PHYSICAL REVIEW B **67**, 085310 (2003)

Electronic structure of monolayer and double-layer Ge on Si(001)

H. W. Yeom* and J. W. Kim
Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea

K. Tono, I. Matsuda, and T. Ohta
Department of Chemistry, The University of Tokyo, Hongo, Tokyo 113, Japan

(Received 27 August 2002; published 18 February 2003)

Electronic structures of the epitaxial Ge layers during the very initial growth on the Si(001)2×1 surface have been studied by angle-resolved photoemission using synchrotron radiation. The surface band structures are investigated in detail for a clean single-domain Si(001)2×1 surface, a single-domain Si(001)1×2-Ge surface at one monolayer of Ge, and a double-domain Si(001)2×1-Ge surface at two monolayers. The two different surface-state bands due to the up-dimer atom states of the buckled dimers on the surface are identified for all three above surfaces with very similar dispersions. In addition, a few surface-resonance bands due to the back bonds of the surface dimers are also identified and their detailed dispersions are determined. These results are compared with the previous experimental and theoretical reports for the band structures of the Si(001), Ge(001), and Ge/Si(001) surfaces in relation to the structure and stoichiometry of the initial Ge layers on Si(001)2×1. The surface band structure is shown to be insensitive to the intermixing of Ge and Si atoms on the surface within the resolution of the present measurement.

DOI: 10.1103/PhysRevB.67.085310 PACS number(s): 73.20.At, 79.60.Dp, 68.43.Fg

I. INTRODUCTION

The growth of Ge on the Si(001) surface has been studied extensively due to its potential in new optoelectronic devices and high-speed electronic devices as well as due to its fundamental importance as a model system for the heteroepitaxial growth of semiconductors.[1,2] Various structural properties of the Ge/Si(001) system have been discussed so far such as the dimer reconstruction on the surface,[2] the surface stress,[3] and the evolution of the early Ge clusters and islands.[4] These issues are directly and indirectly relevant to the noble devices based on quantum well structures.[5]

Despite such a large number of experimental and theoretical studies on Ge/Si(001), the details of the very initial growth are still a subject of controversy, especially when it comes to the monolayer regime. It seems that there had been a wide consensus on the fact that the Ge initial growth proceeds in a layer-by-layer fashion up to the critical thickness of 3–4 monolayers (ML).[3,4,6] The previous scanning tunneling microscopy (STM)[7] and many other studies have reported the initial growth as the Ge-dimer formation on Si(001)2×1.[8–10] However, the recent experimental[11–13] and theoretical studies[13,14] indicated that Ge initially grows as mixed Ge-Si dimers and that Ge atoms intermix with Si atoms on the surface and also at the subsurface layers. Very recently the intermixing on the surface was clearly identified with STM.[15] At the full monolayer coverage, some suggested that the surface is terminated purely by Ge dimers, in contrast to the submonolayer intermixing, due to the gain in the surface free energy,[3] but others reported that a considerable fraction of Ge atoms diffuse to subsurface layers.[11–13,16] Concerning the local geometry of the Ge-Si mixed dimers, a very large buckling angle with Ge atoms buckled-up was reported by a photoelectron diffraction study,[17] which was, however, not reproduced by the subsequent theoretical calculations.[14,18]

In contrast to the large amount of structural studies on Ge/Si(001), there have been very few studies on its electronic structure. A detailed band-structure measurement for this system by angle-resolved photoelectron spectroscopy (ARPES) could be hindered by the double-domain (DD) character of an ordinary Si(001)2×1 substrate. In the present work, the ARPES measurement based on a linearly polarized synchrotron radiation was performed for the Ge/Si(001) surfaces at different Ge coverages using a single-domain (SD) Si(001)2×1 substrate. To investigate the existence and dispersion of surface states (SS's) and resonances on the growth front, we prepared a SD clean Si(001)2×1 surface, a SD Si(001)1×2-Ge surface at 1 ML and a DD Si(001)2×1-Ge surface at 2 ML. The ARPES results on these Ge/Si(001) surfaces are compared with the previous experimental and theoretical studies.

II. EXPERIMENT

The SD Si(001)2×1 substrate was prepared on a specially cut highly flat Si(001) wafer through cycles of high-temperature annealing and Si homoepitaxial growth.[19] The typical LEED pattern of a SD Si(001)2×1 surface is shown in Fig. 1(a), where the ratio of majority 2×1 and minority 1×2 domains is about 8 to 1. Ge atoms were deposited onto the SD Si(001)2×1 surface held at room temperature from a graphite effusion cell. The pressure during deposition was kept below 1.0×10^{-9} mbar. After the Ge deposition, the sample was annealed typically at 600 °C. A completion of the first Ge layer (1 ML) is indicated by a clear SD 1×2 LEED pattern (90°-rotated from the clean surface 2×1) as shown in Fig. 1(b). The SD character of the surface deteriorates for the deposition of more than 1 ML and a completely DD 2×1 LEED pattern is observed from ~2 ML.

