

Strain effect on electronic states of $\sqrt{3}\times\sqrt{3}$ -Ag structure on the (111) surface of Si/Ge system

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Introduction

It is very important to investigate electronic states of nanostructures creating new devices. 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. To control the strain in the surface lattice, we have selected the $\sqrt{3}\times\sqrt{3}$ -Ag (hereafter $\sqrt{3}$) structure which is typically formed on both surfaces of Si(111) and Ge(111) by a Ag adsorption[1,2]. Since the lattice constant of Si is about 4 % smaller than that of the Ge[3,4], the compressive strain is induced in the Ge layer grown on the Si(111) and the tensile strain is induced in the Si layer on the Ge(111) such as a Ge/Si(111) and a Si/Ge(111)[5,6].

We focused on the quasi two-dimensional electron gas (2DEG) state formed on the $\sqrt{3}\times\sqrt{3}$ -Ag structure, 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). We investigated that the electronic states of the compressive and tensile $\sqrt{3}\times\sqrt{3}$ -Ag structure on the Ge/Si(111) and Si/Ge(111) measured with a scanning tunnelling microscope (STM) and an angle resolved ultraviolet photoelectron spectroscopy (ARUPS).

Experimentals

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 \AA^{-1} indicated by a wave number, and the energy resolution was less than 0.05 eV.

Results and Discussion

Figures 1(a)-(d) show the STM images: (a) the Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface, (b) the Si/Ge (111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface (the S- $\sqrt{3}$ Ag) with a coverage of Si at 1.0 BL and (d) the Ge/Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface (the Ge- $\sqrt{3}$ Ag) with a coverage of Ge at 1.0 BL [5,6]. These images show a

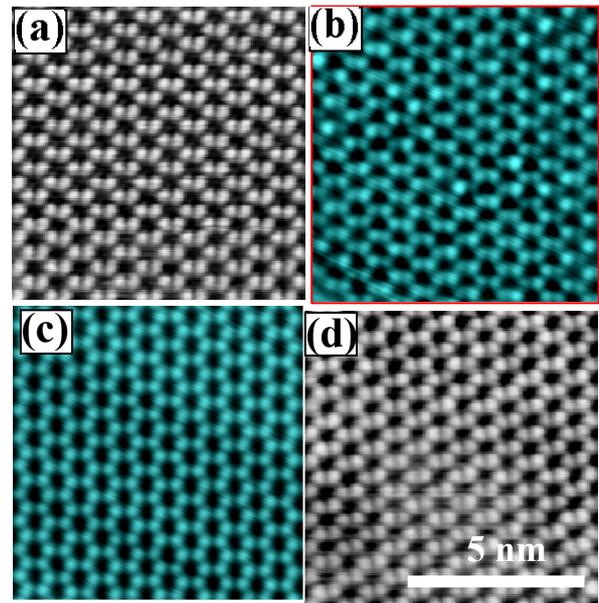


Fig. 1. RT-STM images of (a) Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag, (b) S- $\sqrt{3}$ Ag surface with $\theta_s = 1.0$ BL, (c) Ge(111)- $\sqrt{3}\times\sqrt{3}$ -Ag and (d) G- $\sqrt{3}$ Ag surface with coverage of 1.0 BL ($8 \times 8 \text{ nm}^2$). All STM images show a typical feature of the HCT structure.

same feature from the honeycomb chained trimer (HCT) structure at RT [1], and we have confirmed that each electronic structure observed with the ARUPS is similar to each other.

