PHYSICAL REVIEW B VOLUME 59, NUMBER 24 15 JUNE 1999-II

Electronic structure of the Si(001)$c(6\times2)$-Ag surface studied by angle-resolved photoelectron spectroscopy using synchrotron radiation

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(Received 2 December 1998)

The surface electronic structure of the single-domain Si(001)$c(6\times2)$-Ag surface has been studied by polarization-dependent angle-resolved photoelectron spectroscopy (ARPES) using synchrotron radiation. Through detailed ARPES measurements, the Si(001)$c(6\times2)$-Ag surface is found to be semiconducting with a band gap larger than ~0.7 eV. Three different surface states are identified within the bulk band gap, whose dispersions and symmetry properties are determined. The surface band structures observed have a close resemblance with those of the Si(001)(2×3)-Ag surface reported recently [H. W. Yeom *et al.*, Phys. Rev. B **57**, 3949 (1998)]. This result suggests a similarity between the substrate reconstructions of the $c(6\times2)$-Ag and (2×3)-Ag phases formed at a proximate condition. The surface structure of Si(001)$c(6\times2)$-Ag and the origins of the surface states observed are discussed. [S0163-1829(99)04724-4]

I. INTRODUCTION

Thin films of Ag on Si surfaces have been the prototype system of metal/semiconductor inferfaces due to a minimal chemical interaction between the two elements and due to well-defined interface structures. Because of such technological and fundamental interest, intensive studies have been devoted especially to the Ag/Si(111) surfaces/interfaces over the past two decades.[1] However only a few attempts have so far been made for Ag thin films on the Si(001) surface in spite of the simple surface structure and importance in device technology of the Si(001) substrate. Recently there has been a renewal of interest in the Ag/Si(001) system, which was motivated partly by the observation of the local- or long-range-order structures of the 2×1, 2×2, and 2×3 phases during the initial growth of Ag on Si(001) by scanning tunneling microscopy (STM) and low-energy-electron-diffraction (LEED) studies.[2–4] The surface structures of these surface phases have not been made clear.

Among such order phases, the Si(001)(2×3)-Ag surface has been the main subject of recent interest. Two different structure models have been introduced for the Si(001)(2×3)-Ag surface by STM (Ref. 4) and low-energy electron microscopy[5] studies, based on Ag coverages of $\frac{1}{3}$ and $\frac{1}{2}$ ML, respectively. However, the surface band structure reported recently was not compatible with these previous structure models.[6] This electronic structure study suggested, then, a Ag coverage of $\frac{2}{3}$ ML for the Si(001)(2×3)-Ag surface in order to explain the semiconducting surface band structure.[6] Subsequently, a very recent x-ray photoelectron diffraction (XPD) study successfully introduced a structure, an arrangement of Ag overlayer atoms, based on the $\frac{2}{3}$-ML coverage.[7]

On the other hand, another long-range-order phase $c(6\times2)$ was reported by LEED (Ref. 8) and STM (Ref. 9) at almost identical conditions with the 2×3 phase except for a slightly different temperature during the deposition of Ag. The $c(6\times2)$ phase is metastable, and converts to the 2×3 phase with only a mild post-annealing.[8] In spite of the close similarity in formation conditions of the 2×3 and $c(6\times2)$ phases, Ag $3d$ XPD patterns[8] and STM images[9] of these two surfaces are very different, suggesting a large difference in their local structures. No further information on the $c(6\times2)$ surface has been reported.