Photoemission measurements were carried out for the SD Si(001)1×2-Ge surface formed at 1 ML along most of the

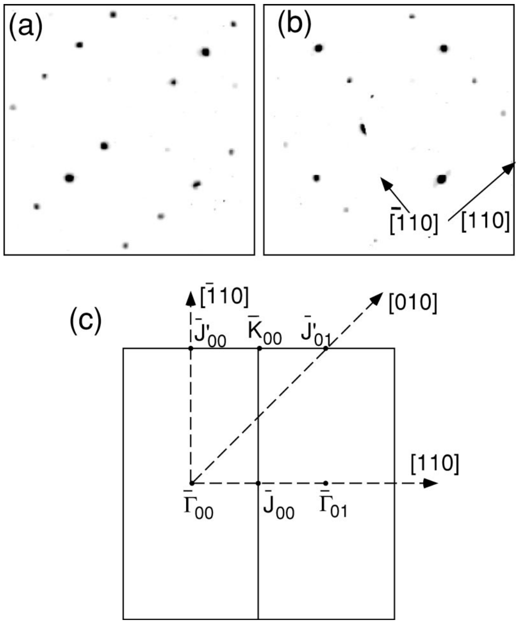

FIG. 1. LEED patterns of (a) the clean SD Si(001)2×1 surface and (b) the SD Si(001)1×2-Ge surface at 1 ML. (c) The surface Brillouin zone of the Si(001)2×1 surface.

symmetry axes of the surface Brillouin zone (SBZ) [Fig. 1(c)] and for DD Si(001)2×1-Ge surface at 2 ML along [010] and [$\bar{1}$10]. ARPES spectra of the clean SD Si(001)2×1 surface were also measured in detail for direct comparison. A linearly polarized synchrotron light (from the beam line BL-7B at Photon Factory, Japan) was used at photon energies ($h\nu$'s) of 17.8 and 13.5 eV at an incidence angle (θ_i) of 45° from the surface normal unless specified. The emission angle θ_e of photoelectrons was scanned with a step of 2°. A commercial ARPES spectrometer (VG ADES-400) was used with an angular resolution of 1°.

III. RESULTS AND DISCUSSION

Figure 2 shows the series of ARPES spectra of (a) the SD clean Si(001)2×1 surface and (b) the SD Si(001)1×2-Ge surface (1 ML) taken along the [010] azimuth [$\bar{\Gamma}_{00}-\bar{J}'_{01}$ direction, see Fig. 1(c)]. The [010] azimuth is common in the **k** space for both 2×1 and 1×2 SBZ's, where a direct comparison of the spectral features of the clean 2×1 and 1×2-Ge surfaces is possible. In both figures, a strongly dispersive feature **b** due to the bulk direct transition is observed. This bulk band is close to the edge of the bulk-band gap and the region with a lower binding energy than **b** roughly corresponds to the bulk-band gap where a surface state is expected. Comparing the binding energy of this bulk band, the valence band maxima are determined to be at ~0.6 eV below the Fermi level (E_F) for both surfaces.[20] That is, no Ge-induced band bending is observed on the 1×2-Ge surface within our spectroscopic resolution of 0.15 eV. Furthermore, this fact does not change for the well-ordered 2-ML Ge film on Si(001) as shown below.

