 keV electron energy. The tunneling experiment has been performed with the commercial Omicron variable temperature STM. The same procedure of the surface preparation was applied both in STM and RHEED experiment.

3. Results

Figure 1a presents the idealised model of the vicinal surface with the uniform monoatomic surface steps. Figure 1b shows the 0-th Laue zone of RHEED pattern

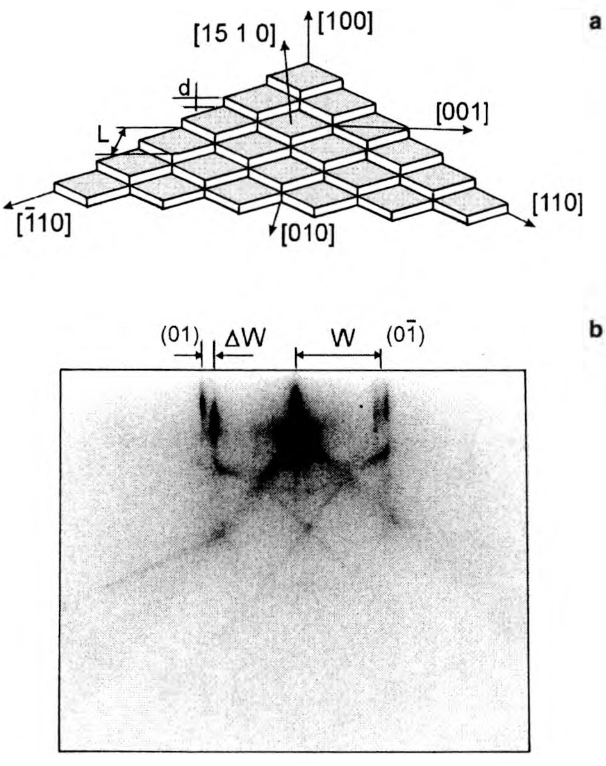

Fig. 1. Schematic model of Si(15 1 0) vicinal surface (**a**), RHEED pattern from this surface taken along [001] direction after flash cleaning at 1500 K and slow cooling (electron energy is 18 keV, and polar angle is equal to 2.5 deg) (**b**).

for the electron beam aligned along [001] azimuth and the polar angle φ equal to 2.5 deg, which satisfies the Bragg condition. Apart from the Kikuchi lines three sets of splitted streaks are clearly visible. The magnitude of this splitting is related to the average size of terraces L, through relation $L/a_{[010]} = W/\Delta W$, where L is the terrace length along [010] azimuth, $a_{[010]}$ – the lattice constant along this direction, W – main streak separation, and ΔW – the splitting of diffraction streaks. The average step edge length L, calculated from this splitting, is equal to 2.1 nm. Accordingly, the average step height d calculated from the tilt angle of the sample is 1.38 Å, nearly equal to $d = 0.25a_{[100]} = 1.37$ Å, the value which agrees with predicted step height for vicinal surface, when monoatomic steps are expected. Figure 2**a** shows RHEED pattern for the surface as in Fig. 1**b**, but taken along [$\bar{1}$ 15 0] (downhill) direction. Here about 2 ML of Au was evaporated on the sample kept at room temperature. After annealing for 2 minutes at temperature about 1000 K the sample was slowly cooled. RHEED pattern in Fig. 2**b** shows that the surface undergoes reconstruction. Surface reconstruction unit cell 5×3.2 was always oriented along [011] or [0$\bar{1}$1] direction. Stress introduced by reconstruction induced formation of the rectangular imbricate terraces with edges

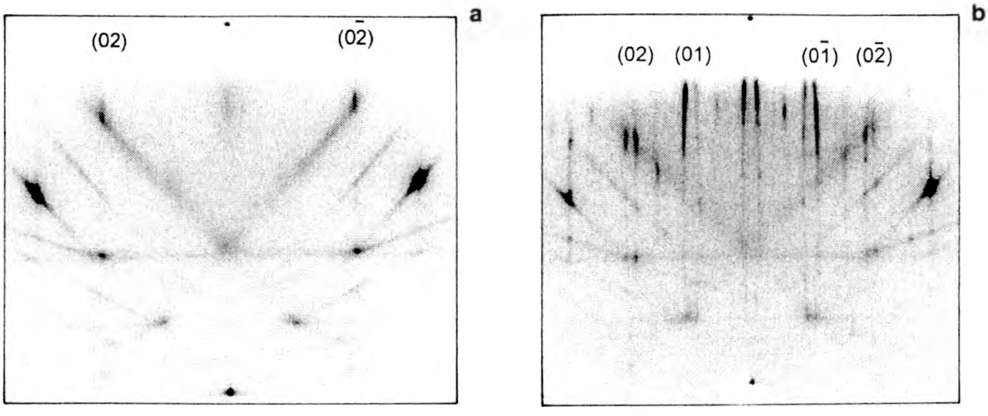

Fig. 2. RHEED pattern of vicinal Si(15 1 0) surface in downhill [$\bar{1}$ 15 0] direction at room temperature: after 1500 K flash cleaning (**a**), after reconstruction at temperature 1000 K with 2 ML of Au coverage (**b**).