In this paper, we extend our previous electronic structure study on the (2×3)-Ag phase[6] to $c(6\times2)$-Ag in order to study the similarity and difference of these two phases and to gain a unified understanding of the bonding and adsorption behaviors of the submonolayer Ag on the Si(001)(2×1) surface. We have prepared a single-domain (SD) Si(001)$c(6\times2)$-Ag surface, and have investigated the surface state band structure of the $c(6\times2)$-Ag phase with polarization-dependent angle-resolved photoelectron spectroscopy (ARPES) using synchrotron radiation (SR). Several surface states are identified, and their dispersions as well as symmetry properties are determined. This result is discussed in comparison with that of the Si(001)(2×3)-Ag surface.[6]

II. EXPERIMENTS

The experiments were performed on the vacuum ultraviolet beam line BL-7B (Research Center for Spectrochemistry, the University of Tokyo) at Photon Factory, KEK, Japan.[10] The detailed experimental setup and procedures for the sample preparation are the same as reported before.[6] A well-ordered SD Si(001)(2×1) surface was prepared as the substrate and a SD Si(001)$c(6\times2)$-Ag surface was formed by a deposition of ~0.6-ML Ag at room temperature and a sub-

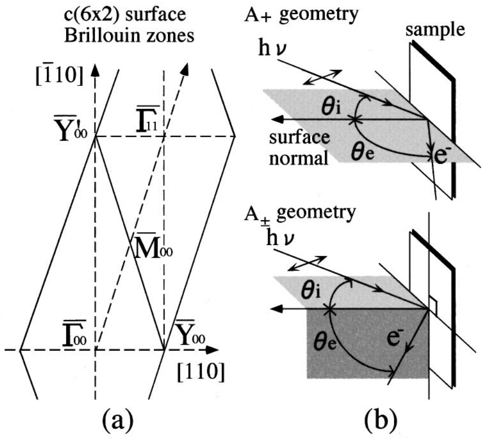

FIG. 1. (a) The surface Brillouin zone of the $c(6\times2)$ surface with symmetry points indicated. (b) Two different geometries of polarization-dependent ARPES measurements for the determination of the symmetry properties of surface states. See text for explanation. In A_+ geometry, the incident synchrotron radiation and its polarization are in the same plane with the surface normal and the direction of photoelectron detection. On the other hand, in the $A_\pm$ geometry, the incident synchrotron radiation and its polarization are in the plane perpendicular to that of the surface normal and the photoelectron detection.

sequent annealing at ~200 °C as reported before.[8] On the other hand, a SD Si(001)(2×3)-Ag surface is prepared by the same procedure but at a substrate temperature of 200 °C during the deposition.

ARPES spectra of the SD Si(001)$c(6\times2)$-Ag surface were measured using linearly polarized SR at photon energies ($h\upsilon$) of 17.4 and 14.7 eV. The spectra shown below were normalized by background intensities above the Fermi level (E_F).[11] ARPES spectra were taken at a step of 2° in the emission angles (θ_e) along the $\bar{\Gamma}_{00}$-$\bar{Y}_{00}$, $\bar{\Gamma}_{00}$-$\bar{Y}'_{00}$, and $\bar{\Gamma}_{00}$-$\bar{M}_{00}$-$\bar{\Gamma}_{11}$ lines of the $c(6\times2)$ surface Brillouin zone (SBZ) [see Fig. 1(a)].

In order to investigate the symmetry properties of surface-state wave functions along the SBZ axes containing mirror symmetry planes, we adopted two different measurement geometries denoted as A_+ [θ_i (the incident angle of SR from the surface normal)$=45°$] and $A_\pm$ ($\theta_i=20°$) as shown in Fig. 1(b).[11] According to the symmetry selection rule,[12] photoelectrons only from even-symmetry initial states are detected in the A_+ geometry while photoelectrons from both even- and odd-symmetry states are probed in the $A_\pm$ geometry. ARPES spectra shown here were recorded in the A_+ geometry, if not specified differently.