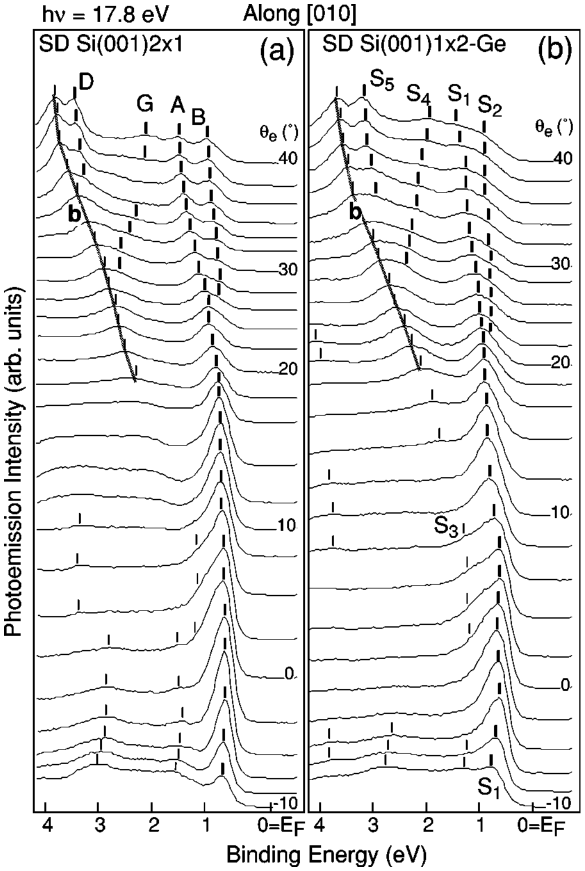

FIG. 2. ARPES spectra taken along the [010] azimuth ($\bar{\Gamma}_{00}-\bar{J}'_{01}$) at a photon energy ($h\nu$) of 17.8 eV for (a) the clean SD Si(001)2×1 surface and (b) the SD Si(001)1×2-Ge surface. The photon incidence angle θ_i is 45° and the step in the emission angle θ_e is 2°. The different bulk- and surface-related spectral features are marked. The gray lines are guides to eyes.

Since the [010] azimuth has a wide bulk-band gap down to 3.6 eV below E_F, it is relatively easy to identify a surface state. Indeed, a few surface-related features are observed in Fig. 2(a). The two dominant spectral features with low binding energies (denoted as A and B following the notation of the previous literature[20]) have been assigned as the dangling-bond surface states of the buckled Si dimers.[20] Feature D close to **b** has been assigned as a surface state due to the back bonds of the dimers. The weak feature G has also been identified as a surface state but its origin is not clear yet: this may correspond to a surface state due to the dimer bond or to the back bonds.[20]

In Fig. 2(b), we find similar four spectral features (denoted as S_1, S_2, S_4, and S_5) for the 1-ML Ge on Si(001) within the bulk-band-gap region. Another state denoted as S_3 is observed as a broad shoulder near S_1 around the normal emission. The surface character of this feature is not clear here but will be made more apparent along the other azimuths. On the Si(001)1×2-Ge surface, the whole surface spectral features appear significantly broader. This broadening might come partly from the increase in the defect density on the surface as observed by STM (Ref. 7) or from the enhanced phonon broadening due to the lower Debye temperature of Ge compared to Si. In particular, the S_1 and S_2 states of 1-ML Ge/Si(001) are not resolved as clear as A and

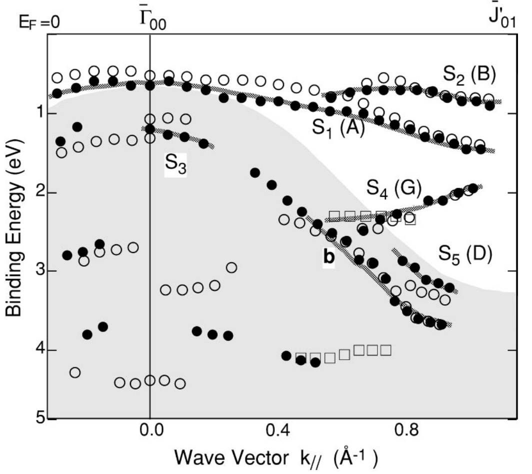

FIG. 3. Experimental dispersions of the spectral features along the [010] azimuth ($\bar{\Gamma}_{00}-\bar{J}'_{01}$) for the clean SD Si(001)2×1 [open circles as taken from the spectra shown in Fig. 2(a)] and the SD Si(001)1×2-Ge surfaces [closed circles from the spectra shown in Fig. 2(a) and open squares taken at $h\nu=17.8$ eV and $\theta_i=0°$]. The shade area corresponds to the bulk bands projected to the 1×1 surface Brillouin zone. The gray lines are guides to eyes.

B on the clean Si(001)2×1 surface due to such broadening. However, the presence of these two states are corroborated from the spectra taken along other azimuthal directions or with different measurement geometries and photon energies. Except for this broadening the overall similarity of the spectral features of clean Si(001)2×1 and 1×2-Ge is remarkable. The experimental dispersions of the bands observed on the SD 1×2-Ge surface along the [010] azimuth are shown together with those of clean Si(001)2×1 in Fig. 3. The shaded area indicates the bulk bands projected into the 1×1 SBZ. As mentioned above, the overall band structure of the 1×2-Ge surface is almost identical to those of the clean Si(001)2×1 surface. As shown below, such a close similarity is also observed along other SBZ lines. The only noticeable differences are the marginal binding energy shift of S_1 from that of A around $k_{\parallel}\sim 0.4$ Å^{-1} and a similar shift of S_5 from that of D.

