Pis'ma v ZhETF, vol. 84, iss. 6, pp. 381 – 384 © 2006 September 25

Ag-induced atomic structures on the Si(110) surface

N. S. Maslova[+], *A. I. Oreshkin*[+1)], *S. I. Oreshkin*[+*], *V. I. Panov*[+], *I. V. Radchenko*[+], *S. V. Savinov*[+]

[+] *Moscow State University, Department of Physics, 119992 Moscow, Russia*

[*] *Sternberg Astronomical Institute, Moscow State University, 119992 Moscow, Russia*

Submitted 17 July 2006

We report the results of STM investigation of initial stage of Ag adsorption on the Si(110) surface. At 0.21 ML Ag coverage the size and orientation of unit cell correspond to parameters of "16 × 2" unit cell of clean Si(110) surface. With increasing of Ag coverage up to 0.42 ML the type of surface reconstruction is changing to 4 × 1-Si(110)-Ag structure.

PACS: 68.37.Ef, 68.47.Fg

Many different surface structures have been experimentally found on Si(110) surface [1, 2], for examples 5 × 4, 1 × 2, 1 × 5, 16 × 2 reconstructions.

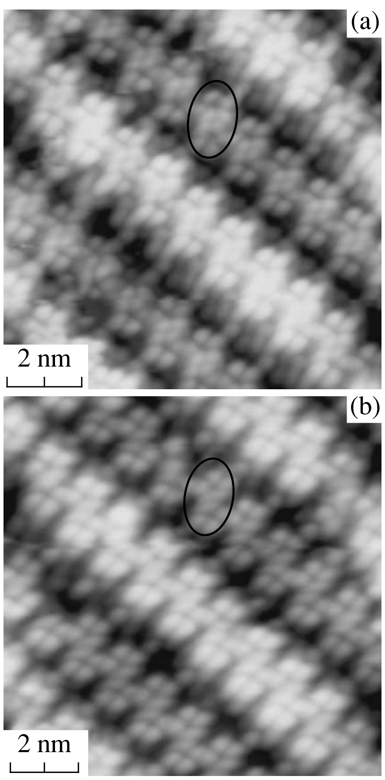

Fig.1. High-resolution STM topographic image of "16 × × 2" structure in the empty states [(a)$V_s = 0.58$ V, $I = 0.085$ nA] and the filled states [(b)$V_s = -0.71$ V, $I = 0.085$ nA]

At the same time there exists the opinion that this variety of surface reconstructions is caused by the absorption of Ni atoms [3], and that Si(110)-("16 × 2") reconstruction should be the only which should be observed on *clean* surface. 0.007 ML of Ni atoms on the surface is enough to transform the Si(110)-("16 × 2") reconstruction into another one [4].

"16 × 2" reconstructed Si(110) surface consists of equally spaced and alternatively raised (up-stripes) and lowered (down-stripes) stripes parallel to the $[\bar{1}12]$ or $[1\bar{1}2]$ directions [5, 6]. Two possible domains of "16 × 2" reconstruction must look as

$$\begin{pmatrix} 5 & 11 \\ -2 & 2 \end{pmatrix} \text{ and } \begin{pmatrix} -5 & 11 \\ 2 & 2 \end{pmatrix}$$

(the basic translation vectors $a = [001]$ and $b = 1/2[1\bar{1}0]$ are used here; $|a| = 0.543$ nm, $|b| = 0.384$ nm).

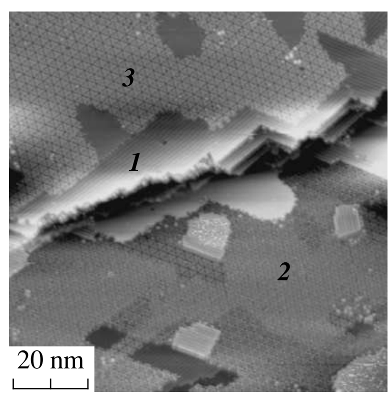

Fig.2. STM image of reconstructed Si(111) surface after Ag deposition [$V_s = -1.57$ V, $I = 0.035$ nA] 1. Si(111)–Ag(3 × 1) 2. Si(111)–Ag($\sqrt{3} \times \sqrt{3}$) 3. Si(111)–(7 × 7)

But until now there is no commonly adopted model of observed atomic structure of the stripes. STM investigation [5, 7, 8] has shown that different local atomic