III. RESULTS

The ARPES spectra of the SD Si(001)$c(6\times2)$-Ag surface are shown in Fig. 2. These spectra were taken along the SBZ line of $\bar{\Gamma}_{00}$-$\bar{Y}'_{00}$ (the [$\bar{1}$10] axis) at a photon energy of 17.4 eV. In these spectra, the most prominent spectral feature is the relatively large and sharp peaks with binding energies of 1.2–1.8 eV at emission angles of 12°–26° and −4° to −10°; this feature is denoted as S_2. Around the normal emission, another spectral feature is observed at smaller binding energies than S_2, which becomes faint at off-normal emissions and is barely observed again at emission angles larger than 24° (denoted as S_1 in Fig. 2). Two other weak features are noticed at $\theta_e>30°$, although they are not so well resolved from each other. One of these features (at a lower binding energy) is denoted as S_3, as explained in detail below. A characteristic band at higher binding energies is the steeply dispersing band **b**, which is due to the well known bulk direct transition.[13]

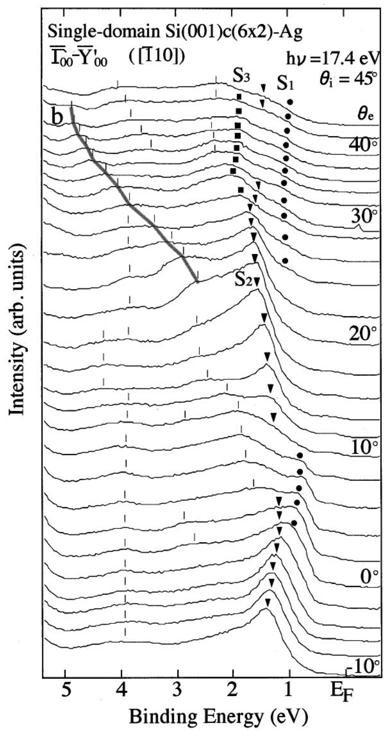

FIG. 2. Normalized ARPES spectra for the single-domain Si(001)$c(6\times2)$-Ag surface taken along the surface Brillouin-zone line of $\bar{\Gamma}_{00}$-$\bar{Y}'_{00}$. The photon energy used is 17.4 eV and the photon incident angle (θ_i) is 45°. The step in emission angles (θ_e's) is 2° between the neighboring spectra. The peak positions of different surface states assigned are marked with different symbols.

Figure 3 shows the experimental dispersion curves for the spectral features observed along the $\bar{\Gamma}_{00}$-$\bar{Y}'_{00}$ line taken at $h\upsilon=14.7$ (open circles) and 17.4 eV (solid circles) in the A_+ geometry, and also at $h\upsilon=17.4$ eV in the $A_\pm$ geometry (solid diamonds). For ARPES scans taken at $h\upsilon=17.4$ eV in the A_+ geometry, the gray-scale E_B-$k_\parallel$ diagram[11,14] is also shown to give a more comprehensive view of the spectral features around the bulk band gap. In this diagram,[11,14] the intensities of the spectral features are approximately represented by the brightness in the gray scale by taking the second derivatives of the spectra. The shaded region in the upper figure is the bulk band projected onto the 1×1 SBZ,[15] and the thin white dashed line in the lower figure is the edge of the projected bulk band. The two uppermost bands S_1 and S_2 have parts of their dispersion curves within the projected bulk band gap, indicating their surface nature. A comparison with ARPES spectra of the clean Si(001)(2×1) surface taken at the same condition confirms that S_1 and S_2 states are intrinsic to the Si(001)$c(6\times2)$-Ag surface. This comparison also reveals that the third band S_3 cannot be assigned to any