Due to such similarity and the common dimer reconstructions, the correspondence between the surface states of 1×2-Ge and clean Si(001)2×1 is very obvious as given in Fig. 3. That is, we can assign S_1 and S_2 to the dangling-bond states of the dimers on 1×2-Ge (A and B) and S_5 to the back bond state (D). Further discussion on the surface states of 1×2-Ge will be given below after we show the ARPES spectra along other azimuths.

Figure 4 compares the ARPES spectra of the SD clean Si(001)2×1 and SD 1×2-Ge surfaces along the $\bar{\Gamma}_{00}-\bar{J}_{00}$ SBZ line (i.e., along the surface dimer bonds). This corresponds to the [110] azimuth on clean Si(001)2×1 but to [$\bar{1}$10] on 1×2-Ge due to the 90° rotation of the dimerization direction. Thus, this comparison applies only for the surface spectral features and the substrate bulk-band dispersions can in principle be different. In these spectra, we also observe the dangling-bond surface state A (S_1) within the bulk-band gap thoughout the SBZ. As previously reported,[20] another surface state is identified at ~1.5 eV on the clean surface (H), which seems to split into I and H around the $\bar{\Gamma}_{01}$ point [Fig. 4(a)]. The corresponding surface state on the 1×2-Ge surface is denoted as S_3 [Fig. 4(b)] but its splitting is not so well resolved.

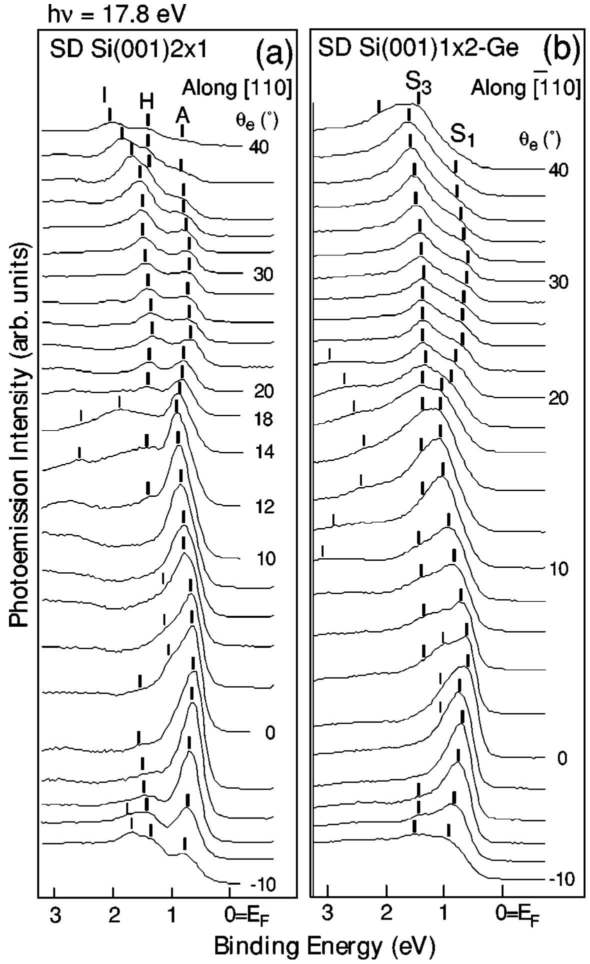

FIG. 4. Similar ARPES spectra to Fig. 2 but along the $\bar{\Gamma}_{00}-\bar{J}_{00}$ surface Brillouin zone line (along the dimer axis) for (a) the clean SD Si(001)2×1 and (b) the SD Si(001)1×2-Ge surfaces.

Figures 5(a) and 5(b) show, respectively, the experimental band dispersion summarized along the direction parallel to the dimer bonds as partly measured from the spectra shown in Fig. 4 and along the dimer-row direction ($\bar{\Gamma}_{00}-\bar{J}'_{00}$ in the SBZ, the raw data are not shown here). Along the $\bar{\Gamma}_{00}-\bar{J}_{00}$ SBZ line, the dispersions of S_1 (S_3) and A (H) are exactly the same as far as the present measurement can tell. A similar degree of proximity is also observed for the S_1 (S_2) and A (B) along the $\bar{\Gamma}_{00}-\bar{J}'_{00}$ direction.

