# MODIFICATION OF ELECTRONIC STATES OF $\sqrt{3} \times \sqrt{3}$ -Ag STRUCTURE BY STRAINED Ge/Si(111) SUBSTRATE

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## **Introduction**

Much interest has been attracted on a microscopic lattice strain, because it has a large possibility to design nanoscale properties. The electronic state of the nanostructure depends on its structure involving the lattice strain to stabilize the nanostructure. To make clear the relation between electronic states and strain in nanoscale, the study in two-dimensional system is very useful and the results will give possibilities for nano-electronics applications.

We focus on the quasi two-dimensional electron gas (2DEG) state formed on the  $\sqrt{3} \times \sqrt{3}$ -Ag structure, which is typically reconstructed by Ag adsorption (1 ML) on the Si(111) or the Ge(111) [1,2], because the dispersion of the 2DEG state could be modified with the lattice strain introduced by hetero-epitaxial growth such as the Ge/Si(111) or the Si/Ge(111). The compressive strain will be induced to the surface layer by the epitaxial growth of the Ge on the Si(111), and the expansive strain will be induced by the growth of the Si on the Ge(111).

We investigated that the electronic states of the compressive  $\sqrt{3} \times \sqrt{3}$ -Ag structure on the Ge/Si(111) at several amounts of the Ge coverage ( $\theta_G$ ) measured with a scanning tunnelling microscope (STM) and an angle resolved ultraviolet photoelectron spectroscopy (ARUPS).

### **Experimental**

The STM observations were performed in our laboratory (U-STM, ULVAC), and the ARUPS observations were performed in BL-18A (Institute for Solid State Physics, University of Tokyo). The STM images were taken in the constant-current mode with a tunnel current  $I_t$ , of 50 pA and several sample bias voltages  $V_s$ , at room temperature (RT). All ARUPS spectra were measured with the polarized light with the photon-energy of 21.2 eV at low temperature (about 120 K). The angular resolution was less than 0.3°, which corresponds to 0.010 Å<sup>-1</sup> indicated by a wave number, and the energy resolution was less than 0.05 eV.

The strained  $\sqrt{3}\times\sqrt{3}$ -Ag surfaces were prepared by two step processes: First, the Ge layer was grown on the clean Si(111) substrate, epitaxially, by the evaporation of Ge with  $\theta_G = 0.8 \sim 3.0$  BL. To create the Ge(111) 5×5 DAS structure on the epitaxial layer, the substrate temperature  $T_S$  was kept at 230 °C during the evaporation, and the sample was annealed ( $T_A$ ) at 350 °C for 5 min. Under the preparation condition, the Ge atoms are almost staying on the surface rather than intermixing with Si substrate [3]. Second, the Ag was evaporated on the strained Ge layer about 0.5 BL at  $T_{\rm S} = \text{RT}$  and  $T_{\rm A} = 350$  °C for 5 min. After the evaporation, we carried out the STM or the ARUPS observations in each chamber.

### **Results and discussion**

Figures 1(a) and 1(b) show the STM images of the Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface and the Ge/Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface with  $\theta_{\rm G} = 1.0$  BL (Here after, we abbreviate as S- $\sqrt{3}$ Ag and G- $\sqrt{3}$ Ag, respectively) [4]. These images show a same feature from the honeycomb chained trimer (HCT) structure at RT [5], and we have confirmed that the shape of ARUPS spectra from both surfaces is similar to each other [4]. We conclude that the HCT structure is also formed on the G- $\sqrt{3}$ Ag.

We also find the dispersion of the  $S_1$  state on the G- $\sqrt{3}$ Ag, which is a metallic band crossing the Fermi level, varies depending on  $\theta_G$ . Figures 2 show gray-scale diagrams of the band dispersion for the  $S_1$  state at (a)  $\theta_G = 0.8$  BL, (b)  $\theta_G = 1.0$  BL, (c)  $\theta_G = 1.6$  BL and (d)  $\theta_G = 3.0$  BL, respectively [4], where the second derivative of the EDC is represented by the contrast according to the scale shown in an upper part. Solid circles represent peak positions of the  $S_1$  state determined from the peak fitting with Lorenz functions.



**Fig. 1** RT-STM images of (a) S- $\sqrt{3}$ Ag surface and (b) G- $\sqrt{3}$ Ag surface with  $\theta_{\rm G} = 1.0$  BL (8 × 8 nm<sup>2</sup>). Both STM images show a typical feature of the HCT structure.

To estimate the lattices strain in each case, we derived the position of  $\overline{\Gamma_1}$  point  $(k_{\Gamma})$  from fitting with a parabolic function to the dispersion of the  $S_1$  state [4]. The value of  $k_{\Gamma}$  is estimated from the bottom of the parabola as shown by a vertical solid line, and the dashed line indicates the position of  $\Gamma_1$  point for the S- $\sqrt{3}$ Ag (1.090 Å<sup>-1</sup>). Each value of  $k_{\Gamma}$  is (a) 1.056 ±0.006 Å<sup>-1</sup>, (b) 1.076 ±0.005 Å<sup>-1</sup>, (c) 1.063 ±0.007 Å<sup>-1</sup> and (d) 1.073 ±0.005 Å<sup>-1</sup>, which corresponds to the lattice expansion about (a) 3.2 %, (b) 1.3 %, (c) 2.5 % and (d) 1.6 %, respectively. And, we re-examined the curvature of each parabola to estimate the value of the effective mass,  $m^*$ . Each calculated value of  $m^*$  is (a) 0.28 ±0.03  $m_e$ , (b) 0.19 ±0.02  $m_e$ , (c) 0.30 ±0.03  $m_e$ , and (d) 0.20 ±0.02  $m_e$ , respectively, where  $m_e$  is the free electron mass.

When the value of  $\theta_G$  is integral,  $k_{\Gamma}$  reaches to the  $\overline{\Gamma_1}$  point of the S- $\sqrt{3}$ Ag (1.090 Å<sup>-1</sup>), the  $S_1$  state disperses steeply and the  $m^*$  becomes light. The compressive strain of the G- $\sqrt{3}$ Ag reaches to maximum with the integral value of  $\theta_G$ . On the other hand, when the value of  $\theta_G$  is fractional,  $k_{\Gamma}$  reaches to that of the Ge(111)- $\sqrt{3} \times \sqrt{3}$ -Ag surface (1.047 Å<sup>-1</sup>) and the dispersion becomes gentle. The relationship means that the relaxation of the compressive strain makes the  $m^*$  to be heavy.

#### **References**

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**Fig. 2** Gray-scale diagrams of band dispersion for  $S_1$  state at (a)  $\theta_G = 0.8$  BL, (b) 1.0 BL, (c) 1.6 BL and (d) 3.0 BL. The solid circle indicates the peak position of  $S_1$  state. The solid curve represents the parabola fitted to the dispersion. The vertical solid line indicates the position of  $\Gamma_1$  point of the G- $\sqrt{3}$ Ag and the dashed line indicates that of the S- $\sqrt{3}$ Ag.