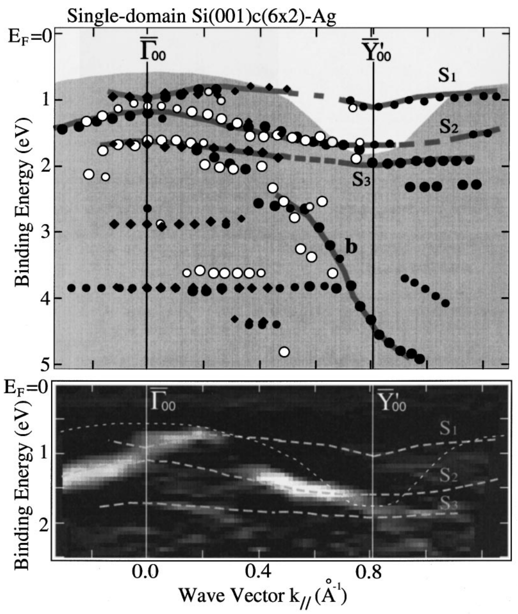

FIG. 3. (Upper) Experimental dispersions for the single-domain Si$(001)c(6\times2)$-Ag surface along the surface Brillouin zone (SBZ) line of $\bar{\Gamma}_{00}$-$\bar{Y}'_{00}$. The small and large symbols represent the rather distinctive and the weak spectral features, respectively. Solid (open) circles and diamonds indicate peak positions obtained in A_+ geometry with $h\nu=17.4$ (14.7) eV and in $A_\pm$ geometry with $h\nu=17.4$ eV, respectively. The shaded region is the bulk band structure projected onto the 1×1 SBZ. The major surface and bulk bands are traced by thick gray lines. (Lower) The gray-scale E_B-$k_\parallel$ diagram (Refs. 11 and 14) for the single-domain Si$(001)c(6\times2)$-Ag surface along $\bar{\Gamma}_{00}$-$\bar{Y}'_{00}$ taken from the ARPES scans at $h\nu=17.4$ eV in the A_+ geometry. The dispersions for the surface states are depicted by white dashed lines. The thin white dashed line is the edge of bulk band projected into 1×1 SBZ.

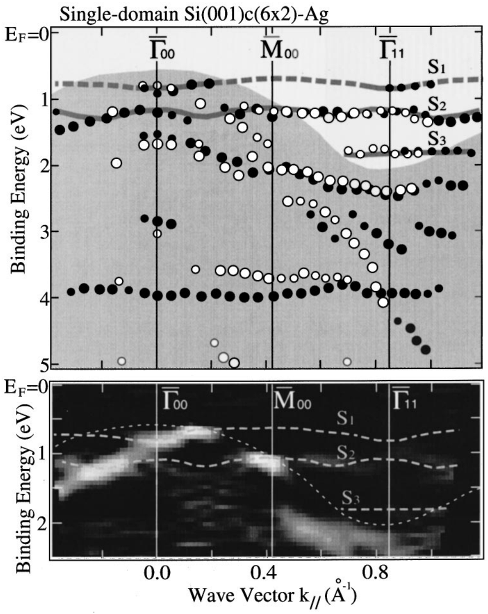

FIG. 4. Experimental dispersions for the single-domain Si$(001)c(6\times2)$-Ag surface along $\bar{\Gamma}_{00}$-$\bar{M}_{00}$-$\bar{\Gamma}_{11}$.

bulk feature of the Si substrate or to a surface state of the clean Si$(001)(2\times1)$ surface. The surface state nature of S_3 will be made more clear below. As shown in Fig. 3, S_1, S_2, and S_3 are observed at the same binding energies for different photon energies, which corroborates them as being surface states.

We observe another band at a binding energy of 2.3 eV around $\bar{Y}'_{00}$, which was also observed on the clean Si$(001)(2\times1)$ surface. Thus this state is thought to originate from the Si substrate. In addition, a characteristic nondispersing band is observed at a binding energy of ~3.8 eV, with $h\nu=17.4$ eV (solid symbols in Fig. 3). This band was also observed for the Si$(001)(2\times3)$-Ag surface, and was suggested to be a surface resonance state (S_5 in Ref. 6). The binding energy of this band shifts slightly for the data taken at $h\nu=14.7$ eV. This seems to suggest the contribution of bulk electronic states to this band in some extent. As mentioned above, the steeply dispersing band **b** is due to the well-known bulk feature. Since the bulk band **b** is observed at almost the same binding energy as that on the clean Si$(001)(2\times1)$ surface, it is estimated that the formation of the $c(6\times2)$-Ag phase does not change the surface band bending. This is similar to the case of the Si$(001)(2\times3)$-Ag surface.[6]