The whole observed dispersions of the 1-ML Ge layer (1×2-Ge) are summarized in Fig. 6. They are compared with the theoretical band dispersions calculated for the Si(001)1×2-Ge surface; the solid lines are for the Ge-Ge dimer structure (1-ML Ge termination),[21] and the dashed lines for Ge-Si mixed dimers (half-monolayer Ge termination).[18] For the latter case, we assume that a half of

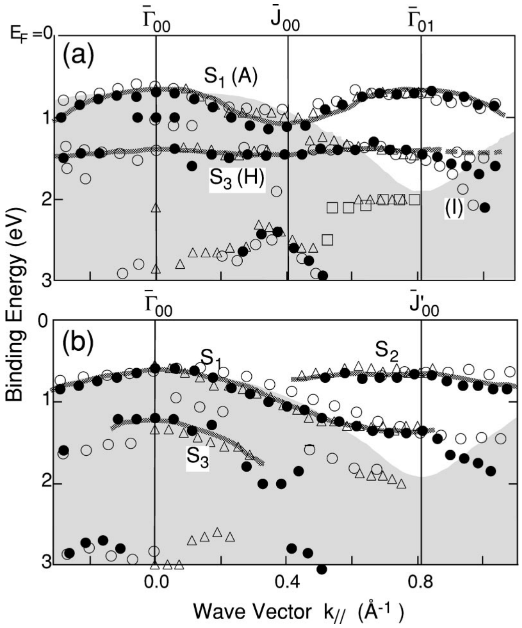

FIG. 5. Experimental dispersion of the spectral features along (a) the $\overline{\Gamma}_{00}-\overline{J}_{00}$ (taken partly from the data shown in Fig. 4) and (b) $\overline{\Gamma}_{00}-\overline{J}'_{00}$ (raw data not shown) surface Brillouin zone lines for the clean SD Si(001)2×1 (open circles taken at $h\nu=17.8$ eV and $\theta_i=45°$) and the SD Si(001)1×2-Ge surfaces (closed circles taken at $h\nu=17.8$ eV and $\theta_i=45°$; open squares taken at $h\nu=17.8$ eV and $\theta_i=0°$; open triangles taken at $h\nu=13.5$ eV and $\theta_i=45°$). The shade area corresponds to the bulk bands projected to the 1×1 surface Brillouin zone. The gray lines are guides to eyes.

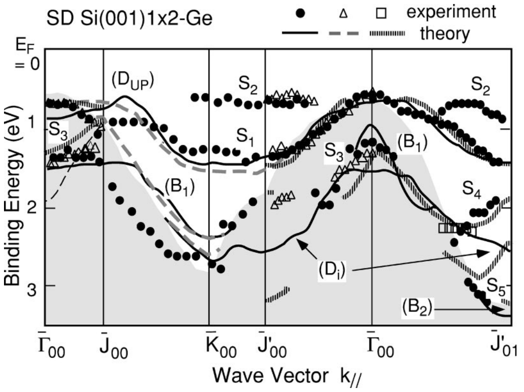

FIG. 6. Summary of the experimental dispersions of the surface states (resonances) for the Si(001)1×2-Ge (1 ML) surface (the symbols and the states S_1, S_2, S_3, S_4, and S_5). The solid line is the theoretical dispersions calculated for the pure Ge-Ge dimers (1 ML) on Si(001) (Ref. 21), the dashed lines for the mixed Ge-Si dimers on Si(001) (Ref. 18), and the hatched lines for the Ge dimers on a clean Ge(001) surface (Ref. 22). In theory, D_{up} corresponds to the up-dimer-atom state, B_1 (B_2) the back-bond states, and D_i the dimer-bond state. The shade area corresponds to the bulk bands projected to the 1×1 surface Brillouin zone.

the Ge adatoms are intermixed into the subsurface layers.[11–13] In addition, the theoretical result for the pure Ge dimers on the clean Ge(001)2×1 surface is given by the hatched lines.[22] A few bulk-related features and unassigned minor peaks observed at 2.5–3.5 eV are taken out for clarity.

At first, one can easily notice the very good overall agreement between the experimental and theoretical results and also the close similarity between the theoretical results of the three largely different dimer configurations; Ge-Ge dimers on Si(001), Ge-Ge dimers on Ge(001), and Ge-Si dimers on Si(001). Note that the surface-band dispersions of the Ge dimers on Ge(001) and that of the Si dimers on Si(001) already have a great similarity.[23] This must be due to the almost identical surface structure of the Ge(001) and Si(001) surfaces but is still surprising considering the different lattice constants and different valence states of Ge and Si. In any case, the close similarity between the theoretical results for the different dimer configurations can, thus, be understood from such structural and electronic proximity of the Ge(001) and Si(001) surfaces. In the experimental point of view, the similarity between the band structure of the Ge and Si dimers has not been established in detail mainly due to the fact that a single-domain Ge(001)2×1 surface could not be prepared so far. Hence the direct comparison of the band dispersion along the $\overline{\Gamma}_{00}-\overline{J}_{00}$ and $\overline{\Gamma}_{00}-\overline{J}'_{00}$ SBZ lines was limited while the comparison along the [010] direction showed the expected similarity. While the present data provides more extensive experimental information over the full SBZ without the ambiguity of coexisting domains, one should note that the stoichiometry of the surface dimers on Si(001)1×2-Ge is not sufficiently clear yet.