We find the dispersion of the S_1 state on each $\sqrt{3}$ surface, which is a metallic band crossing the Fermi level, varies depending on θ_G . Figures 2 show gray-scale diagrams of the band dispersion for the S_1 state at (a) the Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag, (b) the S- $\sqrt{3}$ Ag, (c) the Ge(111)- $\sqrt{3}\times\sqrt{3}$ -Ag and (d) the G- $\sqrt{3}$ Ag. Since the dispersion depends on the amount of excess Ag atom (n_A), each value of excess Ag atom in (a) and (b) is 0.019 ML, and that in (c) and (d) is 0.015 ML. Each solid line indicates the position of the second $\bar{\Gamma}$ point of the $\sqrt{3}\times\sqrt{3}$ Brillouin zone, whose wave number ($k_{\bar{\Gamma}}$) are (a) 1.090 \AA^{-1} , (b) 1.069 \AA^{-1} , (c) 1.049 \AA^{-1} and (d) 1.076 \AA^{-1} , respectively.

The effective mass (m^*) is also estimated from the dispersion fitted by each parabolic function. m^*/m_e for each case are (a) 0.20 ± 0.02 , (b) 0.26 ± 0.03 , (c) 0.30 ± 0.04 and (d) 0.20 ± 0.02 , respectively.

Surface and Interface

The relationship between the m^* and the lattice expansion is plotted with error bars in Fig. 3. The open and closed circles are values obtained from the $\sqrt{3}$ on the Si(111) and the Si/Ge(111), and the open and closed squares are obtained from that on the Ge(111) and the Ge/Si(111). The difference of m^* between on the Si(111) and on the Ge(111) is considered to be attributed to the difference in the n_A .

The relationship is consistent with a model called the “d-band model” [7] on some metal surfaces, qualitatively, in which the reactivity increases with an expansion of interatomic spacing of the lattice parallel to the surface due to an instability of electronic states by missing interaction between the wave functions.

References

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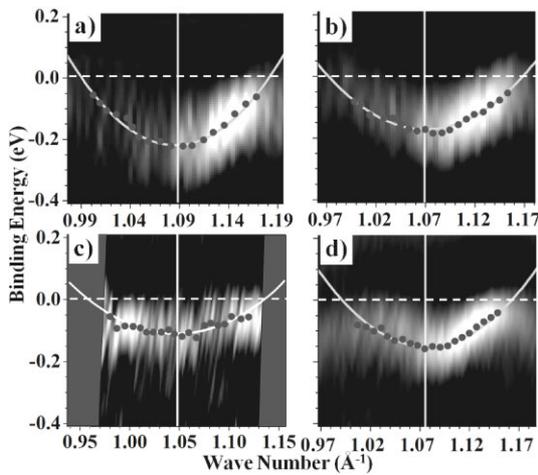


Fig. 2. Dispersions of the S_1 state with ARUPS from (a) the Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag, (b) the S- $\sqrt{3}$ Ag, (c) the Ge(111)- $\sqrt{3}\times\sqrt{3}$ -Ag and (d) the G- $\sqrt{3}$ Ag. Each value of excess Ag atom in (a) and (b) is 0.019 ML, and that in (c) and (d) is 0.015 ML.

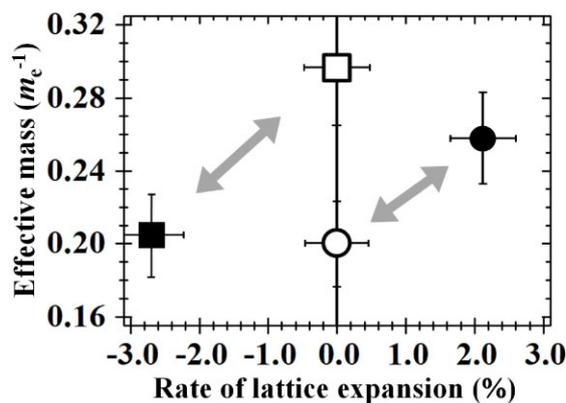


Fig. 3. Relation between m^* and lattice strain. The circles are results for the $\sqrt{3}$ structure from the Si(111) and the Si/Ge(111), and the squares are obtained from that on the Ge(111) and the Ge/Si(111) with error bars. The slope, $\Delta m^*/\Delta k_{\Gamma}$, is estimated to be about $3.1 m_e \text{ \AA}$.