Extended Abstracts of the 1993 International Conference on Solid State Devices and Materials, Makuhari, 1993, pp. 98-100

The Initial Stage of Epitaxial Growth of Al on the Si(111) Surface Observed by Scanning Tunneling Microscopy

Masamichi YOSHIMURA, Katsuya TAKAOKA and Takafumi YAO

Department of Electrical Engineering, Hiroshima University
Higashi-hiroshima 724, Japan

The initial stage of Al epitaxy on the Si(111) surface is investigated by scanning tunneling microscopy (STM), with special attention paid to the α-7x7 and the γ-phase superstructures. It is found for the first time that both structures are based on the dimer-adatom-stacking fault (DAS) model. The possible structural models for both phases are proposed based on the STM results.

1. Introduction

With increasing of packing density in ULSI, the control of the interface structure at an atomistic level is most important for the formation of well-defined metal films, since the initial structure may affect their physical and chemical properties. The Al superstructure on the Si(111) is known to have diverse phases such as /3x/3, α-7x7, β-, and γ- structures depending on the substrate temperature and the Al coverage, as investigated by low-energy electron diffraction (LEED)[1,2], angle-resolved ultra-violet photoelectron spectroscopy (ARPUS)[3]. The atomic structures of some phases have not been determined yet because of the lack of the appropriate structural model for the dynamical LEED calculation.

STM technique has been very useful to elucidate a model for the unknown surface structure because it enables us to get insight into the local atomic arrangement in real space. Recently, Hamers et al. have observed some of these structures by scanning tunneling microscopy (STM), and proposed a possible structural model for the β-phase[4]. Because of the low resolution, however, they have not succeeded in the determination of the atomic structure for the γ-phase. Nor they have observed the α-7x7 superstructure. In this paper we report the STM study of the initial stage of epitaxial growth of Al/Si(111) system with special attention paid to the α-phase[5] and the γ-phase structure.

2. Experimental

The STM used is a commercial UHV-STM (JEOL-4000XV) capable of high temperature operation. It is mounted in an ultrahigh-vacuum chamber with a base pressure of 1.8×10^{-8}Pa. The 1x7mm^2 substrates were cut from the silicon wafers(n-type, P doped, 1~10 Ωcm) and ultrasonically rinsed in acetone before loading into the vacuum chamber. After outgassing the sample overnight, the sample was thermally cleaned at 1200°C for 30 seconds. Al was deposited on the clean surface at various substrate temperatures. STM measurements were performed at room temperature or during heating the substrate.

3. Results and Discussion

3.1 α-7x7 phase

The α-7x7 phase appears at a temperature below 500°C and the coverage below 0.7. Figure 1 shows a Si(111) surface after deposition of submonolayer Al at a temperature of 412°C. The sample voltage is -0.12 V and the average current is 0.1 nA (current mode). As expected from an earlier LEED study[2], the 7x7 periodicity is clearly observable though its features are

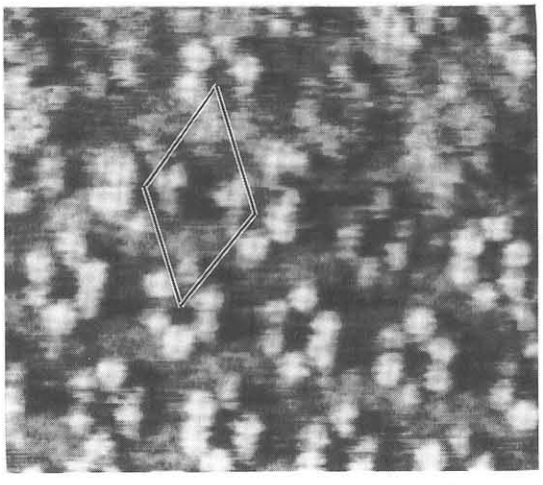

Fig.1. STM image of the α-7x7 surface obtained at -0.12V. (12.5 nm x 9.5 nm)