[1)]e-mail: oreshkin@spmlab.phys.msu.su

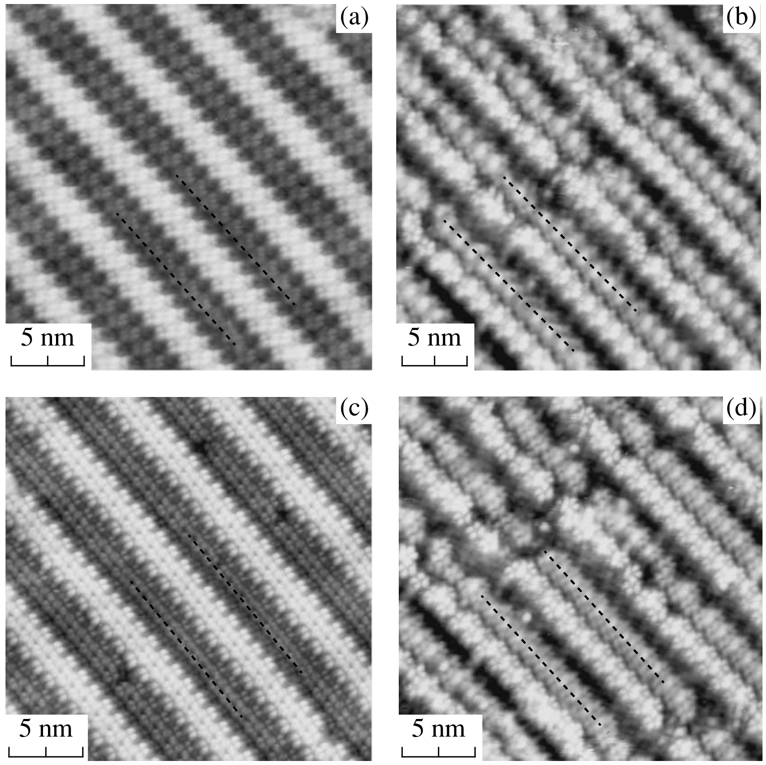

Fig.3. STM images of Si(110)surface reconstructions. (a), (c) – clean surface; (b), (d) – after 0.20 monolayer Ag deposition. (a) $V_s = 0.79$ V, $I = 0.063$ nA; (b) $V_s = 0.79$ V, $I = 0.051$ nA; (c) $V_s = -0.52$ V, $I = 0.101$ nA; (d) $V_s = -0.52$ V, $I = 0.051$ nA

structures can be observed. The stripes are stacks of paired elements whose shape is different in various STM measurements. This shape was interpreted as octets [9], as pentagons [8] and as an arrangement of centered stretched hexagons [7]. So, the precise atomic arrangement has not been elucidated yet.

Samples $(12 \times 2 \times 0.5)\,\mathrm{mm}^3$ in size were cut from P-doped (110) orientated Si wafers with sheet resistance about 1–3 $\Omega \cdot$ cm, the nominal doping concentration was about $3 \cdot 10^{18}\,\mathrm{cm}^{-3}$. Samples were ultrasonically cleaned in acetone and distilled water. With the help of "Ni-free" instrument they were mounted on tantalum sample holder. Samples were degassed at 600 °C during 24 hours and processed with argon-ion-sputtering (5 kV, 50–60 A, 60 min). In the final stage of surface preparation the samples were flash heated at 1200 °C by a direct current.

Typical STM images of Si(110) surface are presented on Fig.1. Elementary structure of Si(110)-("16×2") reconstruction unit cell is clearly resolved. Unit cell contains ten protrusions in the empty states STM image (Fig.1a) while it contains eight protrusions in the filled state STM image (Fig.1b). Our STM measurements data on clean Si(110) surface is consistent with "pentagons" model of Si(110)-("16×2") surface reconstruction suggested in [8]. Besides our data is in good accordance with theoretical calculations of [10].

The Ag/Si(110) Ag evaporation was performed using a Knudsen-cell type of evaporator. The base pressure during Ag deposition was $5 \cdot 10^{-10}$ torr. Empty Knudsen cell was cleaned up by annealing during 48 hours. The evaporation rate was estimated from the experiments with Ag deposition on 7×7-Si(111) surface. Ag deposition was conducted at 820 °C with shutter opening time 10 seconds and subsequent 3 min. annealing at 520 °C. The follow constituent reconstructions of surface have been found: 3×1-Si(111)-Ag, $\sqrt{3} \times \sqrt{3}$-Si(111)-Ag and 7×7-Si(111) (Fig.2). Relative areas occupied by these surface reconstructions are 18%, 42% and 40% correspondingly. Taking into account Ag coverage which induces above mentioned reconstructions [11, 12], we can estimate Ag evaporation rate. In our geometry the Ag evaporation rate at 820 °C equals to $0.4\,\mathrm{nm}^{-2} \cdot \mathrm{sec}^{-1}$.