Figure 4 shows the dispersion curves obtained with the ARPES spectra of the Si$(001)c(6\times2)$-Ag surface along the $\bar{\Gamma}_{00}$-$\bar{M}_{00}$-$\bar{\Gamma}_{11}$ line of the SBZ. Two different photon energies, $h\nu=14.7$ (open circles) and 17.4 eV (solid circles), were used. The gray-scale E_8-$k_\parallel$ diagram[11,14] taken from the ARPES scans at $h\nu=17.4$ eV in the A_+ geometry is also shown in Fig. 4. Along the $\bar{\Gamma}_{00}$-$\bar{M}_{00}$-$\bar{\Gamma}_{11}$ line, the bulk band gap is wider than along the $[\bar{1}10]$ axis: the valence-band maximum is located roughly at a binding energy of ~2 eV at $\bar{\Gamma}_{11}$. Within this wider gap, we observe three rather dispersionless bands, which are identified as the aforementioned S_1, S_2, and S_3 surface states from their binding energies. While the dispersion of S_2 is quite clear throughout the $\bar{\Gamma}_{00}$-$\bar{M}_{00}$-$\bar{\Gamma}_{11}$ line, those for S_1 and S_3 are obvious only within the band-gap region. Along the $\bar{\Gamma}_{00}$-$\bar{M}_{00}$-$\bar{\Gamma}_{11}$ line, a band at a binding energy of ~2.2 eV appears with large intensities, and its dispersion is invariant for the change of photon energy. However, it is not clear whether this is another surface state of the $c(6\times2)$ phase since a similar feature is also observed on the clean Si$(001)(2\times1)$ surface at the same binding energy at similar SBZ points. The nondispersing band at ~3.8 eV and the bulk band **b** at off-normal emission angles mentioned above are also observed along the $\bar{\Gamma}_{00}$-$\bar{M}_{00}$-$\bar{\Gamma}_{11}$ line.

Similar ARPES measurements were also made along yet another major symmetric axis of the $c(6\times2)$ SBZ, $\bar{\Gamma}_{00}$-$\bar{Y}_{00}$ ([110]), which find similar spectral features: S_1, S_2, and S_3. The dispersion curves along the $\bar{\Gamma}_{00}$-$\bar{Y}_{00}$ line are shown in the gray-scale E_b-$k_\parallel$ diagrams[11,14] of Fig. 5. The diagrams are taken from ARPES scans at $h\nu=14.7$ eV in the A_+ geometry (left) and at 17.4 eV in the $A_\pm$ geometry (right).

After establishing the existence and dispersions of the three surface states within the bulk band gap, S_1–S_3, we further studied their symmetry properties. Figure 6 shows a collection of ARPES spectra in the two measurement geometries, A_+ and $A_\pm$, which have different symmetry selection

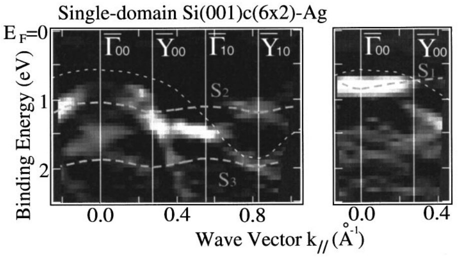

FIG. 5. Gray-scale E_B-$k_\parallel$ diagrams (Refs. 11 and 14) for the single-domain Si(001)$c(6\times2)$-Ag surface along $\overline{\Gamma}_{00}$-$\overline{Y}_{00}$ taken from the ARPES scans at $h\upsilon=14.7$ eV in the A_+ geometry (left), and at 17.4 eV in the $A_\pm$ geometry (right).

rules. It can be clearly found that S_1 and S_2 states are enhanced and quenched, respectively, in the $A_\pm$ geometry along both mirror symmetric axes. This behavior can also be noticed in Fig. 5. This suggests that S_1 (S_2) has odd (even) symmetry along both $\overline{\Gamma}_{00}$-$\overline{Y}_{00}$ and $\overline{\Gamma}_{00}$-$\overline{Y}'_{00}$ lines. The symmetry property of S_3 is rather unclear due to its small intensity.