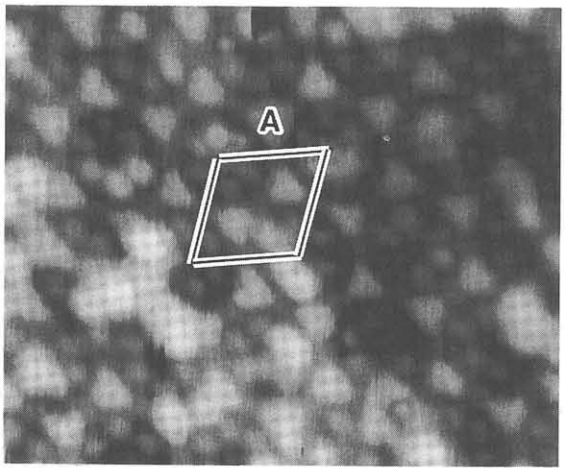

Fig.2. STM image of the α-7x7 surface obtained at -2.0V. (13.5 nm x 11.3 nm)

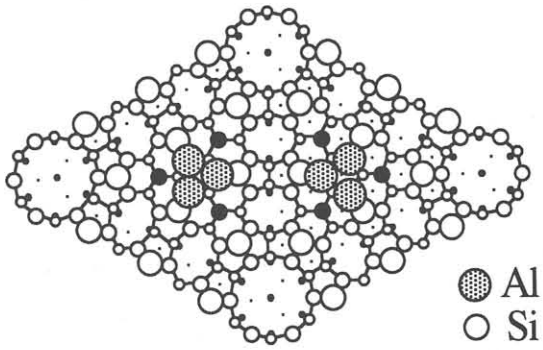

Fig.3. The structural model for the α-7x7 phase.

definitely different from those on the clean Si-7x7 surface. Only corner adatoms can be observed in the image, indicating that Al atoms react preferentially with the center adatom sites.

With increase in the absolute value of the bias voltage the STM image changes dramatically. Figure 2 shows a 16 nm x 15 nm image obtained at the sample voltage of -2.0 V probing the surface occupied state. One recognizes that a triangular shaped protrusion (A) is situated on the center part of each half unit cell. Since this structure was not observed before Al deposition, it is considered to be an Al cluster.

Based on the above observations, the following model is proposed : Al trimer adsorbs on the center position of the half unit of 7x7 DAS structure, with each Al atom being bonded to proximal Si center adatoms(Fig.3). In this situation the number of the dangling bonds is reduced by three per a half unit cell, resulting in lowering the surface energy. The electronic structure of the center adatoms would be modified into non-metallic like because of the saturation of the dangling bonds. That is why the center adatoms are not visible in the image of the surface state near the Fermi energy as is seen in Fig.1.

3.2 γ-phase

The γ-phase structure appears with increasing coverage up to 1ML. Although this phase had long been believed to have nearly 7x7 periodicity, the recent precise LEED study has shown that the periodicity is not ~7x7 but ~9x9[2].

Figure 4 shows the STM image of the γ-phase surface taken at the sample bias voltage of 1V. Individual Al atom is observed to form the triangular unit cell with each side being arranged along the <110> direction. The length of the side is 8.94 times as long as that of the surface unit of the Si(111)-1x1(a=3.84A), and the spacing between Al atoms is nearly equal to the value of a. The periodicity observed is in good agreement with the LEED study[2]. Based on the above findings, we propose the following model for the γ-phase structure (Fig.5): (1) The structure is based on the 9x9 DAS model. (2) Adsorbed Al atoms replace Si atoms in the second layer and terminate on the surface. In this situation, Al atoms adsorb commensurately on the underlying silicon lattice with no dangling bond left on the surface.

Very often are observed the monatomic-height islands of γ-phase as shown in Fig.6. The edge of the

Fig.4. High-resolution image of the γ-phase structure obtained at 1V. (12.4 nm x 7.0 nm)

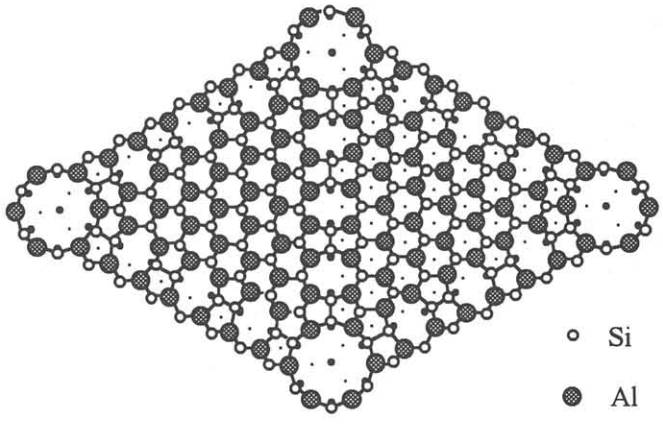

Fig.5. The structural model for the γ-phase surface.