Nevertheless, the comparison given in Fig. 6 makes clear the assignment of the origin of the surface states observed for 1×2-Ge. The S_1 state observed throughout the whole SBZ corresponds to the occupied dangling-bond state as mentioned above. More exactly, it corresponds to the fully occupied p_z state localized on the up-dimer atom of a buckled dimer (D_{up} in theory). This state is known to split into two subbands due to the antiferromagetic order of the buckling (alternate buckling directions between neighboring dimers) on the Si(001) surface.[24,25] Such splittings are clearly observed in the present experiment around $\overline{J}'_{00}$ and $\overline{K}_{00}$ points for both clean Si(001)2×1 (A and B) and 1×2-Ge (S_1 and S_2) (raw data not shown here). Similar splitting for Ge(001)2×1 was also observed, but only along the [010] azimuth around $\overline{J}'_{01}$. This splitting is also consistent to the STM results showing mostly the antiferromagnetic buckling of the dimers on the whole surface even at room temperature after the Ge submonolayer growth.[11] Note that the theoretical results do not show the splitting of the dangling-bond surface state D_{up} (S_1 and S_2 in the experimental data) simply because all the band calculations for the Ge-related surfaces were performed only with the 2×1 surface unit cell instead of more rigorous $c(4\times2)$.

Other than the surface states with the dangling-bond origin, the S_3 state observed around $\overline{\Gamma}$ is identified as one of the back-bond states (B_1 in theory); four fully occupied back-bond surface resonances are expected due to the four back-bond orbitals of a dimer. This state disperses strongly towards $\overline{J}'_{01}$ and is observed as the S_4 state within the band gap around $\overline{J}'_{01}$. The S_5 state around $\overline{J}'_{01}$ is also related to another back-bond state B_2. However, it is not clear whether the strongly dispersing state between $\bar{J}_{00}$ and $\bar{K}_{00}$ at 2–3 eV corresponds to the back-bond state B_1 or the dimer-bond state D_i. If we compare more details of the theoretical band dispersions between the pure Ge dimers and the mixed Ge-Si dimers, there is a noticeable difference for the dispersion of the B_1 state; for the mixed dimers [and also for the Ge dimers on Ge(001)] the binding energy of B_1 at $\bar{J}$ is much lower than that of the pure Ge dimers on Si(001). Then the present result might be interpreted as to favor the pure Ge dimer case over the mixed dimer model although a more systematic theoretical study is required for a clear conclusion. This does not deny the intermixing itself since the intermixing on the surface can occur both through formation of mixed Ge-Si dimers or formation of a mixture of pure Ge and pure Si dimers.

The structural and electronic similarity between the Ge-Ge, Ge-Si, and Si-Si dimers further leads to a very little difference between the corresponding STM images.[7] This fact partly contributed to the misinterpretation of the initial Ge growth as forming simple Ge addimers in the earlier STM studies. Recently, Qin, Swartzentruber, and Lagally reported that Ge intermixing into the topmost Si layer could be identified by STM but only in the empty-state STM images.[15] This indicates that the difference in the band structure can be more than marginal in the empty state bands above the Fermi level. It does not conflict with the present result since we confirm the close similarity of the surface band structure in the filled states. However, even in the empty state imaging the difference between the Ge-Si mixed dimers and the pure Ge dimers was thought to be beyond the resolving power of the STM image.[15]

One can naturally expect that the number of pure Ge-Ge dimers increases for a thicker film, where one may find some difference in the surface band structure. We have prepared a well-ordered 2-ML Ge film which exhibits a DD 2×1 LEED pattern as mentioned above. Figure 7 shows the series of ARPES spectra on the DD Si(001)2×1-Ge surface at 2 ML taken with $h\nu = 17.8$ eV along the [010] azimuth. As evident in this figure, we identify essentially the same surface states with almost the same dispersions with those of the 1×2-Ge (1 ML) surface except for the broadening and weakening of the spectral features. As mentioned above this broadening may come from the increased disorder on the topmost layer or from the enhanced phonon broadening. This result only reconfirms the close similarity between the electronic structures of the Ge-Ge and Ge-Si dimers and the insensitivity of the surface band structure on the stoichiometry and intermixing of the surface dimers. As a different approach, Ku and Nemanich performed an ARPES study on the Si_xGe_{1-x} alloy surfaces grown on a Si(001) surface.[26] In that study, a dangling-bond state (A) and a back-bond state (D) were observed on both $Si_{0.2}Ge_{0.8}$ and $Si_{0.8}Ge_{0.2}$ alloy surfaces (the DD 2×1 surfaces) along the [010] azimuth with proximal dispersions to those of the clean Si(001)2×1 surface. That result is thus fully consistent to the present observation.