STM image of Si(110) surface after 0.21 ML Ag deposition is presented in Fig.3. The size and orientation of unit cell correspond to parameters of "16×2" unit cell on clean Si(110) surface. It can be seen from Fig.3 that Ag atoms precipitate in region of down-stripes. The priority adsorption sites are marked by dashed line on Fig.3. "16×2" unit cell contains 64 atoms in one atomic layer. There should be about 13–14 Ag atoms in the unit cell of "16×2"-Si(110)-Ag structure at 0.21 ML Ag surface coverage. Most probably part of silicon ad-atoms diffuse from original sites of "16×2"-Si(110) structure into bulk of the crystal or precipitate on domain boundaries.

The dependencies of local density of electronic states on bias voltage above "16×2"-Si(110) surface before and

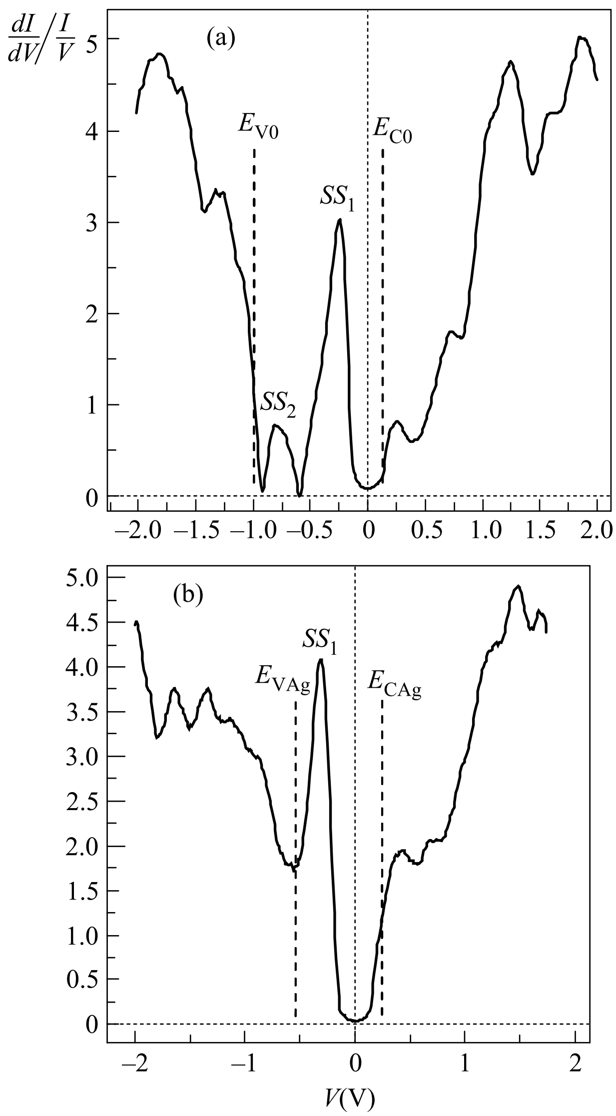

Fig.4. Local density of electronic states depending on bias voltage measured (a) above clean surface Si(110), (b) above surface reconstruction induced by Ag atoms

after Ag deposition are shown on Fig.4. Band gap value derived from Fig.4a for clean silicon surface is about 1.15 eV (which almost coincides with bulk value for Si – 1.1 eV). Surface states peaks SS1 and SS2 (−0.35 eV and −0.8 eV correspondingly) are clearly distinguishable inside the band gap. Fermi level is situated 0.15 eV below the conduction band bottom. After 0.21 ML Ag deposition (Fig.4b) the width of measured band gap becomes smaller by 0.25 eV, most probably due to coupling of surface states SS2 band with electronic states of Ag adatoms. This coupling leads to the shift of surface states band SS2 towards valence band top. Valence band and surface states band SS2 overlap. In tunneling conductivity spectra this results in disappearance of SS2 band and in the shift of the valence band top towards higher energies. The position of surface states SS1 band peak remains unchanged.

With increasing of Ag coverage up to 0.42 ML we are able to observe new type of surface reconstruction (Fig.5) with 5.4 Å periodicity along the [001] direction (~ 5.43 Å of the Si(110) unit cell). The periodicity

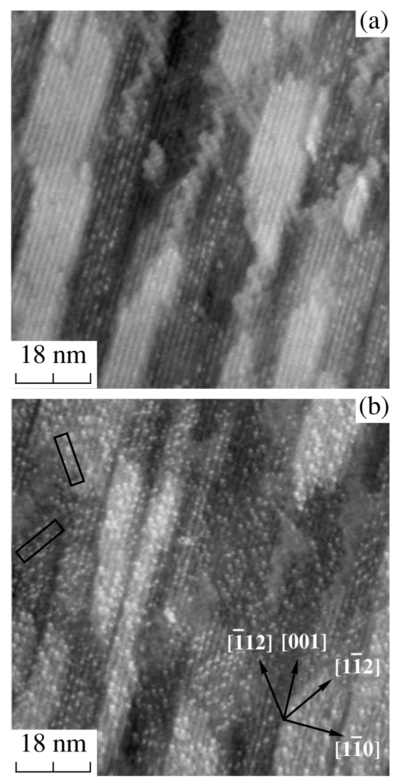

Fig.5. STM images of Ag induced 4×1–Si(110) surface reconstruction in the empty states [(a) $V_s = 1.23$ V, $I = 0.066$ nA] and in the filled states (b) $V_s = -1.14$ V, $I = 0.066$ nA]

