

## Electronic states of strained $\sqrt{3}\times\sqrt{3}$ -Ag structure formed on Ge/Si(111) surfaces

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### Introduction

Much interest has been attracted to what the microscopic lattice strain has an influence on electronic properties on the semiconductor such as the carrier density, the mobility and the effective mass [1,2]. The compressive lattice strain can be introduced by the heteroepitaxial growth of Ge/Si systems [3,4], since the lattice constant differs between Si and Ge about 4 %. It is an attractive study to elucidate the relation between the strain and electronic states, because it has not only an importance in surface science, but also a possibility of the nanoelectronics applications.

We have focused our attention on two-dimensional electron gas (2DEG) states formed on the semiconductor surfaces, because it has unique metallic surface states based on the low-dimensionality [5]. It is well known that the  $\sqrt{3}\times\sqrt{3}$ -Ag structure on the Si(111) or Ge(111) surface has 2DEG states [6-9], and we started to study about the relation between the microscopic lattice strain and the electronic states. First, we confirmed that the strained  $\sqrt{3}\times\sqrt{3}$ -Ag structure is also formed by the adsorption of Ag on the strained Ge/Si(111) surface [10] prepared by the epitaxial growth of the Ge layer on the Si(111)  $7\times 7$  DAS substrate. Then, we measured the electronic states of the strained  $\sqrt{3}\times\sqrt{3}$ -Ag structure at several amounts of the Ge coverage ( $\theta$ ) measured with a scanning tunnelling microscope (STM) and an angle resolved ultraviolet photoelectron spectroscopy (ARUPS).

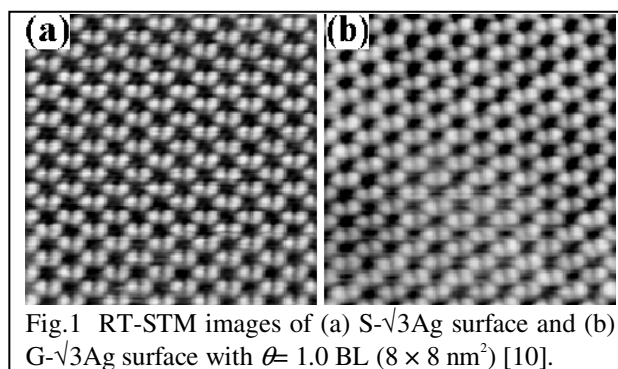
### Experimentals

The STM measurements were performed in an ultrahigh-vacuum chamber (base pressure is less than  $1\times 10^{-8}$  Pa) equipped with reflection high-energy electron diffraction (RHEED) and an electron beam evaporation source at Yokohama City University. STM images were observed with an STM head (ULVAC Japan), controlled by Topsystem 3 (Oxford instruments) at room temperature (RT). The ARUPS measurements were performed by using synchrotron radiation on the beam lines BL-7B and 18A. The experimental chamber, whose base pressure is less than  $1\times 10^{-8}$  Pa, is equipped with an angle-resolved photoelectron spectrometer of Scienta SES-100, evaporation sources, a quartz crystal thickness monitor and a sample manipulator with a cryostat. All the spectra were measured using linearly polarized synchrotron radiation for a photon-energy of 21.2 eV at low temperature (about 120K).

The strained  $\sqrt{3}\times\sqrt{3}$ -Ag surfaces were made by two step processes: First, the heteroepitaxial Ge layer was grown by Ge evaporation with  $\theta=0.5\sim 3.0$  BL on the clean Si(111) substrate. To create the Ge/Si(111)  $5\times 5$  DAS structure, the substrate temperature during the evaporation ( $T_s$ ) was kept at  $230^\circ\text{C}$  and then the sample was annealed ( $T_a$ ) at  $350^\circ\text{C}$  for 5 min. Under the preparation condition, the Ge atoms do not intermix with Si atoms and are almost staying at the surface [11,12]. Second, Ag was evaporated on the strained Ge layer about 0.5 BL at  $T_s = \text{RT}$  and  $T_a = 350^\circ\text{C}$  for 5 min. The substrate temperature was measured with an infrared radiation thermometer (above RT), and a thermocouple installed in the sample holder (below RT).

### Results and discussion

Figures 1(a) and 1(b) show the STM images of the Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface (Here after, we abbreviate as S- $\sqrt{3}\text{Ag}$ ) and the Ge/Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface (G- $\sqrt{3}\text{Ag}$ ) with  $\theta = 1.0$  BL, respectively. They show a same contrast observed from the honeycomb chained trimer (HCT) structure at RT [7]. Hence, we judge that the HCT structure is also formed on the G- $\sqrt{3}\text{Ag}$  surface. The judgment is confirmed by the surface electronic structure of the G- $\sqrt{3}\text{Ag}$  with the ARUPS [10].



For the strain of the G- $\sqrt{3}\text{Ag}$ , one would expect that the interatomic spacing of the Fig. 1(b) is expanded because of the larger lattice constant of the Ge than that of the Si about 4 % [4], but the lattice expansion estimated from such the STM images is less than 1 %. So the interatomic spacing is hardly changed at the condition which is just 1 BL of the Ge deposition. In other words, this surface is compressed considerably by the difference of the lattice constant between the Ge layer and the Si(111) substrate.

Electronic Structure of Condensed Matter

However, the G- $\sqrt{3}$ Ag surface expands when the topmost Ge layer does not form a complete layer, i.e. the value of  $\theta$  is non-integral. Figures 2(a) and 2(b) show the STM images of the S- $\sqrt{3}$ Ag and the G- $\sqrt{3}$ Ag at  $\theta = 0.6$  BL. The lattice of the G- $\sqrt{3}$ Ag in the Fig. 2(b) expands about 3.4 % to the lattice of the S- $\sqrt{3}$ Ag. The value is also confirmed by the fast Fourier transformation (FFT) of the STM images.