IV. DISCUSSION

From Figs. 3–5, it is apparent that the Si(001)$c(6\times2)$-Ag surface is semiconducting with a band gap of larger than ~0.7 eV, which is similar to the case of the Si(001)(2×3)-Ag surface.[6] This indicates an even number of surface electrons in the unit cells of both $c(6\times2)$ and 2×3 phases, consistent with the same Ag coverage of these two phases.[8] From this electron counting, we have suggested that the Si(001)(2×3)-Ag surface has a Ag coverage of $\frac{2}{3}$ ML,[8] in contradiction to the available structure models.[4,5] The Ag coverage of $\frac{2}{3}$ ML also holds for the $c(6\times2)$ phase, although there is no proposed structure model at present.

Due to the lack of structure models and theoretical band-structure calculations for the $c(6\times2)$ phase, it is impossible to assign origins of the surface state bands observed. What can be said is that the three surface states within the band gap, S_1–S_3, would stem from Ag 5s and Si valence electrons (sp). Ag 4d bands are located at a binding energy of ~6 eV, and are thought to have little influence on the states around the bulk band gap.[6,16]

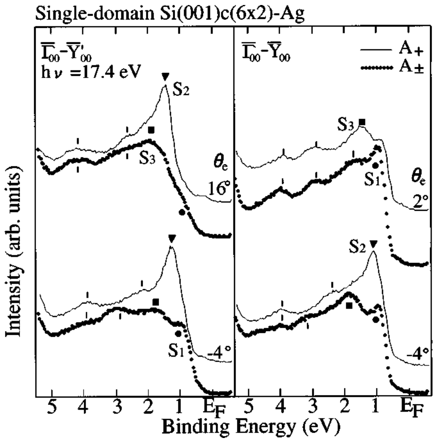

FIG. 6. Selected polarization-dependent ARPES spectra of the single-domain Si(001)$c(6\times2)$-Ag surface recorded with $h\upsilon=17.4$ eV. Spectra depicted with solid lines (dots) are obtained in A_+ ($A_\pm$) geometry. Peak positions of the surface states, S_1, S_2, and S_3, are indicated by circles, triangles, and squares, respectively.

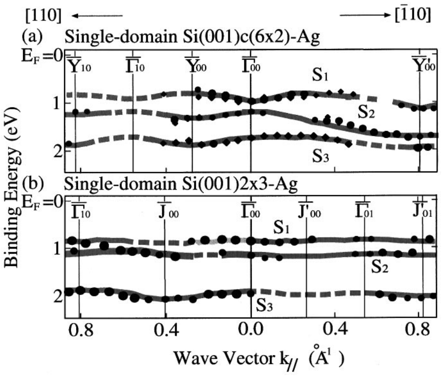

FIG. 7. Summary of the surface-state dispersions of (a) single-domain Si(001)$c(6\times2)$-Ag and (b) single-domain Si(001)(2×3)-Ag surfaces within the bulk band gap. The dispersions of surface states are guided by thick gray lines. The solid circles and diamonds are from the ARPES spectra taken at a photon energy of 17.4 eV in A_+ and $A_\pm$ geometries, respectively.

As mentioned above, the Si(001)$c(6\times2)$-Ag and Si(001)(2×3)-Ag surfaces are prepared at very similar conditions. However, Ag 3d XPD study revealed that the local structures around Ag adsorbates are quite different between these two phases. Thus it is rather surprising that these two surfaces have very similar band bendings and further very similar surface-state bands. The Si(001)(2×3)-Ag and Si(001)$c(6\times2)$-Ag surfaces have three surface states within the bulk band gap at almost the same binding energies, as shown in Fig. 7, although one can notice slight differences in surface-state dispersions reflecting the distinction in the surface periodicity. Furthermore, the intensity distributions of the surface states within the bulk band gap as a function of emission angle closely resemble one another in the Si(001)(2×3)-Ag and Si(001)$c(6\times2)$-Ag surfaces.