along the [1$\bar{1}$0] direction is 15.5 Å, i.e., 4× the length of 3.84 Å of the Si(110) unit cell. We can conclude that with increasing of Ag coverage the basic type of surface reconstruction for Si(110)-Ag system is changing from "16×2"-Si(110)-Ag to 4×1-Si(110)-Ag structure. The unit cell of 4×1-Si(110) reconstruction consists of 8 atoms. Therefore under 0.42 ML Ag coverage the unit cell of formed structure should contain 3–4 atoms of Ag. The atoms of 4×1-Si(110)-Ag structure (Fig.5, marked by rectangles) are aligned in $[1\bar{1}2]$, $[1\bar{1}\bar{2}]$ directions, which correspond to the directions of up- and down-stripes in "16×2"-Si(110) structure. We explain this fact with possible diffusion of Si atoms during the formation the 4×1-Si(110)-Ag surface reconstruction.

To the best of our knowledge there is the only one work dedicated to Ag adsorption on the Si(110) surface [13]. In this work Ag/Si(110) system has been studied by means of reflection high-energy electron diffraction-total reflection angle X-ray spectroscopy. The following structure was reported to be the base surface structure for Ag coverage up to 0.44 ML

$$\begin{pmatrix} 3 & 9 \\ 3 & -9 \end{pmatrix}$$

We were not able to observe this reconstruction at initial stage of Ag adsorption. We suppose that this fact can be explained by different method of sample preparation. The other possibility is the difference in the doping concentration of samples under investigation. Anyway more detailed study of the Ag/Si(110) system with different conditions of surface preparation, different type of bulk conductivity (n-, p-type) and doping concentration is required.

Most probably the lack of reports in the literature on Ag adsorption on the Si(110) surface is caused by very complicated method of substrate preparation. It is also difficult to obtain large uniform area of "16×2"-Si(110) surface.

In conclusion, we report the first time STM/STS experimental observation of initial stages of Ag adsorption on Si(110) surface. We have found substantial difference in STM topographic images as well as in local spectroscopy data before and after Ag adsorption. Our STM measurements of clean Si(110) surface have confirmed the "pentagons" model of clean "16×2" surface reconstruction suggested in [8] and are in good accordance with the theoretical calculations [10]. We suppose that difference in tunneling conductivity spectra is caused by coupling of surface states SS2 with electronic of Ag on the "16×2"-Si(110) surface. We found that up to 0.21 ML Ag surface coverage the surface maintains the original "16×2" unit cell corresponding to clean Si(110) surface. With increasing of Ag coverage the basic type of surface reconstruction for Si(110)-Ag system is changing from "16×2"-Si(110)-Ag to 4×1-Si(110)-Ag structure.

This work was partially supported by RFBR grants # 06-02-17076-a, 06-02-17179-a, 05-02-19806-MF, 06-02-08306-OFI, president grant for scientific school No. 4599.2006.2. Support from Samsung corporation is also gratefully acknowledged. Authors are thankful to A.I. Rudenko, V.V. Gubernov, A.A. Ezhov and D.A. Muzychenko for valuable discussions.

1. F. Jona et al., IBM J. Res. Dev. **9**, 375 (1965).
2. B. Z. Olshanetsky et al., Surf. Sci. **67**, 581 (1977).
3. T. Ichinokawa et al., Phys. Rev. B **31**, 5183 (1985).
4. Y. Yamamoto et al., J. Appl. Phys. **25**, L331 (1986).
5. Y. Yamamoto, Phys. Rev. B **50**, 8534 (1994).
6. H. Ampo et al., Phys. Rev. B **34**, 2329 (1986).
7. William E. Packard et al., Phys. Rev. B **55**, 23, 15643 (1997).
8. T. An et al., Phys. Rev. B **61**, 4, 3006 (2000).
9. E. J. Van Loenen et al., J. Microsc. **152**, 487 (1988).
10. A. A. Stekolnikov et al., Phys. Rev. Lett. **93**, 13, 136104-1 (2004).
11. K. J. Wan et al., Phys. Rew. B **47**, 13700 (1993).
12. T. Fukuda et al., Phys. Rew. B **47**, 13700 (1993). et al. Phys. Rew. B **50**, 1969 (1994).
13. Y. Yamamoto, Jpn. J. Appl. Phys. **31**, 2241 (1992).