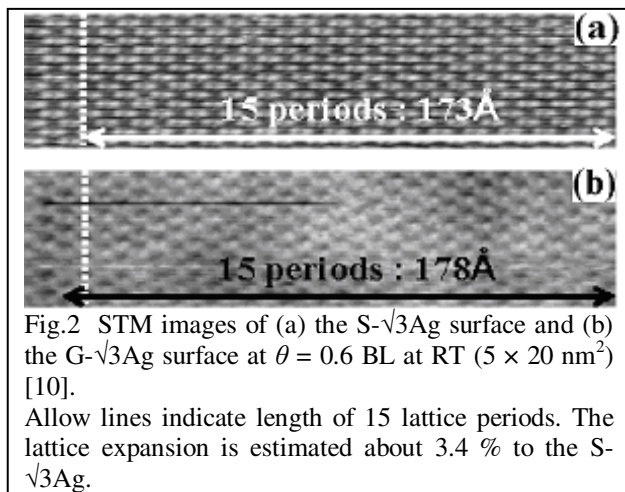


Fig.2 STM images of (a) the S- $\sqrt{3}$ Ag surface and (b) the G- $\sqrt{3}$ Ag surface at  $\theta = 0.6$  BL at RT ( $5 \times 20 \text{ nm}^2$ ) [10].  
 Allow lines indicate length of 15 lattice periods. The lattice expansion is estimated about 3.4 % to the S- $\sqrt{3}$ Ag.

The result indicates that the interatomic spacing,  $l_{\text{Ge}}$ , of the G- $\sqrt{3}$ Ag surface alters depending on the amount of  $\theta$ . When  $\theta$  is integral as shown in Fig. 1(b) ( $\theta = 1.0$  BL), the  $l_{\text{Ge}}$  shrinks and the value approached the interatomic spacing of the S- $\sqrt{3}$ Ag. But when  $\theta$  is non-integral as shown in Fig. 2(b) ( $\theta = 0.6$  BL), the  $l_{\text{Ge}}$  reaches that of the Ge(111)- $\sqrt{3} \times \sqrt{3}$ -Ag surface, which is about 4% larger than that of the S- $\sqrt{3}$ Ag. So, it is expected that the compressive strain on the G- $\sqrt{3}$ Ag becomes maximum at integral amount of  $\theta$  because the Ge film forms a complete layer and cannot release the strain. On the other hand, the strain is released at the non-integral by the structural relaxation.

We also observed ARUPS from the strained and the relaxed G- $\sqrt{3}$ Ag and the S- $\sqrt{3}$ Ag. Figures 3(a) and 3(b) show the gray-scale band dispersion diagrams from the S- $\sqrt{3}$ Ag and the G- $\sqrt{3}$ Ag with  $\theta = 3.0$  BL, respectively. They had taken along the  $[1\bar{1}0]$  direction around the  $\bar{\Gamma}_1$  point, where the  $\bar{\Gamma}_1$  point represents the centre of the adjoining  $\sqrt{3} \times \sqrt{3}$  Surface Brillouin Zone. In the diagrams, the intensity of the spectral features is represented by the brightness. Each symbol in Figs. 3(a) and 3(b) indicates the peak positions from the fitting by the Lorentz function of the energy distribution curve (EDC). The solid curves show the auxiliary conductors of the band dispersions, and the solid curves indicate each  $\bar{\Gamma}_1$  point.

There are five surface states,  $S_1 \sim S_4$  in both spectra. Each shape of dispersion of the  $S_1 \sim S_4$  states is similar to that from the HCT structure as reported previously [6,8]. So we conclude that the G- $\sqrt{3}$ Ag surface is composed of the same electronic structure on the S- $\sqrt{3}$ Ag surface [10].

By the results from detailed measurements, we found that the position of the  $\bar{\Gamma}_1$  point is related to the lattice strain [10].

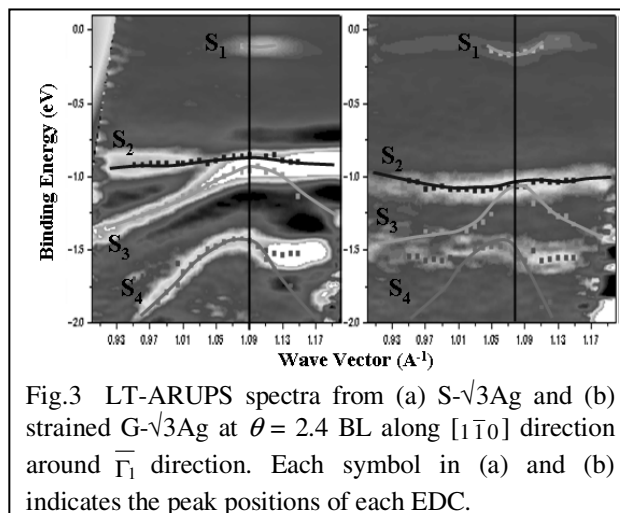


Fig.3 LT-ARUPS spectra from (a) S- $\sqrt{3}$ Ag and (b) strained G- $\sqrt{3}$ Ag at  $\theta = 2.4$  BL along  $[1\bar{1}0]$  direction around  $\bar{\Gamma}_1$  direction. Each symbol in (a) and (b) indicates the peak positions of each EDC.

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