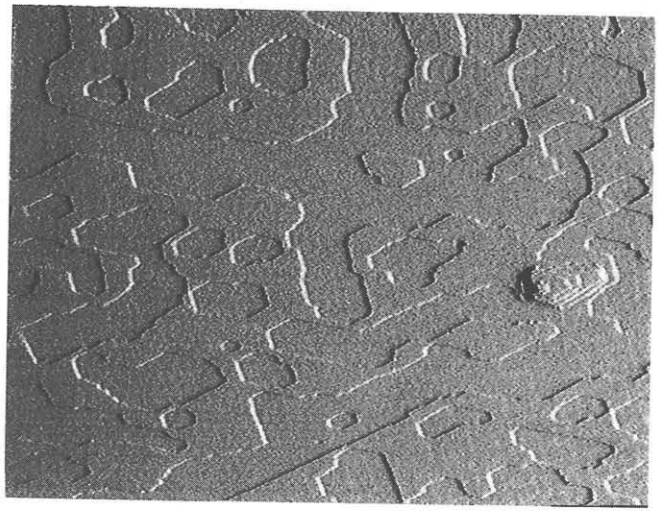

Fig.6. Island structure on the γ-phase surface. (200 nm x 200 nm)

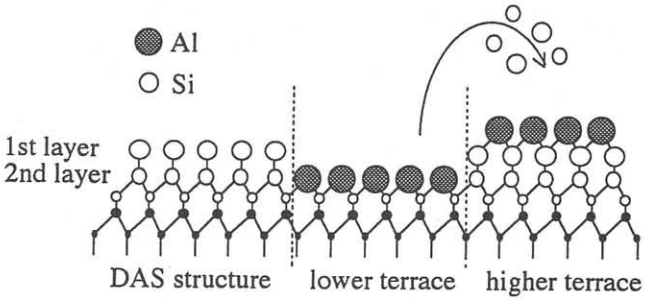

Fig.7. Schematic of the formation mechanism of the monatomic-height island.

islands is along the <110> direction. We consider the formation of the islands as follows: The replaced Si atoms such as the adatoms and the rest atoms diffuse out to form monatomic-height islands with Al atoms being situated at the topmost surface (Fig.7). This can be supported by the fact that the area ratio of the higher terrace to the lower terrace obtained experimentally is 1.26, which is very close to the expected value of 1.23 (=54/44).

4. Conclusions

We have investigated the atomic arrangement of the α-7x7 and the γ- surface structures by STM, and have proposed the possible structural models for both superstructures. In the α-7x7 structure, Al trimers adsorb on the center position of the half units of the 7x7 DAS surface, with each Al atom being bonded to proximal Si center adatoms. This situation reduces the number of surface dangling bonds, and modifies the electronic state of the proximal Si center adatoms. In the γ-phase structure, Al atoms adsorb commensurately to terminate on the surface by replacing the Si center adatoms of the 9x9 DAS structure.

Acknowledgement

We would like to acknowledge Prof. A. Kawazu and Dr. H. Sakama of the University of Tokyo for the valuable discussion. Thanks are also due to the T.Sueyoshi, T.Sato and M.Iwatsuki for their help with the STM experiments.

References

1)J.J.Lander and J.Morrison, Surf.Sci.2(1964)553.
2)K.Nishikata, K.Murakami, M.Yoshimura and A.Kawazu, Surf.Sci.269/270(1992)995.
3)R.I.G.Uhrberg, G.V.Hasson, J.M.Nicholls and F.Jona, Phys.Rev.B31(1985)3805.
4)R.J.Hamers, Phys.Rev.B40(1989)1657.
5)M.Yoshimura, K.Takaoka, T.Yao, T.Sato, T.Sueyoshi and M.Iwatsuki, Phys.Rev.B, in print.