Recently Si 2p core levels of the Si(001)$c(6\times2)$-Ag and Si(001)(2×3)-Ag surfaces were found to be very similar, indicating a close similarity of the reconstructions of outermost Si layers for these two surfaces.[17] Thus the resemblance between the surface band structures of these two phases is thought to reflect the similarity in the Si substrate reconstructions. This interpretation is natural, since surface-state bands with monovalent adsorbates are generally governed by substrate reconstructions, as shown in the well established examples of alkali adsorption on Si(001) (Ref. 18) and Ag adsorption on Si(111).[19] Then the distinctive difference in the Ag 3d XPD patterns of the Si(001)(2×3)-Ag and Si(001)$c(6\times2)$-Ag surfaces is interpreted to reflect the different arrangements of Ag adsorbates. This is plausible since XPD patterns are not sensitive to the substrate reconstructions beneath the adsorbate layer when the adsorbates form an overlayer.[7] That is, it is suggested that the Si(001)$c(6\times2)$-Ag and Si(001)(2×3)-Ag surfaces have similar Si substrate reconstructions but different adsorbate arrangements. The substrate reconstruction is definitely not based on the dimerization of the Si top-layer atoms, since (1) the $c(6\times2)$ periodicity cannot be incorporated with the 2×1 dimer reconstruction, and (2) surface states related to the Si dimers of the clean Si(001) surface (such as D, I, H, and G in Ref. 13) are not observed for both (2×3)-Ag and $c(6\times2)$-Ag phases.[6] The similarity in the substrate reconstructions of Si$(001)(2\times3)$-Ag and Si$(001)c(6\times2)$-Ag surfaces naturally explain the proximity in the preparation conditions of these two phases. That is, converting the metastable $c(6\times2)$ structure to 2×3 does not require much energy since it accompanies only a rearrangement of Ag adsorbates. The detailed structure analyses of the Si$(001)c(6\times2)$-Ag and the Si$(001)(2\times3)$-Ag surfaces remain to be investigated.

V. CONCLUSIONS

Polarization-dependent ARPES with synchrotron radiation was applied to the SD Si$(001)c(6\times2)$-Ag surface in order to investigate its surface band structure. From detailed ARPES measurements along the important symmetric axes of the $c(6\times2)$ surface Brillouin zone, three different surface states (S_1, S_2, and S_3) are identified, and their symmetry properties along the mirror symmetric axes were determined. The Si$(001)c(6\times2)$-Ag surface is found to be semiconducting in consistent with the previous ARPES result for the Si$(001)(2\times3)$-Ag surface formed at the same Ag coverage.[6] This result is interpreted as evidence of the $\frac{2}{3}$-ML coverage for these two Ag-induced phases. The surface band structure of the $c(6\times2)$ surface is found to be similar to that of the Si$(001)(2\times3)$-Ag surface, suggesting that these two surfaces have similar Si substrate reconstructions. This suggestion does not contradict the Ag $3d$ XPD result,[8] and is consistent with a recent high-resolution Si $2p$ photoemission result.[17] Proper theoretical calculations on the surface structures and surface-state bands are required.

ACKNOWLEDGMENTS

The authors are grateful to Dr. K. Sakamoto and Dr. T. Sakamoto for providing us with a well-oriented Si wafer, and to Dr. A. Kimura and A.Harasawa for their help during the experiments.

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[1] J. Nogami, Surf. Rev. Lett. **1**, 395 (1994).

[2] X.F. Lin, K.J. Wan, and J. Nogami, Phys. Rev. B **47**, 13 491 (1993).

[3] X.F. Lin, K.J. Wan, and J. Nogami, Phys. Rev. B **49**, 7385 (1994).