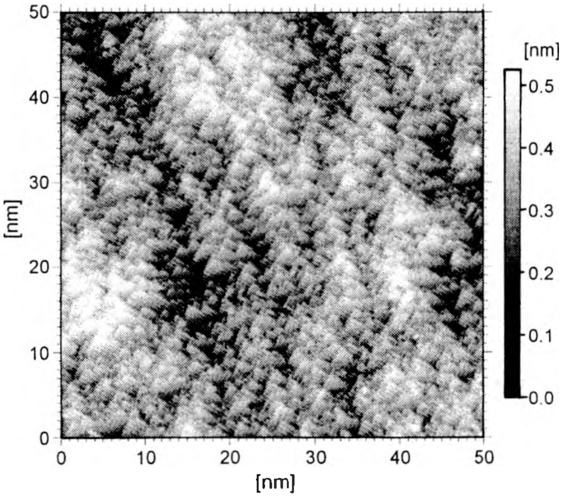

Fig. 3. Topographic STM image of clean Si(15 1 0) surface after annealing. Bias voltage is equal to –2 V. Monoatomic steps and dimmers 2×1 and 1×2 on imbricate rectangular terraces are well resolved.

parallel to 5×3.2 surface unit cell. Visible curved streks are due to the intersection of (0 0), ($\bar{1}$ 0), (0 1) reciprocal lattice of the reconstructed surface with the Ewald sphere.

STM experiment. To find the step distribution in the real space a direct observation is more convenient. Figure 3 shows a STM image of Si(15 1 0) surface after high temperature flash cleaning. The surface is composed of fine terraces with their edges oriented along [$\bar{1}$10] and [110] azimuths. The average size of these terraces is about 2 nm in both orthogonal directions. Most of the steps are $0.25a_{[100]}$ high, as it was calculated from the RHEED experiment. Dimers on neighboring terraces are perpendicular to each other as expected. No step bunches are formed during the high

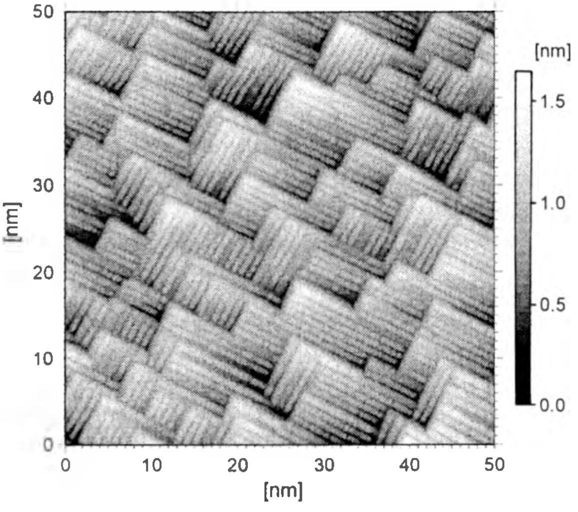

Fig. 4. Topographic STM image of Si(15 1 0) surface covered with 2 ML of Au and annealed at 1000 K. Visible (5×3.2) unit cells are oriented orthogonally to [01$\bar{1}$] and [011] direction.

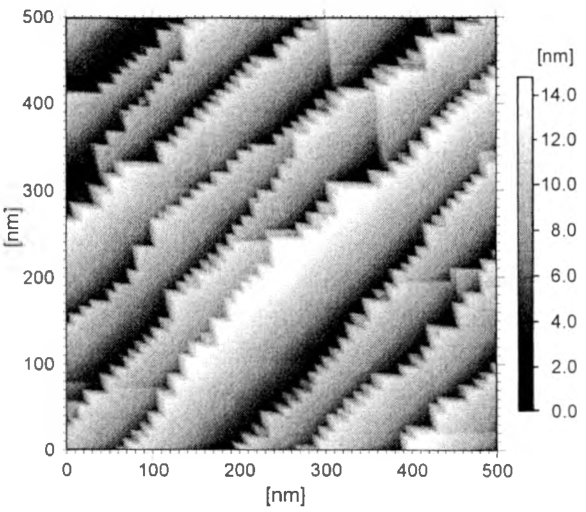

Fig. 5. Topographic STM image of Si(15 1 0) surface covered with 4 ML Au after annealing at 1000 K. Large sawtooth-like terraces with broad [100] facets and zigzag edges were formed.

temperature cleaning. After deposition of 2 ML Au and the subsequent annealing at 1000 K the surface undergoes reconstruction, as shown in Fig. 4. Large flat (100) terraces with 5×3.2 Au reconstruction are formed on the top of each terrace. Step edges are well defined but not uniform in size. Average rectangle terrace size and step height are equal to 9 nm and 0.8 nm, respectively. At even higher Au coverage, equal to 4 ML of Au, the rectangular terraces transform into broad [100] facets with zigzag edges, as it is shown in Fig.5.

4. Conclusions

Self-organization process conditions on vicinal Si(100) based surface with gold as surfactant has been presented. This process is controlled directly by anisotropic property of 5×3.2 surface reconstruction. Depending on the treatment conditions and Au coverage the Si(15 1 0) surface can be modelled as composed of fine rectangular imbricate terraces with their average size about 2 nm or as composed of wide (100) terraces separated by step bunches. When the Au coverage is equal to 2 ML the terraces grow in size several times. Simultaneously the step height increases. Due to richness of well defined corners this structure can be used for growth of quantum dots in predefined sites.

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