IV. SUMMARY

An angle-resolved photoelectron spectroscopy study was devoted to study systematically the electronic structures of the epitaxial Ge layers during the very initial growth on the Si(001)2×1 surface. The surface band structures are investigated in detail for a clean single-domain Si(001)2×1 surface, a single-domain Si(001)1×2-Ge surface with one monolayer of Ge, and a double-domain Si(001)2×1-Ge surface at two monolayers. The two different surface-state bands due to the up-dimer atom states (S_1 and S_2) of the buckled dimers and the three other surface-states bands due to the back bonds (S_2, S_3, and S_5) are identified clearly for all three above surfaces with very similar dispersions. These results are compared with the previous experimental and theoretical reports for the band structures of the Si(001)2×1 and the Ge(001)2×1 surfaces and further with the theoretical band structures of the Si(001)1×2-Ge surfaces with the pure Ge dimers or the mixed Ge-Si dimers on top. The surface band structure is shown to be insensitive to the inter-

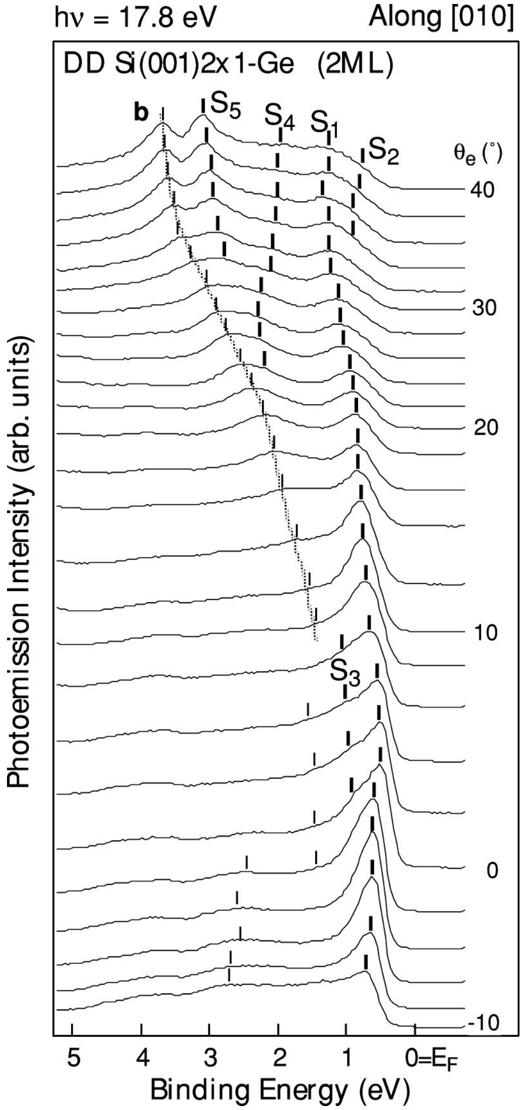

FIG. 7. Similar ARPES spectra to Fig. 2 but for the DD Si(001)2×1-Ge surface formed by 2-ML Ge deposition. The gray lines are guides to eyes. The surface states and their dispersions are almost identical to the SD Si(001)1×2-Ge surface at 1 ML.

mixing of Ge and Si atoms on the surface within the resolution of the present measurement while a part of the dispersions of the back-bond state S_3 seems to favor the pure Ge-Ge dimer model. This insensitivity is thought to be due mainly to the striking similarity of the surface-state dispersions of the Ge(001) and Si(001) surfaces. In addition, the band bending by the Ge layers on Si(001) is shown to be negligible (<0.1 eV) up to 2 ML.

ACKNOWLEDGMENTS

We are grateful to Dr. K. Sakamoto and Dr. T. Sakamoto for providing us with a well-oriented Si wafer. This work was performed under the Photon Factory Proposal No. 96-G150. H.W.Y. and J.W.K. are supported by KOSEF through ASSRC at Yonsei University and by MOST through Tera-level Nano Device project of 21 century Frontier program.

---

*Author to whom correspondence should be addressed. Email address: yeom@phya.yonsei.ac.kr

[1] For example, T. E. Whall and E. H. C. Parker, J. Mater. Sci.: Mater. Electron **6**, 249 (1995).