[4] D. Winau, H. Itoh, A.K. Schmid, and T. Ichinokawa, Surf. Sci. **303**, 139 (1994).

[5] R.M. Tromp and T. Michely, Nature (London) **373**, 499 (1995); T. Michely, M.C. Reuter, M. Copel, and R.M. Tromp, Phys. Rev. Lett. **73**, 2095 (1994).

[6] H.W. Yeom, I. Matsuda, K. Tono, and T. Ohta, Phys. Rev. B **57**, 3949 (1998).

[7] M. Shimomura, T. Abukawa, M. Higa, M. Nakamura, S.M. Shivaprasad, H.W. Yeom, S. Suzuki, S. Sato, J. Tani, and S. Kono, Surf. Rev. Lett. **5**, 953 (1998).

[8] S.M. Shivaprasad, T. Abukawa, H.W. Yeom, M. Nakamura, S. Suzuki, S. Sato, K. Sakamoto, T. Sakamoto, and S. Kono, Surf. Sci. **344**, L1245 (1995).

[9] A. Kawazu (private communication).

[10] H. Namba, M. Masuda, H. Kuroda, T. Ohta, and H. Noda, Rev. Sci. Instrum. **60**, 1917 (1989).

[11] H.W. Yeom, T. Abukawa, Y. Takakuwa, Y. Mori, T. Shimatani, A. Kakizaki, and S. Kono, Phys. Rev. B **53**, 1948 (1996).

[12] J. Hermanson, Solid State Commun. **22**, 9 (1977).

[13] L.S.O. Johansson, R.I.G. Uhrberg, P. Mårtensson, and G.V. Hansson, Phys. Rev. B **42**, 1305 (1990).

[14] H.W. Yeom, T. Abukawa, Y. Takakuwa, M. Nakamura, M. Kimura, A. Kakizaki, and S. Kono, Surf. Sci. **321**, L177 (1994); H. W. Yeom, T. Abukawa, Y. Takakuwa, Y. Mori, T. Shimatani, A. Kakizaki, and S. Kono, Phys. Rev. B **55**, 15 669 (1997); T. Abukawa, M. Sasaki, T. Hisamatsu, T. Goto, T. Kinoshita, A. Kakizaki, and S. Kono, Surf. Sci. **325**, 33 (1995).

[15] J. Pollmann, R. Kalla, P. Krüger, A. Mazur, and G. Wolfgarten, Appl. Phys. A: Solids Surf. **41**, 21 (1986); J. Pollmann, P. Krüger, and A. Mazur, J. Vac. Sci. Technol. B **5**, 945 (1987).

[16] I. Matsuda, H.W. Yeom, K.Tono, and T. Ohta (unpublished).

[17] H.W. Yeom, I. Matsuda, Y.-C. Chao, S. Terada, and R.I.G. Uhrberg (unpublished).

[18] For example, T. Abukawa, T. Kashiwakura, T. Okane, H. Takahashi, S. Suzuki, S. Kono, S. Sato, T. Kinoshita, A. Kakizaki, T. Ishii, C.Y. Park, K.A. Kang, K. Sakamoto, and T. Sakamoto, Surf. Sci. **303**, 146 (1994); T. Abukawa, T. Kashiwakura, T. Okane, Y. Sasaki, H. Takahashi, Y. Enta, S. Suzuki, S. Kono, S. Sato, T. Kinoshita, A. Kakizaki, T. Ishii, C.Y. Park, S.W. Yu, K. Sakamoto, and T. Sakamoto, *ibid.* **261**, 217 (1992).

[19] T. Yokotsuka, S. Kono, S. Suzuki, and T. Sagawa, Surf. Sci. **127**, 35 (1983); E.J.J. Kirchner, E.J. Baerends, and E. Vlieg *ibid.* **304**, 12 (1994); E.J.J. Kirchner, E.J. Baerends, G. te Velde, and E. Vlieg, *ibid.* **330**, 113 (1995).