[2] M. Asai, H. Ueda, and C. Tatsuyama, J. Appl. Phys. **58**, 2577 (1985); H.-J. Gossmann, L. C. Feldman, and W. M. Gibson, Surf. Sci. **155**, 413 (1985).

[3] F. Liu, F. Wu, and M. G. Lagally, Chem. Rev. **97**, 1045 (1997), and references therein.

[4] D. J. Eaglesham and M. Cerullo, Phys. Rev. Lett. **64**, 1943 (1990); Y.-W. Mo, D. E. Savage, B. S. Swartzentruber, and M. G. Lagally, *ibid.* **65**, 1020 (1990).

[5] T. I. Kamins, K. Nauka, and R. S. Williams, Appl. Phys. A: Mater. Sci. Process. **73**, 1 (2001).

[6] M. Copel, M. C. Reuter, M. Horn von Hoegen, and R. M. Tromp, Phys. Rev. B **42**, 11 682 (1990); S. S. Iyer, J. C. Tsang, M. W. Copel, P. R. Pukite, and R. M. Tromp, Appl. Phys. Lett. **54**, 219 (1989).

[7] F. Iwakami, M. Tomitori, and O. Nishikawa, Surf. Sci. **266**, 285 (1992); Ultramicroscopy **42**, 895 (1992).

[8] E. Fontes, J. R. Patel, and F. Comin, Phys. Rev. Lett. **70**, 2790 (1993), and references therein.

[9] J.-H. Cho, S.-M. Jeong, and M.-H. Kang, Phys. Rev. B **50**, 17 139 (1994); J.-M. Jin and L. J. Lewis, *ibid.* **49**, 2201 (1994).

[10] L. Patthey, E. L. Bullock, T. Abukawa, S. Kono, and L. S. O. Johansson, Phys. Rev. Lett. **75**, 2538 (1995).

[11] H. W. Yeom, M. Sasaki, S. Suzuki, S. Sata, S. Hosoi, M. Iwabuchi, K. Higashiyama, F. Fukutani, M. Nakamura, T. Abukawa, and S. Kono, Surf. Sci. Lett. **381**, L533 (1997).

[12] A. Ikeda, K. Sumitomo, T. Nishioka, T. Yause, and Y. Kido, Surf. Sci. **385**, 200 (1997); K. Nakajima, A. Konishi, and K. Kimura, Phys. Rev. Lett. **83**, 1802 (1999).

[13] B. P. Uberuaga, M. Leskovar, A. P. Smith, H. Jonsson, and M. Olmstead, Phys. Rev. Lett. **84**, 2441 (2000).

[14] S. J. Jenkins and G. P. Srivastava, Surf. Sci. **377–379**, 887 (1997); Y. Yoshimoto and M. Tsukada, *ibid.* **423**, 32 (1999).

[15] X. R. Qin, B. S. Swartzentruber, and M. G. Lagally, Phys. Rev. Lett. **84**, 4645 (2000).

[16] X. Y. Zhu and Y. H. Lee, Phys. Rev. B **59**, 9764 (1999).

[17] X. Chen, D. K. Saldin, E. L. Bullock, L. Patthey, L. S. O. Johansson, J. Tani, T. Abukawa, and S. Kono, Phys. Rev. B **55**, R7319 (1997).

[18] S. C. A. Gay and G. P. Strivastava, Surf. Sci. **433–435**, 909 (1999).

[19] T. Abukawa and S. Kono, Phys. Rev. B **37**, 9097 (1988); T. Abukawa, T. Okane, and S. Kono, Surf. Sci. **256**, 370 (1991).

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

[21] P. Krüger and J. Pollmann, Appl. Phys. A: Mater. Sci. Process. **59**, 487 (1994).

[22] E. Landemark, R. I. G. Uhrberg, P. Kruger, and J. Pollmann, Surf. Sci. Lett. **236**, L359 (1990); E. Landemark, C. J. Karlsson, L. S. O. Johansson, and R. I. G. Uhrberg, Phys. Rev. B **49**, 16 523 (1994).

[23] P. Krüger and J. Pollmann, Phys. Rev. Lett. **74**, 1155 (1995).

[24] Y. Enta, S. Suzuki, and S. Kono, Phys. Rev. Lett. **65**, 2704 (1990).

[25] K. C. Low and C. K. Ong, Phys. Rev. B **50**, 5352 (1994); J. E. Northrup, *ibid.* **47**, 10 032 (1993).

[26] J.-H. Ku and R. J. Nemanich, Phys. Rev. B **54**, 14 102 (1996).